



Exploring Quantum Wave Propagation and Scattering

Jess Winterborne

Supervised by Roman Schubert

Level 7

40 Credit Points

May 2, 2023

Acknowledgement of Sources

Acknowledgement of Sources

For all ideas taken from other sources (books, articles, internet),
the source of the ideas is mentioned in the main text and fully
referenced at the end of the report.

All material which is quoted essentially word-for-word from
other sources is given in quotation marks and referenced.

Pictures and diagrams copied from the internet or other sources
are labelled with a reference to the web page or book, article etc.

Signed 

Date 02/05/2023

Contents

1	Introduction	4
2	Background	5
2.1	Classical Mechanics	5
2.2	Quantum Mechanics	8
2.2.1	Dirac Notation	11
2.2.2	Pictures	15
3	Numerical Methods	17
3.1	Split Operator Method	17
4	Scattering Theory	22
4.1	The Continuity Equation	27
4.2	S and M Matrices	28
4.3	Reflection and Transmission Coefficients	32
4.3.1	Examples	32
5	Semiclassical Methods	48
5.1	WKB Theory	48
5.1.1	Implications	51
5.2	Airy Functions for Linear Potential	53
5.3	Connecting WKB and Airy Functions	59
6	The Wigner Function	74
6.1	Examples	75
7	Animation Analyses	82
7.1	Single Gaussian Potential	83
7.2	Double Gaussian Potential	88
7.2.1	Equal Heights	88
7.2.2	Unequal Heights	92
7.3	Potential Wells	97
8	Further Topics	101
8.1	Time Dependent WKB	101
9	Conclusion	105
10	Appendix	106
10.1	Evolving and Animating Wave Packets	106
10.2	Plotting, Evolving and Animating the Wigner Function	111
10.3	Figures	116

1 Introduction

This project aims to provide an overview of wave propagation in quantum mechanics. Through this, we will cover some fascinating quantum phenomena such as superposition and tunneling effects. We begin with an introduction to quantum mechanics and its fundamental differences from classical mechanics. We set out some postulates of quantum mechanics that are relevant to the rest of the paper. We also examine how plane waves and wave packets can be used to describe the behavior of particles. Unlike classical particles, which can be described as having a definite position and momentum at any given time, quantum particles are subject to the Heisenberg uncertainty principle. This means that their position and momentum cannot both be known with arbitrary precision at the same time. Instead, they must be described using probability distributions known as wave functions. Wave packet propagation is a way of describing how these probability distributions evolve over time.

We cover numerical methods in §3, that allow us to simulate the evolution of a wave packet and gain insights into how quantum particles behave under different conditions. Additionally, we look at analytical methods of how plane waves as well as wave functions (super positions of plane waves) evolve by various other propagation methods, valid for each region of a system as a state approaches a barrier. First, we deal with when a state is far away from the barrier in the classically allowed regions in §4. Then, we deal with when it is far away from the barrier in both the classically allowed and classically forbidden regions in §5.1. Lastly, we cover when it is close to the barrier in §5.2. We subsequently attempt to unify these methods to create a complete picture.

To gain further insight into the evolution of wave packets, we introduce the Wigner function as a way to visualise systems in phase space. Finally, we analyse and compare some snapshots of simulations of wave functions and Wigner functions, in the context of what we have learned during the paper. We can compare some of the results found numerically to the analytical solutions, visualising some of the phenomena that arise in the quantum world. We also touch on how one can extend and further develop some of the approximation methods we have introduced in the final section.

2 Background

2.1 Classical Mechanics

The ideas presented in this section, along with further reading, can be seen in [1], chapter 4 and chapter 10 of [2], as well as in chapter 1.5 of [3].

Classical mechanics is used to describe the motion of macroscopic objects - that is objects visible to the human eye. We will introduce some different formulations of classical mechanics that will be relevant to quantum mechanics later down the line.

Lagrangian Mechanics

Lagrangian mechanics is a formulation of classical mechanics and is based on the principle of least action. The Lagrangian is defined as

$$L(\mathbf{q}, \dot{\mathbf{q}}, t) = T - V, \quad (1)$$

where the dot represents a time derivative, $T = \frac{1}{2}m\mathbf{v}^2 = \frac{1}{2}m\dot{\mathbf{q}}^2$ is the kinetic energy and $V = V(\mathbf{q})$ is the potential energy. From here on, we will be working in one dimension and so we drop the bold notation, and change the dot time derivative to $\frac{d}{dt}$.

Lagrange's equations are

$$\frac{\partial L}{\partial q} = \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \quad (2)$$

or

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) = \frac{\partial L}{\partial q}, \quad (3)$$

and are used to derive the equations of motion.

The action is defined as

$$S = \int_{t_1}^{t_2} L(q, \dot{q}, t) dt. \quad (4)$$

You can read more on the classical action in chapter 10.1 of [2].

Hamiltonian Mechanics

Another formulation (or rather a reformulation of Lagrangian mechanics) which is useful in studying quantum mechanics, is Hamiltonian mechanics. Hamiltonian mechanics is set

in phase space where coordinates are given in momentum p as well as position q . We can define that $p := \frac{\partial L}{\partial \dot{q}}$.

In terms of the Lagrangian, the Hamiltonian is $H(q, p, t) = p\dot{q} - L$. Since $p = mv = m\dot{q} \Rightarrow \dot{q} = \frac{p}{m}$ we have that $H(q, p, t) = \frac{p^2}{m} - (\frac{m}{2}\dot{q}^2 - V) = \frac{p^2}{m} - \frac{p^2}{2m} + V = \frac{p^2}{2m} + V$. Thus, the Hamiltonian is

$$H(q, p, t) = \frac{1}{2m}p^2 + V(q) = T + V \quad (5)$$

Where m is mass, T is the kinetic energy and V is the potential energy. The kinetic energy plus the potential energy gives the total energy of the system E , hence we have that $H(q, p, t) = E$. It's also important to note that the energy, and so the Hamiltonian, is conserved.

Hamilton's equations of motion are:

$$\dot{q} = \frac{\partial H}{\partial p} \quad , \quad \dot{p} = -\frac{\partial H}{\partial q} \quad (6)$$

Hamilton-Jacobi Equation

The Hamilton-Jacobi equation is yet another reformulation of classical mechanics. Its a useful formulation to consider, as its the only one where we can think of motion in terms of a wave. Due to this it is considered to be one of the closest approaches to quantum mechanics [1].

It is defined as

$$H(q, p, t) + \frac{\partial S}{\partial t} = 0 \quad \text{or} \quad H\left(q, \frac{\partial S}{\partial q}, t\right) + \frac{\partial S}{\partial t} = 0, \quad (7)$$

where S is the action and H is the Hamiltonian, both defined above. Here, $\frac{\partial S}{\partial q}$ plays the role of momentum p .

We can make a guess solution, or an Ansatz, for the Hamilton-Jacobi equation

$$S(q, t) = S(q) - Et$$

where $S(q)$ is the action for a given energy E . Plugging this into the Hamilton-Jacobi equation gives

$$H\left(q, \frac{\partial S}{\partial q}, t\right) = E.$$

Since $H(q, p, t) = T + V = E$, from the Hamiltonian in (5), we have that

$$\left(\frac{\partial S}{\partial q}\right)^2 \frac{1}{2m} + V(q) = E \Leftrightarrow \frac{\partial S}{\partial q} = \pm \sqrt{2m(E - V(q))}.$$

Level Sets

Given a potential and wave function with a certain energy, there are classical constraints on what a particle or wave can do, for example, if the energy is below the maximum energy of the potential, a particle with an energy below this will not be able to move past it. This idea is shown in Fig. 1, where we have shown an example of a potential barrier, and different energy level sets corresponding to what a particle can do with a given energy.

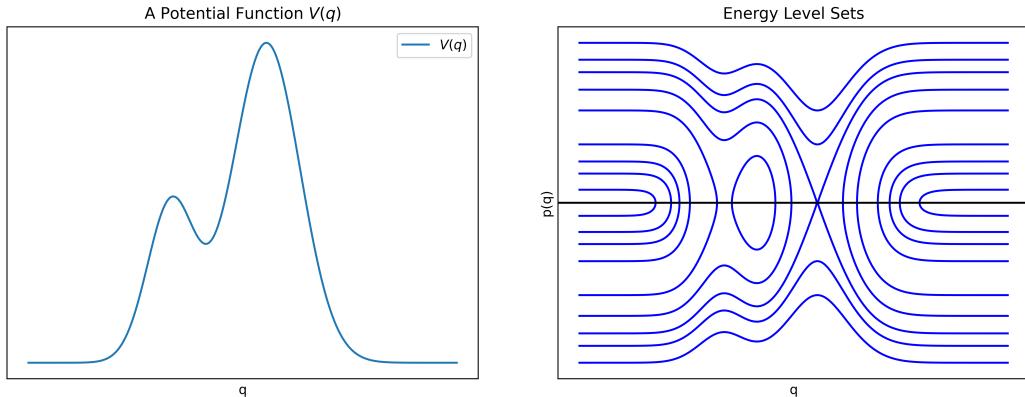


Figure 1: On the left hand side a generic potential is shown. On the right hand side, the energy level sets corresponding to the potential on the left is shown.

In Fig. 1, you can see that particles with a higher energy, and thus a larger momentum $p(q)$, can travel over and past the barrier, and particles with a lower energy or momentum, reach the barrier and are reflected back in the opposite direction. Alternatively, if the particle is located in the dip between the peaks, and has a lower energy than the peaks, then it will oscillate back and forth being reflected off of the potential at either side. This can be seen visually by the circle in the level set graph on the right of Fig. 1.

In the next section we introduce quantum mechanics. In contrast to classical mechanics, particles are able to pass through potential barriers, even if they do not have enough energy to overcome the peaks classically. This phenomenon is referred to as quantum tunnelling, and will be a recurring topic in this paper.

2.2 Quantum Mechanics

The concepts introduced here, as well as supplementary reading, can be found in chapters 2, 6 and 9 of [2], chapter 3 of [3], chapter 1 and 3.3 of [4], and in chapter 2 of [5]. See also [6].

Operators

An important postulate in quantum mechanics, is that for every observable in classical mechanics, there is a corresponding observable self adjoint operator. Self adjoint, or Hermitian, refers to the conjugate transpose, and the adjoint of an operator \hat{A} is denoted A^\dagger . By self adjoint, we mean $\hat{A}^\dagger = \hat{A}$. We can define the position and momentum operators as $\hat{q} = q$ and $\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial q}$. We can get the quantum mechanical Hamiltonian operator from the classical Hamiltonian equation by $\hat{H} = \frac{1}{2m} \hat{p}^2 + V(\hat{q}) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} + V(q)$. Setting $\hat{T} = \frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2}$ and $\hat{V} = V(q)$, the Hamiltonian operator is given by

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} + V(q) = \hat{T} + \hat{V}. \quad (8)$$

From here on, we drop the hat notation on the Hamiltonian and other operators (bar certain exceptions) since we are generally working within a quantum setting.

One important point on observables or Hermitian operators, is that their eigenvectors form a complete basis, or an orthonormal basis (ONB) on the space. This means that any function on the space can be written as a linear combination of the eigenvectors of an observable in the same space.

Wave Functions

In the quantum world, we can think of a particle as a wave packet. A wave packet is like a superposition of multiple sinusoidal plane waves with slightly different wave lengths, and hence momenta. This is because the wave length λ is related to the wave number k from $k = \frac{1}{\lambda}$ and thus the momentum $p = \hbar k$ via the de Broglie formula (see chapter 1.6 of [4]). This superposition then localises the infinite plane waves over a finite region of space, as shown in Fig. 2.

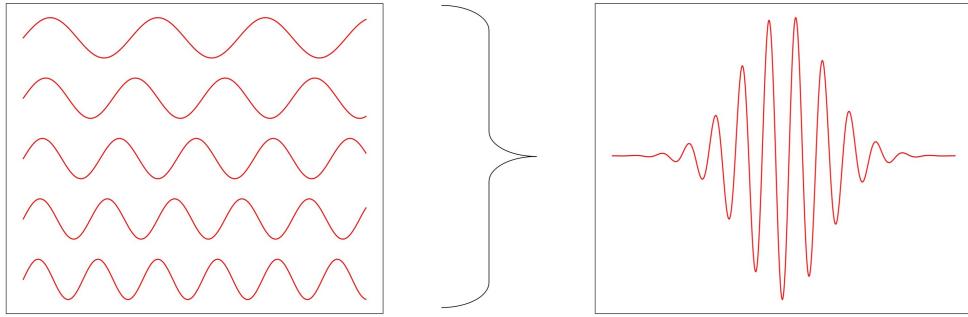


Figure 2: Multiple sinusoidal plane waves with different wave lengths are superposed into a single wave packet over finite space.

The reason for this is due to the well-known Heisenberg's uncertainty principle, which states that we cannot simultaneously know the exact position and momentum of the particle (see chapter 2.2 of [5]). This may sound strange, but this is what quantum superposition is - the idea that a system can exist in multiple states simultaneously until measured (see section 3.6 of [3]). We refer to measurement as gaining information about the system - in doing so the wave function 'collapses' to a certain state.

Finally, we represent a wave packet by a wave function $\psi(q)$ or $\psi(q, t)$. What's important about ψ is that it gives us the probability density of the particle being at a certain position via the modulus squared $|\psi|^2$. This is due to Born's statistical interpretation (see chapter 1.2 of [4]) which says that the probability that a particle is at a point q at time t is given by

$$\rho(q, t) := |\psi(q, t)|^2 = \psi(q, t)\bar{\psi}(q, t).$$

This probability interpretation requires that

$$\int_{-\infty}^{+\infty} |\psi(q, t)|^2 dq = 1. \quad (9)$$

The Schrödinger Equation

The Schrödinger equation is one of the most fundamental equations in quantum mechanics, which describes the behaviour of particles / waves. There are two different forms - the time independent Schrödinger equation (TISE), and the time dependent Schrödinger equation (TDSE).

The time independent Schrödinger equation is a partial differential equation that describes the stationary states of a quantum system. It is defined as

$$E\psi(q) = H\psi(q), \quad (10)$$

and inserting the Hamiltonian from (8) gives us

$$E\psi(q) = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} + V(q) \right) \psi(q). \quad (11)$$

Similarly, the time dependent Schrödinger equation is also a partial differential equation, but it describes the evolution in time of a wave in a specific quantum system. It is defined as

$$i\hbar \frac{\partial}{\partial t} \psi(q, t) = H\psi(q, t), \quad (12)$$

where H is the (quantum) Hamiltonian operator as above. Inserting the Hamiltonian gives us

$$i\hbar \frac{\partial}{\partial t} \psi(q, t) = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} + V(q) \right) \psi(q, t). \quad (13)$$

This implies that the energy operator is given by

$$E = i\hbar \frac{\partial}{\partial t}. \quad (14)$$

Fourier Transform

A helpful tool in quantum mechanics is the Fourier transform. To understand the Fourier transform, its important to recognise there is a duality between position and momentum space - a function in position space can be Fourier transformed into momentum space, and then functions in momentum space can be inverse Fourier transformed back into position space. We call q and p conjugate variables, because they are duals in this way.

Given a function $\psi(q)$, we can Fourier transform (FT) it into momentum space by

$$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \psi(q) e^{-\frac{i}{\hbar} pq} dq. \quad (15)$$

Likewise, for a function $\tilde{\psi}(p)$ we can convert from momentum space back to position space with the inverse Fourier transform (iFT)

$$\psi(q) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \tilde{\psi}(p) e^{\frac{i}{\hbar} pq} dp. \quad (16)$$

Dirac Delta function

Another useful tool in quantum calculations is the Dirac delta function. It is hard to define formally, since it is not a conventional function, but it is often loosely defined such that

$$\delta(q) = \begin{cases} 0 & q \neq 0 \\ \infty & q = 0 \end{cases} \quad (17)$$

and further, it can also be defined by the following integrals (see §2.5.1 of [5])

$$\int f(q)\delta(q)dq = f(0) \quad (18)$$

$$\int f(q)\delta(q - q')dq = f(q'). \quad (19)$$

Lastly, we have that

$$\frac{1}{2\pi\hbar} \int e^{\frac{i}{\hbar}pq}dp = \delta(q) \quad (20)$$

in one dimension. This is an interesting form, since it is very closely related to the Fourier and inverse Fourier transforms as defined in (15) and (16). Importantly, this definition of the delta function is key in the derivations of them (see §2.5.1 of [5]).

2.2.1 Dirac Notation

Dirac notation is an initially strange but undoubtedly useful way to write quantum mechanics, and allows us to solve initially complicated equations quite simply. We will use Dirac notation in this section to derive some important properties of wave functions, specifically related to position and momentum eigenfunctions shown below. In Dirac notation, we represent a wave function $\psi(q)$ as $|\psi\rangle$ which we call ‘ket psi’. We also denote the inner product as $\langle\phi|\psi\rangle$ where

$$\langle\phi|\psi\rangle = \int \bar{\phi}\psi dq.$$

The norm of a wave function ψ is defined as $||\psi|| = \sqrt{\langle\psi|\psi\rangle}$, so the norm squared is the inner product, or

$$||\psi||^2 = \langle\psi|\psi\rangle = \int |\psi|^2 dq.$$

Position and Momentum Eigenfunctions

Let us denote $|q\rangle$ and $|p\rangle$ as the eigenstates of the position and momentum operators respectively,

$$\begin{aligned}\hat{q}|q\rangle &= q|q\rangle \\ \hat{p}|p\rangle &= p|p\rangle.\end{aligned}$$

The eigenfunctions of the position operator are given by delta functions

$$|q'\rangle = \psi_{q'}(q) = \delta(q - q'). \quad (21)$$

Proof.

$$\hat{q}|q'\rangle = q\delta(q - q') = q'\delta(q - q') = q'|q'\rangle,$$

as the delta function is zero unless $q = q'$. □

The eigenstates of the momentum operator are given by

$$|p\rangle = \psi_p(q) = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}pq}. \quad (22)$$

Proof.

$$\hat{p}|p\rangle = \frac{\hbar}{i}\frac{\partial}{\partial q}\frac{1}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}pq} = \frac{p}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}pq} = p|p\rangle.$$

□

The prefactor $\frac{1}{\sqrt{2\pi\hbar}}$ is used for normalisation, since

$$\begin{aligned}\langle p|p'\rangle &= \frac{1}{2\pi\hbar}\langle e^{\frac{i}{\hbar}pq}|e^{\frac{i}{\hbar}p'q}\rangle \\ &= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}e^{-\frac{i}{\hbar}pq}e^{\frac{i}{\hbar}p'q}dq \\ &= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}e^{\frac{i}{\hbar}q(p'-p)}dq \\ &= \delta(p' - p),\end{aligned}$$

where we have used definition (20) for the Dirac delta function.

We introduce the resolution of the identity (in position and in momentum), as well as Lemma 2.2 in the following, as it will come in handy when proving some properties of wave functions in Lemma 2.4 and Lemma 2.5. These will be beneficial later on when solving the Schrödinger equation by Fourier transforms in section 5.2. We also make use of them and other ideas from this section in §4.

Theorem 2.1 (Resolution of the Identity in Position).

$$I = \int |q\rangle\langle q| dq \quad (23)$$

Proof.

$$\langle \phi | \int |q\rangle\langle q| dq | \psi \rangle = \int \langle \phi | q \rangle \langle q | \psi \rangle dq = \int \overline{\langle q | \phi \rangle} \langle q | \psi \rangle dq = \int \bar{\phi}(q) \psi(q) dq = \langle \phi | \psi \rangle = \langle \phi | I | \psi \rangle.$$

□

Now we introduce the fact

Lemma 2.2.

$$\langle q | p \rangle = \psi_p(q).$$

Proof. Consider $\langle q | \hat{p} | p \rangle$. On one hand we have that

$$\langle q | \hat{p} | p \rangle = p \langle q | p \rangle.$$

On the other hand, using the resolution of the identity in position (23), we have that

$$\begin{aligned} \langle q | \hat{p} I | p \rangle &= \langle q | \hat{p} \int |q'\rangle\langle q' | dq' | p \rangle = \int \langle q | \hat{p} | q' \rangle \langle q' | p \rangle dq' = \int -i\hbar \frac{\partial}{\partial q} \langle q | q' \rangle \langle q' | p \rangle dq' \\ &= -i\hbar \frac{\partial}{\partial q} \int \delta(q' - q) \langle q' | p \rangle dq' = -i\hbar \frac{\partial}{\partial q} \langle q | p \rangle, \end{aligned}$$

by the definition of the delta function in (19).

Now, we can equate these to get

$$\begin{aligned} p \langle q | p \rangle = -i\hbar \frac{\partial}{\partial q} \langle q | p \rangle &\Leftrightarrow \frac{i}{\hbar} p = \frac{\frac{\partial}{\partial q} \langle q | p \rangle}{\langle q | p \rangle} \Leftrightarrow \frac{i}{\hbar} p = \frac{d}{dq} (\ln \langle q | p \rangle) \\ &\Leftrightarrow \frac{i}{\hbar} pq + c = \ln \langle q | p \rangle \Leftrightarrow ce^{\frac{i}{\hbar} pq} = \langle q | p \rangle, \end{aligned}$$

and set $c = \frac{1}{\sqrt{2\pi\hbar}}$ for normalisation of the resolution of the identity in momentum, which we define momentarily. Thus,

$$\langle q|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}pq} = \psi_p(q)$$

as required. \square

Similarly to the resolution of the identity in position, we have

Theorem 2.3 (Resolution of the Identity in Momentum).

$$I = \int |p\rangle\langle p|dp. \quad (24)$$

Proof.

$$\begin{aligned} \langle q| \int |p\rangle\langle p|dp|\psi\rangle &= \int \langle q|p\rangle\langle p|\psi\rangle dp = \int \psi_p(q)\langle p|I|\psi\rangle dp = \int \int \psi_p(q)\langle p|q'\rangle\langle q'|\psi\rangle dpdq' \\ &= \int \int \psi_p(q)\overline{\psi_p}(q')\psi(q')dpdq' = \int \int \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}pq} \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar}pq'} \psi(q')dpdq' \\ &= \int \int \frac{1}{2\pi\hbar} e^{\frac{i}{\hbar}p(q-q')} \psi(q')dpdq' = \int \delta(q-q')\psi(q')dq' = \psi(q) = \langle q|\psi\rangle \\ &= \langle q|I|\psi\rangle, \end{aligned}$$

where we have inserted the equation for the eigenstate of the momentum operator $\psi_p(q)$ from equation (22) in place of $\langle q|p\rangle$. \square

Useful Properties

We can now use the lemmas and theorem above to prove some useful properties when using Dirac notation. First, we have that

Lemma 2.4.

$$\langle q|\psi\rangle = \psi(q).$$

Proof.

$$\langle q|\psi\rangle = \int \bar{\delta}(q'-q)\psi(q')dq' = \int \delta(q'-q)\psi(q')dq' = \psi(q),$$

using the definition of the delta function (19), and since the delta function is real. \square

Another useful property is that we can write the Fourier transform of $\psi(q)$ similarly,

Lemma 2.5.

$$\langle p|\psi\rangle = \tilde{\psi}(p).$$

Proof.

$$\begin{aligned}\langle p|\psi \rangle &= \langle p| \int |q\rangle\langle q| dq |\psi \rangle = \int \langle p|q\rangle\langle q|\psi \rangle dq = \int \overline{\langle q|p\rangle} \langle q|\psi \rangle dq = \int \overline{\psi_p}(p) \langle q|\psi \rangle dq \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int e^{-\frac{i}{\hbar}pq} \psi(q) dq = \tilde{\psi}(p),\end{aligned}$$

using the resolution of the identity in q as in (23), the definition of $\psi_p(q)$ (22) and the definition of the Fourier transform as in (15). \square

2.2.2 Pictures

Pictures are different ways we can formulate quantum mechanics (just like Hamiltonian and Lagrangian mechanics are different formulations of classical mechanics). We use different pictures depending on the ease of solving problems in that picture.

Schrödinger Picture

In the Schrödinger picture, the states evolve in time and the operators remain constant. We will mostly be using the Schrödinger picture in this project. Recall that the evolution of a state is governed by the TDSE (12), and we generally assume H is time independent. In this case, time evolution is brought about by the unitary time evolution operator, $U(t - t_0)$, or $U(t)$ assuming $t = 0$. When H is time-independent, $U(t - t_0) = e^{-\frac{i}{\hbar}H(t-t_0)}$ or $U(t) = e^{-\frac{i}{\hbar}Ht}$ if $t_0 = 0$. From here on, we generally assume $t_0 = 0$, and then

$$\psi(t) = U(t)\psi(0) = e^{-\frac{i}{\hbar}Ht}\psi(0), \quad (25)$$

which is also often written $\psi(t) = e^{-\frac{i}{\hbar}Ht}\psi_0$ or just $\psi(t) = e^{-\frac{i}{\hbar}Ht}\psi$.

We can write this slightly differently, by considering the TISE (10), and recalling that any state can be written as a linear combination of eigenfunctions of the Hamiltonian, ψ_n , where

$$H\psi_n = E\psi_n.$$

Heisenberg Picture

In the Heisenberg picture, in contrast to the Schrödinger picture, the states are time independent and the operators evolve in time.

In this picture, operators A evolve according to

$$A_H(t) := U^\dagger(t)A_SU(t).$$

The H and S here represent ‘Heisenberg’ and ‘Schrödinger’, and from here on we will denote $A_H(t) = A(t)$ and $A_S = A(0) = A$. If the Hamiltonian is time independent, $U(t)$ is the time evolution operator as in the Schrödinger picture. Then we also have

$$A(t) = e^{\frac{i}{\hbar}Ht} A e^{-\frac{i}{\hbar}Ht}.$$

The operator A then satisfies Heisenberg’s equation of motion (where we assume in this paper that A is time-independent initially)

$$\frac{d}{dt} A(t) = \frac{i}{\hbar} [H, A(t)], \quad (26)$$

where the square brackets indicate the commutator of two operators $[X, Y] = XY - YX$.

Proof. The evolution operator satisfies the Schrödinger equation $\frac{d}{dt}U(t) = -\frac{i}{\hbar}HU(t)$. Then,

$$\begin{aligned} \frac{d}{dt} A(t) &= \frac{d}{dt} U^\dagger(t) A U(t) = \frac{d}{dt} (U^\dagger(t)) A U(t) + U^\dagger(t) A \frac{d}{dt} (U(t)) \\ &= \left(-\frac{i}{\hbar} H U(t) \right)^\dagger A U(t) + U^\dagger(t) A \left(-\frac{i}{\hbar} H U(t) \right) \\ &= \frac{i}{\hbar} U^\dagger(t) H^\dagger A U(t) - \frac{i}{\hbar} U^\dagger(t) A H U(t) = \frac{i}{\hbar} U^\dagger(t) (HA) U(t) - \frac{i}{\hbar} U^\dagger(t) (AH) U(t) \\ &= \frac{i}{\hbar} e^{\frac{i}{\hbar}Ht} (HA) e^{-\frac{i}{\hbar}Ht} - \frac{i}{\hbar} e^{\frac{i}{\hbar}Ht} (AH) e^{-\frac{i}{\hbar}Ht} \\ &= \frac{i}{\hbar} \left(H e^{\frac{i}{\hbar}Ht} A e^{-\frac{i}{\hbar}Ht} \right) - \frac{i}{\hbar} \left(e^{\frac{i}{\hbar}Ht} A e^{-\frac{i}{\hbar}Ht} H \right) = \frac{i}{\hbar} (HA(t) - A(t)H) = \frac{i}{\hbar} [H, A(t)], \end{aligned}$$

where we have used that H is self adjoint, H commutes with $e^{-\frac{i}{\hbar}Ht}$, and $(XY)^\dagger = Y^\dagger X^\dagger$. Thus we have the equation as in (26) as required. \square

Interaction Picture

The interaction or Dirac picture can be thought of as a combination of the Schrödinger picture and the Heisenberg picture, since both the states and operators have time dependence. For the interaction picture, the Hamiltonian in the Schrödinger equation has two parts

$$i\hbar \frac{\partial}{\partial t} \psi = (H_1 + H_2)\psi. \quad (27)$$

Usually, H_1 is some solvable Hamiltonian and H_2 is some harder to solve Hamiltonian involving a perturbation or interaction (see chapter 11 of [6]).

3 Numerical Methods

Gaussian Wave

A Gaussian wave (see chapter 3 of [2]) has the form

$$\psi(q) = \frac{1}{\sqrt{a\sqrt{\pi}}} e^{-\frac{(q-q_0)^2}{4a^2}} e^{ikq}, \quad (28)$$

where a is the width, q_0 is the centre, and $k = p\hbar$ is the wave number. As usual, p is the momentum. The energy of the state is given by $E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$ since $p = \sqrt{2mE}$ and $p = \hbar k$. In most of our calculations we will model the initial wave packet as a normalised Gaussian wave as above, or some variation of this.

3.1 Split Operator Method

The ideas and methods presented in this section can be seen and furthered explored in chapter 11 of [2], chapter 3.7, 14.2 and 20.1 of [3] and also in chapter 3.3 of [7].

The split operator method, also known as Strang splitting, is a numerical method used to solve partial differential equations, such as the Schrödinger equation. We solve the Schrödinger equation in time steps, dt , via (25) using a half time step in potential, followed by a full time step in kinetic and then another half step in potential

$$\psi(q, t + dt) = e^{-\frac{i}{\hbar} H dt} \psi(q, t) = e^{-\frac{i}{\hbar}(T+V)dt} \psi(q, t) \approx e^{-\frac{i}{\hbar} \frac{V}{2} dt} e^{\frac{i}{\hbar} T dt} e^{-\frac{i}{\hbar} \frac{V}{2} dt} \psi(q, t).$$

To explain why we can split the exponentials in such a way we use the Trotter product formula (see chapter 20.1 of [3]), and the Baker-Campbell-Hausdorff (BCH) formula (see chapter 14.2 of [3]).

The Trotter product formula says

$$e^{A+B} = \lim_{N \rightarrow \infty} \left(e^{\frac{A}{N}} e^{\frac{B}{N}} \right)^N, \quad (29)$$

so this explains why we can split t up into N smaller time steps $dt := \frac{t}{N}$, as then

$$e^{(A+B)t} = \lim_{N \rightarrow \infty} \left(e^{A \frac{t}{N}} e^{B \frac{t}{N}} \right)^N = \lim_{N \rightarrow \infty} (e^{Adt} e^{Bdt})^N.$$

Thus, with repeated applications of $e^{Adt} e^{Bdt}$, we can approximate $e^{(A+B)t}$. However we are not doing infinite time steps in our method, so it's also important to note that in general, $e^{A+B} \neq e^A e^B$ for operators A and B if they do not commute (i.e. if $[A, B] = AB - BA \neq 0$). Before we can continue, it is necessary to introduce some properties of the commutator.

Lemma 3.1.

- (i) $[A, B] = -[B, A]$
- (ii) $[\alpha A + \beta B, \gamma C + \delta D] = \alpha\gamma[A, C] + \alpha\delta[A, D] + \beta\gamma[B, C] + \beta\delta[B, D]$

Proof.

$$\begin{aligned}
(i) \quad [A, B] &= AB - BA = -(BA - AB) = -[B, A]. \\
(ii) \quad [\alpha A + \beta B, \gamma C + \delta D] &= (\alpha A + \beta B)(\gamma C + \delta D) - (\gamma C + \delta D)(\alpha A + \beta B) \\
&= \alpha\gamma AC + \alpha\delta AD + \beta\gamma BC + \beta\delta BD \\
&\quad - \alpha\gamma CA - \beta\gamma CB - \alpha\delta DA - \beta\delta DB \\
&= \alpha\gamma(AC - CA) + \alpha\delta(AD - DA) + \beta\gamma(BC - CB) \\
&\quad + \beta\delta(BD - DB) \\
&= \alpha\gamma[A, C] + \alpha\delta[A, D] + \beta\gamma[B, C] + \beta\delta[B, D].
\end{aligned}$$

□

Since T and V do not commute, we show that we can write the exponentials in this way using the Baker-Campbell-Hausdorff formula

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\dots}, \quad (30)$$

where further terms involve $[A, B]$. This means that

$$e^{Adt} e^{Bdt} = e^{(A+B)dt+\frac{1}{2}[Adt, Bdt]+\dots} = e^{(A+B)dt+\frac{1}{2}[A, B]dt^2+\dots},$$

so we can approximate $e^{(A+B)dt}$ by $e^{Adt} e^{Bdt}$ with an error of $\mathcal{O}(dt^2)$. However, via Strang splitting, we can achieve an even smaller error of order $\mathcal{O}(dt^3)$. We show this by applying the BCH formula twice

$$\begin{aligned}
e^{\frac{A}{2}dt} e^{Bdt} e^{\frac{A}{2}dt} &= e^{\frac{A}{2}dt} \left(e^{Bdt} e^{\frac{A}{2}dt} \right) \\
&= e^{\frac{A}{2}dt} \left(e^{(B+\frac{A}{2})dt+\frac{1}{4}[B,A]dt^2+\mathcal{O}(dt^3)} \right) \\
&= e^{(A+B)dt+\frac{1}{4}[B,A]dt^2+\mathcal{O}(dt^3)+\frac{1}{2}\left[\frac{A}{2}dt, Bdt+\frac{A}{2}dt+\frac{1}{4}[B,A]dt^2+\mathcal{O}(dt^3)\right]} \\
&= e^{(A+B)dt+\frac{1}{4}[B,A]dt^2+\frac{1}{4}[A,B]dt^2+\frac{1}{8}[A,A]dt^2+\mathcal{O}(dt^3)} \\
&= e^{(A+B)dt+\mathcal{O}(dt^3)},
\end{aligned}$$

where we have used Lemma 3.1 to show that the terms involving dt^2 cancel.

Because the potential V is a function of position q , and T is a function of momentum p , we have to switch between position and momentum space via the Fourier and inverse Fourier transforms. Then the whole process becomes

$$\begin{aligned} \psi(q, t) &\xrightarrow{\frac{1}{2} \text{ step in } V} e^{-\frac{i}{\hbar} \frac{V}{2} dt} \psi(q, t) \xrightarrow{\text{FT}} e^{-\frac{i}{\hbar} \frac{V}{2} dt} \psi(p, t) \xrightarrow{\text{step in } T} e^{-\frac{i}{\hbar} T dt} e^{\frac{i}{\hbar} \frac{V}{2} dt} \psi(p, t) \xrightarrow{\text{iFT}} \\ &e^{-\frac{i}{\hbar} T dt} e^{\frac{i}{\hbar} \frac{V}{2} dt} \psi(q, t) \xrightarrow{\frac{1}{2} \text{ step in } V} e^{\frac{i}{\hbar} \frac{V}{2} dt} e^{-\frac{i}{\hbar} T dt} e^{\frac{i}{\hbar} \frac{V}{2} dt} \psi(q, t) \approx \psi(q, t + dt). \end{aligned}$$

A computationally efficient way to perform the Fourier transform is the use the fast Fourier transform (FFT). This is a quick and effective way to compute the discrete Fourier transform (DFT) (see [2] chapter 6.2.4) given by

$$\tilde{\psi}(k_l) = \sum_{j=0}^{N-1} \psi(q_j) e^{-2\pi i \frac{j l}{N}}, \quad (31)$$

and the inverse discrete Fourier transform (iDFT) given by

$$\psi(q_j) = \frac{1}{N} \sum_{l=0}^{N-1} \tilde{\psi}(k_l) e^{2\pi i \frac{j l}{N}}. \quad (32)$$

This, coupled with the split operator method, allows us to simulate interactions between quantum states and potentials efficiently and accurately. In order to do so, we first have to discretise a position grid, and define a Gaussian wave packet on it. This can then be fed into a function that computes the position and momentum time steps, and the Fourier and inverse Fourier transforms in between. Since we are using the FFT and iFFT, we have to modify our wave function slightly so that it still acts like a continuous Fourier transform.

Recall the continuous FT from (15) and note that it can be rewritten slightly differently in terms of $k = p/\hbar$

$$\tilde{\psi}(k) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \psi(q) e^{-ikq} dq.$$

To make this look like the DFT, we first assume it can be approximated by the integral

$$\tilde{\psi}(k) \approx \frac{1}{\sqrt{2\pi\hbar}} \int_a^b \psi(q) e^{-ikq} dq$$

for some a and b . We can then approximate this integral using a Riemann sum [8].

$$\tilde{\psi}(k) \approx \frac{1}{\sqrt{2\pi\hbar}} \sum_{j=0}^{N-1} \psi(q_j) e^{-ikq_j} \Delta q,$$

where $q_j = q_0 + j\Delta q = a + j\Delta q$ and $\Delta q = \frac{b-a}{N}$, so we have discretised the position space. We have to discretise k space too, by setting $k_l = k_0 + l\Delta k$ where $\Delta k = \frac{2\pi}{N\Delta q} = \frac{2\pi}{b-a}$. Thus,

$$\tilde{\psi}(k_l) \approx \frac{1}{\sqrt{2\pi\hbar}} \sum_{j=0}^{N-1} \psi(q_j) e^{-ik_l q_j} \Delta q.$$

Now, we can first sub in $k_l = k_0 + l\Delta k$

$$\tilde{\psi}(k_l) \approx \frac{1}{\sqrt{2\pi\hbar}} \sum_{j=0}^{N-1} \psi(q_j) e^{-ik_0 q_j} e^{-ilj\Delta k q_j} \Delta q$$

and then we can sub $q_j = q_0 + j\Delta q$ into the last q_j

$$\tilde{\psi}(k_l) \approx \frac{1}{\sqrt{2\pi\hbar}} \sum_{j=0}^{N-1} \psi(q_j) e^{-ik_0 q_j} e^{-ilq_0 \Delta k} e^{-ilj\Delta k \Delta q} \Delta q$$

and finally, we sub $\Delta k = \frac{2\pi}{N\Delta q}$ into the last Δp and rearrange to get

$$\begin{aligned} \tilde{\psi}(k_l) &\approx \frac{1}{\sqrt{2\pi\hbar}} \sum_{j=0}^{N-1} \psi(q_j) e^{-ik_0 q_j} e^{-ilq_0 \Delta k} e^{-2\pi i \frac{lq_j}{N}} \Delta q \Rightarrow \\ e^{ilq_0 \Delta k} \tilde{\psi}(k_l) &\approx \frac{1}{\sqrt{2\pi\hbar}} \sum_{j=0}^{N-1} \psi(q_j) e^{-2\pi i \frac{lq_j}{N}} e^{-ik_0 q_j} \Delta q. \end{aligned}$$

We can do similar calculations for the iFT and get

$$\frac{1}{\sqrt{2\pi\hbar}} \psi(q_j) e^{-ik_0 q_j} \Delta q = \frac{1}{N} \sum_{l=0}^{N-1} \tilde{\psi}(k_l) e^{2\pi i \frac{jl}{N}} e^{ilq_0 \Delta k}.$$

Thus, comparing this to the definitions in (31) and (32), we have the discrete Fourier pair

$$\frac{1}{\sqrt{2\pi\hbar}} \psi(q_j) e^{-ik_0 q_j} \Delta q \longleftrightarrow \tilde{\psi}(k_l) e^{ilq_0 \Delta k},$$

corresponding to the continuous Fourier pair $\psi(q) \longleftrightarrow \tilde{\psi}(k)$. We have to take these extra factors into account when fast Fourier transforming in the split operator method. This was all executed in Python code and the FFT along with other numerical tools were implemented using the NumPy and SciPy libraries [9] [10]. The code was further visualised in animations using the Matplotlib library [11]. This code can all be seen in Appendix 10.1, and some resulting animation snapshots can be seen throughout the project as well as a more detailed analysis of them in §7.

4 Scattering Theory

You can find the ideas discussed in this section and additional reading material in chapter 6 and 7 of [2], as well as in chapter 3 of [5].

In this section we introduce quantum scattering theory. The basic idea is to observe how an incident wave with a given energy interacts with a potential barrier, where it can split into reflected and transmitted parts. This is another way to describe how states evolve in a quantum system over time. So far, we have seen that the evolution of a system defined by a Hamiltonian H is given by the TDSE (12),

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi.$$

We also have the TISE as in (10),

$$H\psi = E\psi,$$

which describes the stationary states of the system. Since H is self adjoint, recall that there exists an orthonormal basis (ONB) of eigenfunctions ψ_n of H such that

$$H\psi_n = E_n\psi_n \quad , \quad \langle \psi_m | \psi_n \rangle = \delta_{nm}$$

where δ is the Kronecker delta defined

$$\delta_{nm} = \begin{cases} 0 & \text{if } m \neq n \\ 1 & \text{if } m = n. \end{cases}$$

We can use these eigenfunctions to solve the TDSE. Recall that the evolution of a wave is given by

$$\psi(q, t) = e^{-\frac{i}{\hbar} H t} \psi_0(q),$$

and since $\{\psi_n\}$ from a complete basis, we can write ψ_0 as a linear combination of them. Then

$$|\psi_0\rangle = \sum_n c_n |\psi_n\rangle \Rightarrow c_n = \langle \psi_n | \psi_0 \rangle,$$

therefore

$$|\psi_0\rangle = \sum_n \langle\psi_n|\psi_0\rangle |\psi_n\rangle,$$

and then using lemma 2.4, we can apply $\langle q|$ to get,

$$\psi_0(q) = \sum_n \langle\psi_n|\psi_0\rangle \psi_n(q).$$

Thus, we have that the time evolution of $\psi_0(q)$ is given by

$$\psi(q, t) = \sum_n \langle\psi_n|\psi_0\rangle e^{-\frac{i}{\hbar}Ht} \psi_n(q) = \sum_n \langle\psi_n|\psi_0\rangle e^{-\frac{i}{\hbar}E_n t} \psi_n(q),$$

We use the power expansion of e^H to show

$$e^H \psi_n = \sum_m \frac{H^n}{n!} \psi_n = \left(1 + H + \frac{H^2}{2!} + \dots\right) \psi_n = \left(1 + E + \frac{E^2}{2!} + \dots\right) \psi_n = e^E \psi_n,$$

since ψ_n are eigenvectors of H with eigenvalues E_n .

This is the time evolution for a discrete spectrum of eigenfunctions, however, a similar case holds for a continuous spectrum of eigenfunctions ψ_E (for every energy $E > 0$). In this case the TISE is

$$H\psi_E = E\psi_E \quad , \quad \langle\psi_{E'}|\psi_E\rangle = \delta(E - E'),$$

where this time, δ is the Dirac delta function from §2.2. Then, the time evolution is given by

$$\psi(q, t) = \int e^{-\frac{i}{\hbar}Et} \langle\psi_E|\psi_0\rangle \psi_E(q) dE.$$

The eigenstates ψ_E are called scattering states. They are related to something called the scattering matrix or the S -matrix. We define S and show the connection in the following.

Consider a situation where we have a general potential barrier $V(q)$, for example like the one shown in Fig. 3. We can split this system into three regions L , C and R standing for left, centre and right. Region L is the region where $V = 0$ to the left of the barrier, and region R is where $V = 0$ to the right of the barrier. In region C , $V(q) \neq 0$ and varies spatially - we deal with this case using the WKB approximation in §5.1. Now, if we send in particles from the left and right, we can observe how they interact with the barrier, as

they will either be transmitted past it, or reflected back off of it. We can find the wave functions in L and R by considering the TISE

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial q^2} = E\psi \Leftrightarrow \frac{\partial^2 \psi}{\partial q^2} + \frac{2mE}{\hbar^2} \psi = 0 \Leftrightarrow \frac{\partial^2 \psi}{\partial q^2} + k^2 \psi = 0,$$

where $k = \frac{p}{\hbar} = \frac{\sqrt{2mE}}{\hbar}$. Solving this second order differential equation gives us the general solutions for the region L

$$\psi_E = Ae^{ikq} + Be^{-ikq},$$

and for region R ,

$$\psi_E = Ce^{ikq} + De^{-ikq}.$$

Notice that Ae^{ikq} and Ce^{ikq} have positive momentum $p = \sqrt{2mE}$ (which in this setup indicates traveling to the right), whereas Be^{-ikq} and De^{-ikq} have negative momentum $p = -\sqrt{2mE}$ (this indicates motion to the left). This means that we interpret Ae^{ikq} as representing a wave of incoming particles from the left with intensity $|A|^2$ and Be^{-ikq} as outgoing particles to the left with intensity $|B|^2$. Similarly, Ce^{ikq} represents outgoing particles to the right with intensity $|C|^2$, and De^{-ikq} represents incoming particles from the right with intensity $|D|^2$.

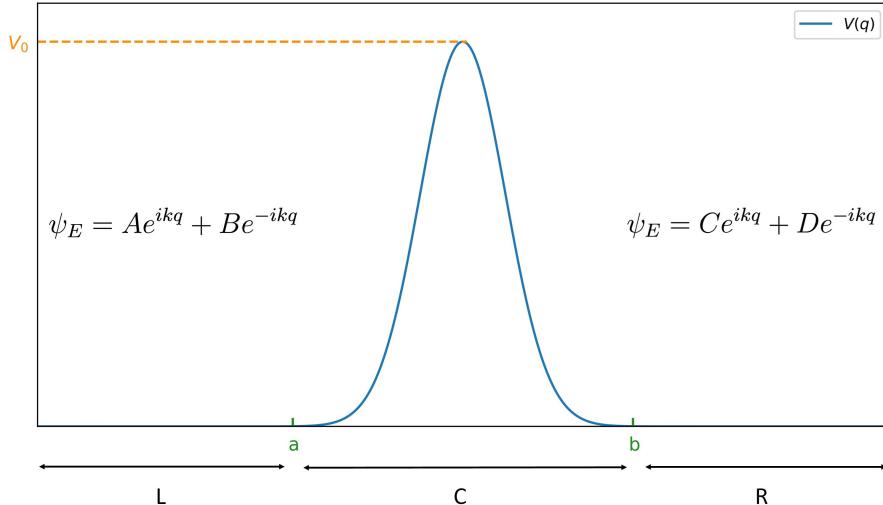


Figure 3: The different regions of a system split with respect to where the potential is zero or non-zero. Also indicated are the wave functions to the left and right of the potential.

In physical terms, we can think about a situation where we send in particles from the left and right and observe what is outputted (how they are transmitted or reflected). So given A and D , we want to determine B and C . We defined the S -matrix as a way to interpret this transition from incoming to outgoing waves. S is a 2×2 matrix defined such that $\psi_{\text{out}} = S\psi_{\text{in}}$ so,

$$\begin{bmatrix} B \\ C \end{bmatrix} = S \begin{bmatrix} A \\ D \end{bmatrix}.$$

In more mathematical terms, since the TISE is a second order differential equation, there are exactly two linearly independent solutions for any $E > 0$, and therefore there must be two linear relations between the four constants A , B , C and D . This is encoded in the S -matrix, which also implies that S depends on E .

Now if we consider sending a wave in from the left, then A is given and $D = 0$. Then,

$$\begin{bmatrix} B \\ C \end{bmatrix} = S \begin{bmatrix} A \\ 0 \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} A \\ 0 \end{bmatrix} = \begin{bmatrix} S_{11}A \\ S_{21}A \end{bmatrix}.$$

Thus, in region L , $\psi_E(q) = Ae^{ikq} + S_{11}Ae^{-ikq}$ and in region R , $\psi_E(q) = AS_{21}e^{ikq}$. Also note that $E = \frac{\hbar^2 k^2}{2m}$ and $\psi_E(q, t) = e^{-\frac{i}{\hbar}Et}\psi_E(q) = e^{-\frac{i\hbar k^2}{2m}t}\psi_E(q)$ is a solution of the TISE.

We can now connect the plane wave scattering eigenstates with wave packets. We assume that we have a incident wave packet from the left, so it is a superposition of plane waves

$$\psi_0(q) = \frac{1}{\sqrt{2\pi\hbar}} \int A(k)e^{ikq}dk.$$

This is because the incoming wave is given by Ae^{ikq} , with a range of energies and thus we integrate over k . The constant at the front can be thought of as a normalisation constant, and $A(k)$ is an envelope function centred at k_0 . Note that $\psi_0(q)$ is of the form of a Fourier transform of $A(k)$ in k . Then,

$$\psi(q, t) = e^{-\frac{i}{\hbar}Et}\psi_0(q) = \frac{1}{\sqrt{2\pi\hbar}} \int e^{-\frac{i\hbar k^2}{2m}t} A(k)e^{ikq}dk.$$

Also, we have that in region L ,

$$\psi(q, t) = \frac{1}{\sqrt{2\pi\hbar}} \int e^{-\frac{i\hbar k^2}{2m}t} A(k)(e^{ikq} + S_{11}e^{-ikq})dk$$

and in region R ,

$$\psi(q, t) = \frac{1}{\sqrt{2\pi\hbar}} \int e^{-\frac{i\hbar k^2}{2m}t} A(k) S_{21} e^{ikq} dk.$$

Now, for large enough t , the waves will have left the centre region C and be fully transmitted or reflected, giving us

$$\lim_{t \rightarrow \infty} = \begin{cases} \frac{1}{\sqrt{2\pi\hbar}} \int S_{11}(k) e^{-\frac{i\hbar k^2}{2m}t} A(k) e^{-ikq} & \text{if } q < a \\ \frac{1}{\sqrt{2\pi\hbar}} \int S_{21}(k) e^{-\frac{i\hbar k^2}{2m}t} A(k) e^{ikq} dk & \text{if } q > b. \end{cases}$$

These equations give the reflected and transmitted parts of the wave packet respectively, which we denote $\psi_R(q, t)$ and $\psi_T(q, t)$. So,

$$\psi_R(q, t) = \frac{1}{\sqrt{2\pi\hbar}} \int S_{11}(k) e^{-\frac{i\hbar k^2}{2m}t} A(k) e^{-ikq} , \quad \psi_T(q, t) = \frac{1}{\sqrt{2\pi\hbar}} \int S_{21}(k) e^{-\frac{i\hbar k^2}{2m}t} A(k) e^{ikq} dk.$$

Since $\psi_0(q)$ is a Fourier transform of $A(k)$, we can inverse Fourier transform to get

$$A(k) = \frac{1}{\sqrt{2\pi\hbar}} \int \psi_0(q) e^{-ikq} dq.$$

We assume $A(k) \approx 0$ for $k < 0$, since we are assuming we have a incident wave travelling to the right with positive momentum only.

By conservation of probability, since the wave can either be reflected or transmitted for large enough t , we have that

$$\lim_{t \rightarrow \infty} (\|\psi_R(q, t)\|^2 + \|\psi_T(q, t)\|^2) = 1.$$

This is related to the reflection and transmission coefficients $R(E)$ and $T(E)$, which are defined as the ratios of the reflected and transmitted probability currents over the incoming probability current respectively - we see this in more detail in §33. They can also be defined as $R(E) = |S_{11}(E)|^2$ and $T(E) = |S_{21}(E)|^2$ and we explain this in more detail in §4.2. Then we have the following theorem

Theorem 4.1.

$$\lim_{t \rightarrow \infty} \|\psi_R(q, t)\|^2 = \int R(k) |A(k)|^2 dk , \quad \lim_{t \rightarrow \infty} \|\psi_T(q, t)\|^2 = \int T(k) |A(k)|^2 dk.$$

Proof. We have

$$\begin{aligned} \|\psi_R(q, t)\|^2 &= \frac{1}{\sqrt{2\pi\hbar}} \int \int \int S_{11}(k) \overline{S}_{11}(k') A(k) \overline{A}(k') e^{-\frac{i\hbar}{2m}(k^2 - k'^2)t} e^{iq(k-k')} dk dk' dq \\ &= \int |S_{11}(k)|^2 |A(k)|^2 dk = \int R(k) |A(k)|^2 dk, \end{aligned}$$

where we have used that $\frac{1}{\sqrt{2\pi\hbar}} \int e^{iq(k-k')} dq = \delta(k - k')$. The proof for ψ_T is similar. \square

To summarise, we have shown that scattering states can be used to study time evolution and vice versa, the time evolution of wave packets can be used to obtain information about scattering states and the S -matrix. You can read more on this in chapter 7 of [2].

4.1 The Continuity Equation

The continuity equation is given by

$$\frac{\partial}{\partial t} \rho(q, t) + \frac{\partial}{\partial q} j(q, t) = 0, \quad (33)$$

where $\rho(q, t) = |\psi(q, t)|^2$ is the probability density of the wave function ψ and $j(q, t)$ is the probability current,

$$j(q, t) = \frac{\hbar}{2mi} \left(\overline{\psi} \frac{\partial \psi}{\partial q} - \psi \frac{\partial \overline{\psi}}{\partial q} \right) = \frac{\hbar}{m} \operatorname{Re} \left(\frac{1}{i} \overline{\psi} \frac{\partial \psi}{\partial q} \right) = \frac{\hbar}{m} \operatorname{Im} \left(\overline{\psi} \frac{\partial \psi}{\partial q} \right). \quad (34)$$

We can see this since $\rho(q, t) = |\psi(q, t)|^2 = \overline{\psi}(q, t)\psi(q, t)$ and so

$$\begin{aligned} \frac{\partial}{\partial t} \rho(q, t) &= \frac{\partial}{\partial t} (\overline{\psi}\psi) = \frac{\partial \overline{\psi}}{\partial t} \psi + \overline{\psi} \frac{\partial \psi}{\partial t} \\ &= \overline{\psi} \frac{1}{i\hbar} \left(-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial q^2} + V\psi \right) - \frac{1}{i\hbar} \left(-\frac{\hbar^2}{2m} \frac{\partial^2 \overline{\psi}}{\partial q^2} + V\overline{\psi} \right) \psi \\ &= -\frac{\hbar}{2mi} \left(\frac{\partial^2 \psi}{\partial q^2} \overline{\psi} - \psi \frac{\partial^2 \overline{\psi}}{\partial q^2} \right) = -\frac{\hbar}{2mi} \frac{\partial}{\partial q} \left(\frac{\partial \psi}{\partial q} \overline{\psi} - \psi \frac{\partial \overline{\psi}}{\partial q} \right) \\ &= -\frac{\partial}{\partial q} j(q, t). \end{aligned}$$

We have worked this out by using the TDSE (13) and the product rule, so that

$$\frac{\partial \psi}{\partial t} = \frac{1}{i\hbar} \left(-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial q^2} + V\psi \right), \quad \frac{\partial \overline{\psi}}{\partial t} = -\frac{1}{i\hbar} \left(-\frac{\hbar^2}{2m} \frac{\partial^2 \overline{\psi}}{\partial q^2} + V\overline{\psi} \right).$$

Reflection and Transmission Coefficients

As we saw earlier, the reflection and transmission coefficients are formally defined as the ratios of the reflected and transmitted probability currents over the incoming probability current.

Recall the definition of the probability current from (34)

$$j(q, t) = \frac{\hbar}{m} \operatorname{Re} \left(\frac{1}{i} \bar{\psi} \frac{\partial \psi}{\partial q} \right).$$

Then, for example, the probability current for a wave travelling to the right in region L is given by

$$j = \frac{\hbar}{m} \operatorname{Re} \left(\frac{1}{i} \bar{A} e^{-ikq} (ik A e^{ikq}) \right) = \frac{\hbar k}{m} |A|^2.$$

Similarly, the probability current for a wave travelling to the left in region L is $j = \frac{\hbar k}{m} |B|^2$, for a wave travelling to the right in region R is $j = \frac{\hbar k}{m} |C|^2$ and for a wave travelling to the left in region R is $j = \frac{\hbar k}{m} |D|^2$. Thus, since the wave number k is equivalent in each region (as we have $V(q) = 0$ in L and R), we have the definitions

$$R_L = \frac{|B|^2}{|A|^2}, \quad T_L = \frac{|C|^2}{|A|^2}, \quad R_R = \frac{|C|^2}{|D|^2}, \quad T_R = \frac{|B|^2}{|D|^2}, \quad (35)$$

where the subscripts L and R indicate what region the incident wave came from.

4.2 S and M Matrices

The scattering and transfer matrices are denoted S and M respectively. These matrices are both closely related to the reflection and transmission coefficients. The S -matrix essentially relates incoming waves to outgoing waves, and the M -matrix relates waves in different regions. So, $\psi_{out} = S\psi_{in}$ and $\psi_L = M\psi_R$ (or vice versa, depending on what convention you use). Thus, in the context of the wave functions as in Fig. 3, we have

$$\begin{bmatrix} B \\ C \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} A \\ D \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix}.$$

Importantly, the S -matrix elements can give us the reflection and transmission coefficients R and T , which we show in the following. For an incoming wave travelling to the right in region L (Ae^{ikq}), we set $D = 0$. Then, we can find R_L and T_L by expanding the matrix multiplication out

$$S_{11}A = B \Rightarrow S_{11} = \frac{B}{A} \quad , \quad S_{21}A = C \Rightarrow S_{21} = \frac{C}{A}.$$

Therefore

$$|S_{11}|^2 = \frac{|B|^2}{|A|^2} = R_L \quad , \quad |S_{21}|^2 = \frac{|C|^2}{|A|^2} = T_L,$$

where we have used the definitions in (35) and the subscript indicates what region the incident wave is from. Similarly, for an incoming wave in region R (De^{-ikq}), we set $A = 0$ and then we can find R_R and T_R in a similar manner

$$S_{12}D = B \Rightarrow S_{12} = \frac{B}{D} \quad , \quad S_{22}D = C \Rightarrow S_{22} = \frac{C}{D},$$

so

$$|S_{12}|^2 = \frac{|B|^2}{|D|^2} = T_R \quad , \quad |S_{22}|^2 = \frac{|C|^2}{|D|^2} = R_R,$$

where we have used the definitions in (35). Thus we have

$$S = \begin{bmatrix} r_L & t_R \\ t_L & r_R \end{bmatrix},$$

where $R_L = r_L \bar{r}_L$, $T_L = t_L \bar{t}_L$, and analogous relations hold for R_R and T_R .

If we consider the fact that probability current is conserved across the regions L and R , we can use this to show that S is unitary, i.e. $SS^\dagger = I$.

If we consider a wave incident from region L , then $\psi_L = Ae^{ikq} + Be^{-ikq}$, and we set $D = 0$. Then we can work out the probability current as

$$\begin{aligned} j &= \frac{\hbar}{m} \operatorname{Re} \left(\frac{1}{i} (\overline{A} e^{-ikq} + \overline{B} e^{ikq}) (ik A e^{ikq} - ik B e^{-ikq}) \right) \\ &= \frac{\hbar}{m} \operatorname{Re} (k|A|^2 - k \overline{A} B e^{-2ikq} + k A \overline{B} e^{2ikq} - k|B|^2) \\ &= \frac{\hbar k}{m} (|A|^2 - |B|^2), \end{aligned}$$

where we have cancelled the imaginary terms of the middle terms since we are taking the real part, and taking the difference of them cancels the real terms. Likewise the probability current in region R is given by

$$j_R = \frac{\hbar}{m} \operatorname{Re} \left(\frac{1}{i} \bar{\psi}_R \frac{\partial \psi_R}{\partial q} \right) = \frac{\hbar k}{m} (|C|^2 - |D|^2).$$

Because we have defined regions L and R such that $V(q) = 0$, we have that $k = \frac{\sqrt{2mE}}{\hbar}$ for both regions (i.e. they are equal in both regions). Then requiring continuity of the probability current, and using the fact that $\psi_{out} = S\psi_{in}$ and also, $\psi_{out}^\dagger = (S\psi_{in})^\dagger = \psi_{in}^\dagger S^\dagger$ we have that

$$\begin{aligned} j_L = j_R &\Leftrightarrow |A|^2 - |B|^2 = |C|^2 - |D|^2 \Leftrightarrow |A|^2 + |D|^2 = |B|^2 + |C|^2 \\ &\Leftrightarrow \psi_{in}^\dagger \psi_{in} = \psi_{out}^\dagger \psi_{out} \Leftrightarrow \psi_{in}^\dagger \psi_{in} = \psi_{in} S^\dagger S \psi_{in} \Leftrightarrow S^\dagger S = I, \end{aligned}$$

thus proving that the S -matrix is unitary.

We can obtain the elements of either the scattering or transfer matrix from the other by solving the simultaneous equations

$$S_{11}A + S_{12}D = B \tag{36}$$

$$S_{21}A + S_{22}D = C \tag{37}$$

$$M_{11}A + M_{12}B = C \tag{38}$$

$$M_{21}A + M_{22}B = D \tag{39}$$

We can solve (36) for D and sub this into (37)

$$-\frac{S_{11}}{S_{12}}A + \frac{1}{S_{12}}B = D.$$

Then,

$$\begin{aligned} S_{21}A + S_{22} \left(-\frac{S_{11}}{S_{12}}A + \frac{1}{S_{12}}B \right) &= C \Leftrightarrow \frac{S_{12}S_{21} - S_{11}S_{22}}{S_{12}}A + \frac{S_{22}}{S_{12}}B = C \\ &\Leftrightarrow -\frac{\det(S)}{S_{12}}A + \frac{S_{22}}{S_{12}}B = C. \end{aligned}$$

Thus, comparing this with (38), since we now have the same coefficients, we have that

$$M_{11} = -\frac{\det(S)}{S_{12}}, \quad M_{12} = \frac{S_{22}}{S_{12}}.$$

Next, notice that (36) and (39) involve the same coefficients, so we can rearrange (36) to get

$$-\frac{S_{11}}{S_{12}}A + \frac{1}{S_{12}}B = D.$$

Then we can compare this with (39) to obtain

$$M_{21} = -\frac{S_{11}}{S_{12}}, \quad M_{22} = \frac{1}{S_{12}}.$$

Therefore,

$$M = \begin{bmatrix} -\frac{\det(S)}{S_{12}} & \frac{S_{22}}{S_{12}} \\ -\frac{S_{11}}{S_{12}} & \frac{1}{S_{12}} \end{bmatrix} = \frac{1}{S_{12}} \begin{bmatrix} -\det(S) & S_{22} \\ -S_{11} & 1 \end{bmatrix}.$$

We can do something similar and get the S matrix elements from the M matrix by first rearranging and comparing (36) and (39)

$$-\frac{M_{21}}{M_{22}}A + \frac{1}{M_{22}}D = B.$$

Therefore

$$S_{11} = -\frac{M_{21}}{M_{22}}, \quad S_{12} = \frac{1}{M_{22}}.$$

Then we can rearrange (38) for B and insert it into (39) so,

$$B = -\frac{M_{11}}{M_{12}}A + \frac{1}{M_{12}}C,$$

therefore

$$M_{21}A + M_{22} \left(-\frac{M_{11}}{M_{12}}A + \frac{1}{M_{12}}C \right) = C \Leftrightarrow \frac{\det(M)}{M_{22}}A + \frac{M_{12}}{M_{22}}D = C$$

Now, we have the same coefficients as equation (37) so we can compare and get

$$S_{21} = \frac{\det(M)}{M_{22}}, \quad S_{22} = \frac{M_{12}}{M_{22}}.$$

So finally,

$$S = \begin{bmatrix} -\frac{M_{21}}{M_{22}} & \frac{1}{M_{22}} \\ \frac{\det(M)}{M_{22}} & \frac{M_{12}}{M_{22}} \end{bmatrix} = \frac{1}{M_{22}} \begin{bmatrix} -M_{21} & 1 \\ \det(M) & M_{12} \end{bmatrix}. \quad (40)$$

4.3 Reflection and Transmission Coefficients

The reflection and transmission coefficients (defined in (35)) can be thought of as the probability that an incident wave will be reflected off of, or transmitted through a potential barrier. This makes sense when we recall that the probability density of a wave is the modulus squared, or the inner product, as we saw in §2.2. We know from the laws of probability that it is conserved, so we expect that $R + T = 1$. We will give a proof of this in the following, using the idea of conservation of probability current.

Recall from earlier in §4.2 that the probability current in region L is given by

$$j_L = \frac{\hbar}{m} \operatorname{Re} \left(\frac{1}{i} \bar{\psi}_L \frac{\partial \psi_L}{\partial q} \right) = \frac{\hbar k}{m} (|A|^2 - |B|^2).$$

Then if we require continuity of the probability current, we have that

$$|A|^2 - |B|^2 = |C|^2 \Rightarrow 1 - \frac{|B|^2}{|A|^2} = \frac{|C|^2}{|A|^2} \Rightarrow \frac{|B|^2}{|A|^2} + \frac{|C|^2}{|A|^2} = 1 \Rightarrow R_L + T_L = 1,$$

where we have cancelled \hbar , k and m . Similarly, if we have a wave incident from region R , we have $\psi_R = Ce^{ikq} + De^{-ikq}$, and $A = 0$. Then,

$$|C|^2 - |D|^2 = -|B|^2 \Rightarrow \frac{|C|^2}{|D|^2} - 1 = -\frac{|B|^2}{|D|^2} \Rightarrow \frac{|C|^2}{|D|^2} + \frac{|B|^2}{|D|^2} = 1 \Rightarrow R_R + T_R = 1.$$

This aligns with the idea that R and T are probabilities, and by conservation of probabilities we know that they must sum to one.

4.3.1 Examples

Note that in our examples we tend to set one of the coordinate points splitting the regions to be at $q = 0$ for simplicity, as it will simplify some of the resulting equations. However, this is not a necessary condition, and we would end up with similar results if we used an arbitrary point, although the calculations to get there would be more convoluted (than they already are). Another point to consider is that so far we have been dealing with wave numbers k that are equal in the regions we consider, however in the following, the wave numbers in different regions are not necessarily the same. This is because the potential will

not always be equal to zero, however it is still valid to use wave numbers in the solution since within each region, $V(q)$ is still spatially constant.

Example - Step Potential

We will first consider a simple example of a step potential and show how to calculate the reflection and transmission coefficients. To do so, consider that the particle is free up to a point where the potential equals V_0 , which is some non-zero constant, and then imagine that this potential extends to infinity in the positive q -direction. This is shown visually in Fig. 4. Thus consider the potential

$$V(q) = \begin{cases} 0 & \text{if } q < 0 \\ V_0 & \text{if } q > 0 \end{cases}.$$

When $V(q) = 0$ we call this region I and when $V(q) = V_0$ we call this region II. Also, consider the TISE (11)

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial q^2} + V(q) = E\psi.$$

In region I, we have that $k_0 = \frac{\sqrt{2mE}}{\hbar}$ and so the TISE becomes

$$\frac{\partial^2 \psi}{\partial q^2} = -\frac{2mE_n}{\hbar} \Leftrightarrow \frac{\partial^2 \psi}{\partial q^2} + k_0^2 = 0.$$

In region II we have to distinguish between when $E > V_0$ and when $E < V_0$.

We first consider the case when $\mathbf{E} > \mathbf{V}_0$.

Then we have that $k_+ = \frac{\sqrt{2m(E-V_0)}}{\hbar}$ and so the TISE becomes

$$\frac{\partial^2 \psi}{\partial q^2} = -\frac{2m(E-V_0)}{\hbar} \psi \Leftrightarrow \frac{\partial^2 \psi}{\partial q^2} + k_+^2 = 0.$$

These are second order differential equations and have general solutions of the form

$$\psi_I = A e^{ik_0 q} + B e^{-ik_0 q}, \quad \psi_{II} = C e^{ik_+ q} + D e^{-ik_+ q}.$$

Since this is a step potential as pictured in Fig. 4, we only consider incoming waves from region I, as an incoming wave from region II is illogical as the potential extends to infinity. Hence we set $D = 0$.

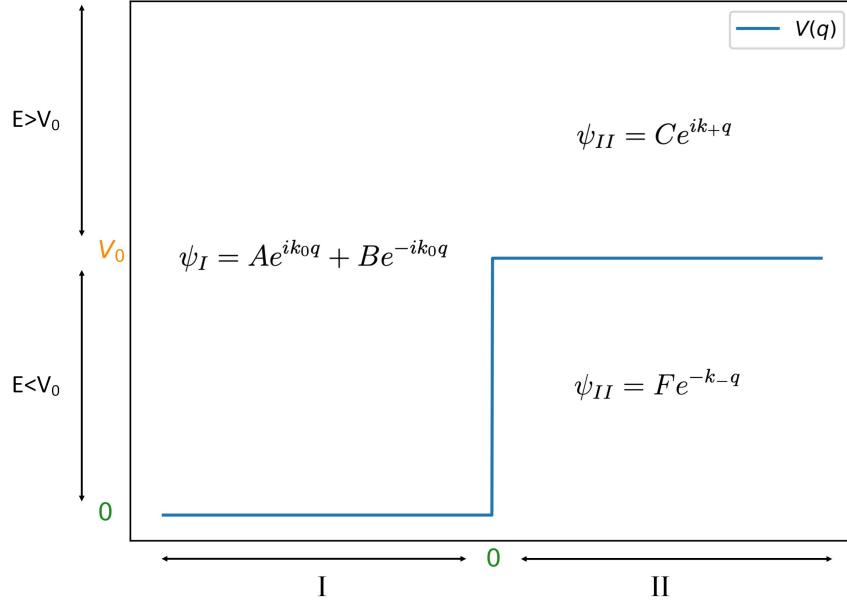


Figure 4: A step potential with $V = 0$ in region I and $V = V_0$ in region II. Further, we have the wave equations for each region, depending if $E > V_0$ or $E < V_0$.

Now we require continuity of the wave functions as well as their derivatives at the boundary of the potential. So at $q = 0$, we require that

$$\psi_I|_{q=0} = \psi_{II}|_{q=0} \Leftrightarrow A + B = C \quad (41)$$

and

$$\frac{\partial \psi_I}{\partial q} \Big|_{q=0} = \frac{\partial \psi_{II}}{\partial q} \Big|_{q=0} \Leftrightarrow k_0 A - k_0 B = k_+ C. \quad (42)$$

Using these two equations, we can find B and C in terms of A , k_0 and k_+ by first substituting $C = A + B$ into (42)

$$\begin{aligned} k_0 A + k_0 B &= k_+(A + B) \Leftrightarrow (k_0 - k_+)A = (k_0 + k_+)B \\ &\Leftrightarrow B = \frac{k_0 - k_+}{k_0 + k_+} A, \end{aligned}$$

and then we can sub this equation for B into (41) to get

$$\begin{aligned} A + \frac{k_0 - k_+}{k_0 + k_+} A = C &\Leftrightarrow \frac{Ak_0 + Ak_+ + Ak_0 - Ak_+}{k_0 + k_+} = C \\ &\Leftrightarrow C = \frac{2k_0}{k_0 + k_+} A. \end{aligned}$$

Now finally, we recall the reflection and transmission coefficients are defined as the ratios of the reflected and transmitted probability currents over the incoming probability current, so

$$R = \frac{|B|^2}{|A|^2}, \quad T = \frac{k_+ |C|^2}{k_0 |A|^2}.$$

Thus, we can insert our values in for B and C to get the reflection and transmission coefficients in terms of k_0 and k_+ below

$$R = \left(\frac{k_0 - k_+}{k_0 + k_+} \right)^2, \quad T = \frac{4k_0 k_+}{(k_0 + k_+)^2}.$$

We can check now that $R + T = 1$ since

$$R + T = \frac{k_0^2 - 2k_0 k_+ + k_+^2 + 4k_0 k_+}{(k_0 + k_+)^2} = \frac{(k_0 + k_+)^2}{(k_0 + k_+)^2} = 1.$$

Some more animation snapshots for a step potential when $E > V_0$ are provided in Fig. 5 to get a better picture of what is happening. It is clear in these snapshots that most of the wave has been transmitted through the barrier, with a small amount being reflected back.

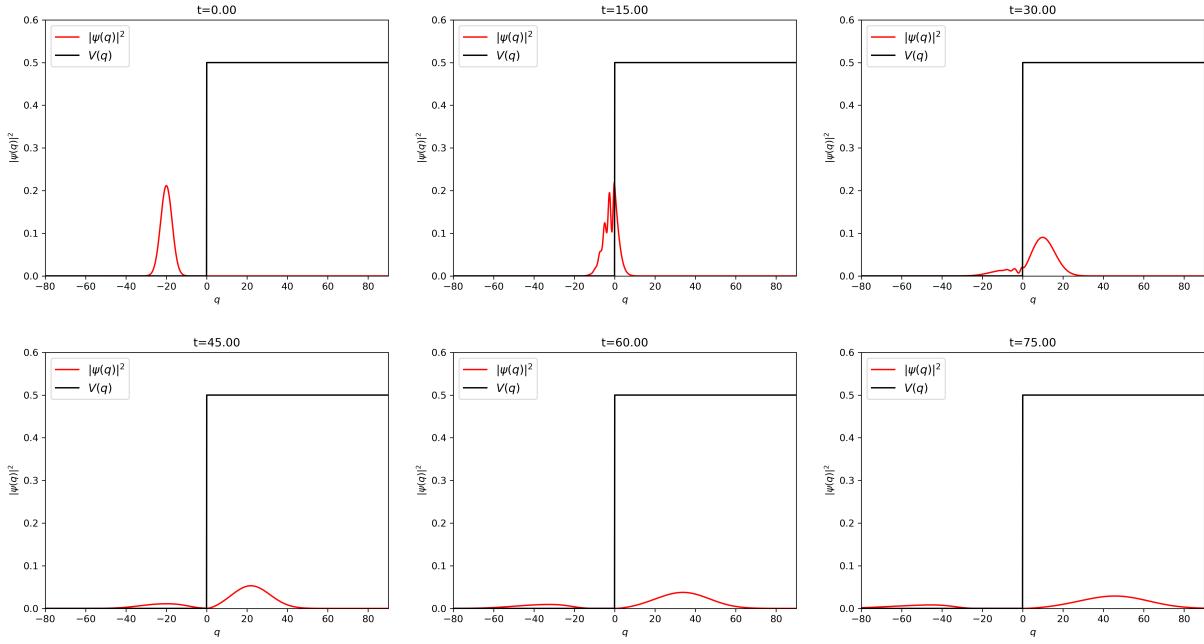


Figure 5: Pictured are some snapshots of an initially Gaussian wave packet interacting with a step potential. The potential has a maximum V_0 which is 0.5 in this case, and the energy of the wave E is such that $E > V_0$.

Next we consider the case when $\mathbf{E}_n < \mathbf{V}_0$.

In this scenario, we have that $k_- = \frac{\sqrt{2m(V_0 - E_n)}}{\hbar}$ and so the TISE (in region II) becomes

$$\frac{\partial^2 \psi}{\partial q^2} - \frac{2m(V_0 - E_n)}{\hbar} \psi = 0 \Leftrightarrow \frac{\partial^2 \psi}{\partial q^2} - k_-^2 = 0.$$

In this case, we have the general solutions

$$\psi_I = A e^{ik_0 q} + B e^{-ik_0 q} \quad , \quad \psi_{II} = E e^{k_- q} + F e^{-k_- q}.$$

ψ_{II} is a superposition of two exponential functions - one with a positive exponent and one with a negative exponent. As $q \rightarrow +\infty$, the term with the positive exponent will go to infinity, so we require that it's coefficient $E = 0$ and thus,

$$\psi_{II} = F e^{-k_- q}.$$

Then, if we require the matching conditions from before (that the wave and its derivative are continuous at the boundary at $q = 0$), we have that

$$\psi_I|_{q=0} = \psi_{II}|_{q=0} \Leftrightarrow A + B = F \quad (43)$$

and

$$\frac{\partial\psi_I}{\partial q}\Bigg|_{q=0} = \frac{\partial\psi_{II}}{\partial q}\Bigg|_{q=0} \Leftrightarrow ik_0A - ik_0B = -k_-F. \quad (44)$$

We can make substitutions of (43) and (44) in a similar way as before to obtain

$$B = \frac{k_0 - ik_-}{k_0 + ik_-}A \quad , \quad F = \frac{2k_0}{k_0 + ik_-}A.$$

Finally, we can sub B into our reflection coefficient as before to get

$$R = \frac{|B|^2}{|A|^2} = \left| \frac{k_0 - ik_-}{k_0 + ik_-} \right|^2 = \frac{k_0^2 + k_-^2}{k_0^2 + k_-^2} = 1.$$

This implies $T = 0$ since $R + T = 1$. We can't substitute F into the transmission coefficient equation, because ψ_{II} does not represent a wave with probability current like ψ_I does. There is no transmission since the barrier extends to infinity. This means that even though the wave may penetrate the barrier at first, it will never reach the end and thus will never be transmitted, so it will always be reflected back eventually. This also explains why even though $T = 0$, the probability density of the wave in region II is $|\psi_{II}|^2 = |F|^2 e^{-2k_- q}$. Thus, there is a non zero probability of measuring the wave inside the potential. This probability exponentially decreases as q increases i.e. as we get further away from the barrier. We can see a visual representation of this in Fig. 6.

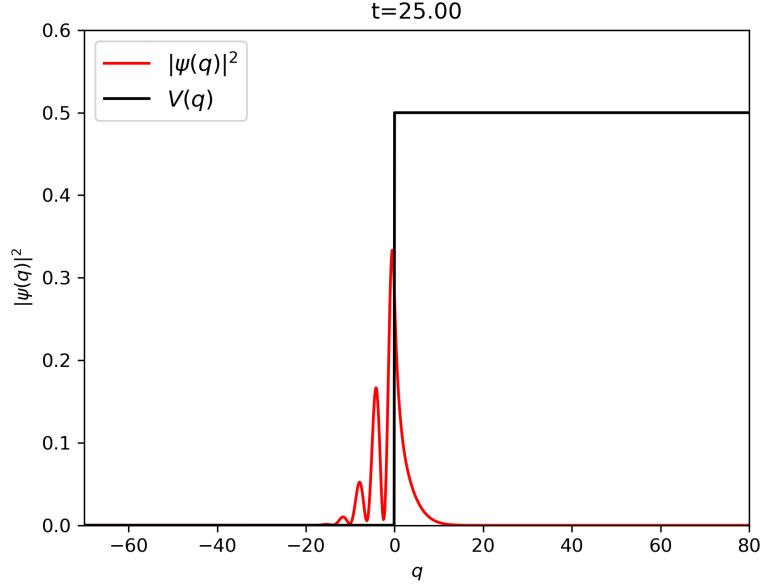


Figure 6: A snapshot of a wave packet at the point of interaction with a step potential. In this particular example, $V_0 = 0.5$, but we can generalise this to any V_0 .

Some more animation snapshots for a step potential when $E < V_0$ are shown in Fig. 7.

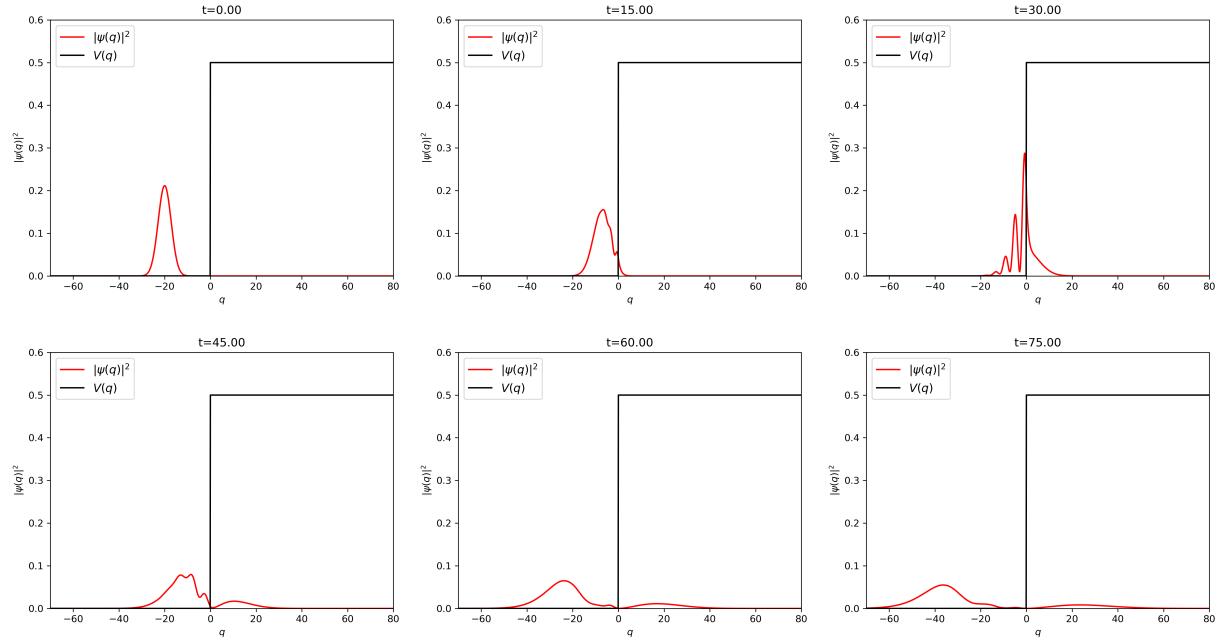


Figure 7: Snapshots of a wave packet interacting with a step potential where $E < V_0$.

Example - Rectangular Potential

In this example we consider a similar simple scenario as in the step potential, however this time the potential does not extend to infinity, but rather drops back off to equal zero at another point. This means that we expect the transmission coefficient to be non zero in this situation. So, we consider the simple rectangular potential barrier

$$V(q) = \begin{cases} 0 & \text{if } q < a \\ V_0 & \text{if } 0 < q < a \\ 0 & \text{if } q > a. \end{cases}$$

Like with the step potential, we have to distinguish between the very different cases when $E_n > V_0$ and when $E_n < V_0$. We show this scenario with the wave functions labelled in each section in Fig. 8. These wave functions are calculated in the following pages.

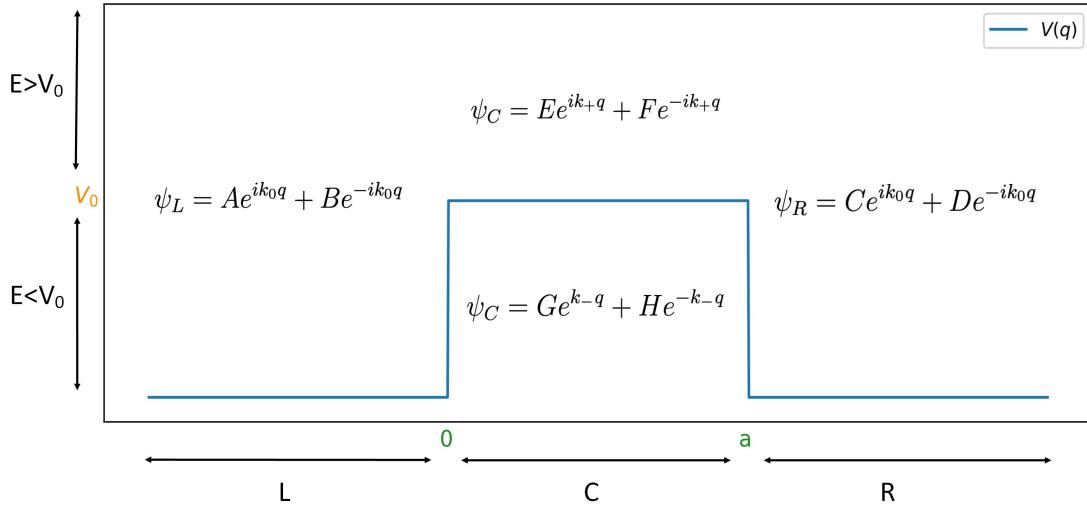


Figure 8: Pictured is an example of a rectangular potential with the different wave function in their corresponding regions.

We start with the case when $E_n > V_0$.

Consider splitting the system into three sections again: L, C and R standing for left, centre and right. Just as in the beginning of the section, we can solve the TISE to get wave functions of the form

$$\begin{aligned}\psi_L &= A e^{ik_0 q} + B e^{-ik_0 q} \\ \psi_R &= C e^{ik_0 q} + D e^{-ik_0 q} \\ \psi_C &= E e^{ik_+ q} + F e^{-ik_+ q},\end{aligned}$$

where

$$k_0 = \frac{\sqrt{2mE}}{\hbar} \quad , \quad k_+ = \frac{\sqrt{2m(E - V_0)}}{\hbar}.$$

Now we can also consider two different situations in this case, one where a wave is incident from the left, implying that $D = 0$ and one where a wave is incident from the right, implying that $A = 0$. We consider the first scenario, but both cases are analogous. We require continuity of the wave and its derivative at the boundaries again. Thus, at $q = 0$, we require that

$$\psi_L|_{q=0} = \psi_C|_{q=0} \Leftrightarrow A + B = E + F \quad (45)$$

and

$$\left. \frac{\partial \psi_L}{\partial q} \right|_{q=0} = \left. \frac{\partial \psi_C}{\partial q} \right|_{q=0} \Leftrightarrow ik_0A - ik_0B = ik_+E - ik_+F. \quad (46)$$

Similarly, at $q = a$, for continuity we require that

$$\psi_C|_{q=a} = \psi_R|_{q=a} \Leftrightarrow Ee^{ik_+a} + Fe^{-ik_+a} = Ce^{ik_0a} \quad (47)$$

and

$$\left. \frac{\partial \psi_C}{\partial q} \right|_{q=a} = \left. \frac{\partial \psi_R}{\partial q} \right|_{q=a} \Leftrightarrow ik_+Ee^{ik_+a} - ik_+Fe^{-ik_+a} = ik_0Ce^{ik_0a}. \quad (48)$$

So we have four matching equations, (45), (46), (47) and (48). We will try and find equations for the reflection and transmission coefficients in terms of k_0 and k_+ and thus E and V_0 from these. We first recall that

$$R_L = \frac{|B|^2}{|A|^2} = \frac{B\bar{B}}{A\bar{A}} = r_L\bar{r}_L \quad , \quad T_L = \frac{|C|^2}{|A|^2} = \frac{C\bar{C}}{A\bar{A}} = t_L\bar{t}_L,$$

where $r_L = \frac{B}{A}$ and $t_L = \frac{C}{A}$. From now on we drop the subscripts as we are only dealing with an incoming wave from region L in this example. We start by dividing (45), (46), (47) and (48) by A , giving us

$$1 + r = \frac{E}{A} + \frac{F}{A} \quad (49)$$

$$ik_0 - ik_0 r = ik_+ \frac{E}{A} - k_+ \frac{F}{A} \quad (50)$$

$$\frac{E}{A} e^{ik_+ a} + \frac{F}{A} e^{-ik_+ a} = t e^{ik_0 a} \quad (51)$$

$$ik_+ \frac{E}{A} e^{ik_+ a} - ik_+ \frac{F}{A} e^{-ik_+ a} = ik_0 t e^{ik_0 a}. \quad (52)$$

We want to find expressions for $\frac{E}{A}$ and $\frac{F}{A}$, and to do so we first multiply (51) by ik_+ and add (52)

$$2ik_+ \frac{E}{A} e^{ik_+ a} = i(k_0 + k_+) t e^{ik_0 a}.$$

We can rearrange this for $\frac{E}{A}$

$$\frac{E}{A} = \frac{k_0 + k_+}{2k_+} t e^{i(k_0 - k_+) a}. \quad (53)$$

Next, we multiply (51) by ik_+ again, but then subtract (52) and rearrange for $\frac{F}{A}$

$$\frac{F}{A} = \frac{k_+ - k_0}{2k_+} t e^{i(k_0 + k_+) a}. \quad (54)$$

Last, we can multiply (49) by ik_0 and add (50)

$$2ik_0 = i(k_0 + k_+) \frac{E}{A} + i(k_0 - k_+) \frac{F}{A}.$$

Now we can substitute our expressions for $\frac{E}{A}$ and $\frac{F}{A}$ from (53) and (54) into this

$$2ik_0 = \frac{t}{2k_+} (i(k_0 + k_+)^2 e^{i(k_0 - k_+) a} - i(k_0 - k_+)^2 e^{i(k_0 + k_+) a}).$$

Using the Euler forms of the trigonometric functions sin and cos

$$\sin(x) = \frac{e^{ix} - e^{-ix}}{2i} \quad , \quad \cos(x) = \frac{e^{ix} + e^{-ix}}{2}, \quad (55)$$

we can solve this equation for t

$$\begin{aligned}
2ik_0 &= \frac{t}{2k_+} (i(k_0 + k_+)^2 e^{i(k_0 - k_+)a} - i(k_0 - k_+)^2 e^{i(k_0 + k_+)a}) \Rightarrow \\
2ik_0 &= \frac{te^{ik_0a}}{2k_+} (-i(k_0^2 + k_+^2)(e^{ik_+a} - e^{-ik_+a}) + 2ik_0k_+(e^{ik_+a} + e^{-ik_+a})) \Rightarrow \\
2ik_0 &= \frac{te^{ik_+a}}{2k_+} (2(k_0^2 + k_+^2) \sin(k_+a) + 4ik_0k_+ \cos(k_+a)) \Rightarrow \\
t &= \frac{2ik_0k_+e^{-ik_+a}}{(k_0^2 + k_+^2) \sin(k_+a) + 2ik_0k_+ \cos(k_+a)}.
\end{aligned}$$

Finally, we can work out the reflection and transmission coefficients using the trigonometric identity

$$\sin^2(x) + \cos^2(x) = 1. \quad (56)$$

Since $T = t\bar{t}$ and $R = 1 - T$ we have that

$$\begin{aligned}
T &= t\bar{t} \\
&= \left(\frac{2ik_0k_+e^{-ik_+a}}{(k_0^2 + k_+^2) \sin(k_+a) + 2ik_0k_+ \cos(k_+a)} \right) \left(\frac{-2ik_0k_+e^{ik_+a}}{(k_0^2 + k_+^2) \sin(k_+a) - 2ik_0k_+ \cos(k_+a)} \right) \\
&= \frac{4k_0^2k_+^2}{(k_0^2 + k_+^2)^2 \sin^2(k_+a) + 4k_0^2k_+^2 \cos^2(k_+a)} = \frac{4k_0^2k_+^2}{((k_0^2 + k_+^2)^2 - 4k_0^2k_+^2) \sin^2(k_+a) + 4k_0^2k_+^2} \\
&= \frac{1}{\left(\frac{(k_0^2 + k_+^2)^2}{4k_0^2k_+^2} - 1\right) \sin^2(k_+a) + 1}.
\end{aligned}$$

Now we can substitute $k_0 = \frac{\sqrt{2mE}}{\hbar}$ and $k_+ = \frac{\sqrt{2m(E-V_0)}}{\hbar}$ into $\frac{(k_0^2 + k_+^2)^2}{4k_0^2k_+^2} - 1$ to simplify it

$$\begin{aligned}
\frac{(k_0^2 + k_+^2)^2}{4k_0^2k_+^2} - 1 &= \frac{k_0^4 + 2k_0k_+ + k_+^4}{4k_0^2k_+^2} = \frac{k_0^2}{4k_+^2} - \frac{1}{2} + \frac{k_+^2}{4k_0^2} = \frac{E}{4(E-V_0)} - \frac{1}{2} + \frac{E-V_0}{4E} \\
&= \frac{(E - (E - V_0))^2}{4E(E - V_0)} = \frac{V_0^2}{4E(E - V_0)}.
\end{aligned}$$

Thus, we have an expression for T and R in terms of E and V_0

$$T = \frac{1}{\frac{V_0^2}{4E(E-V_0)} \sin^2(k_+a) + 1}, \quad R = 1 - T = 1 - \frac{1}{\frac{V_0^2}{4E(E-V_0)} \sin^2(k_+a) + 1}. \quad (57)$$

We can see some animation snapshots for a rectangular potential when $E > V_0$ in Fig. 9. As expected, when the energy of the wave is greater than the potential, the majority of the wave is transmitted past the barrier.

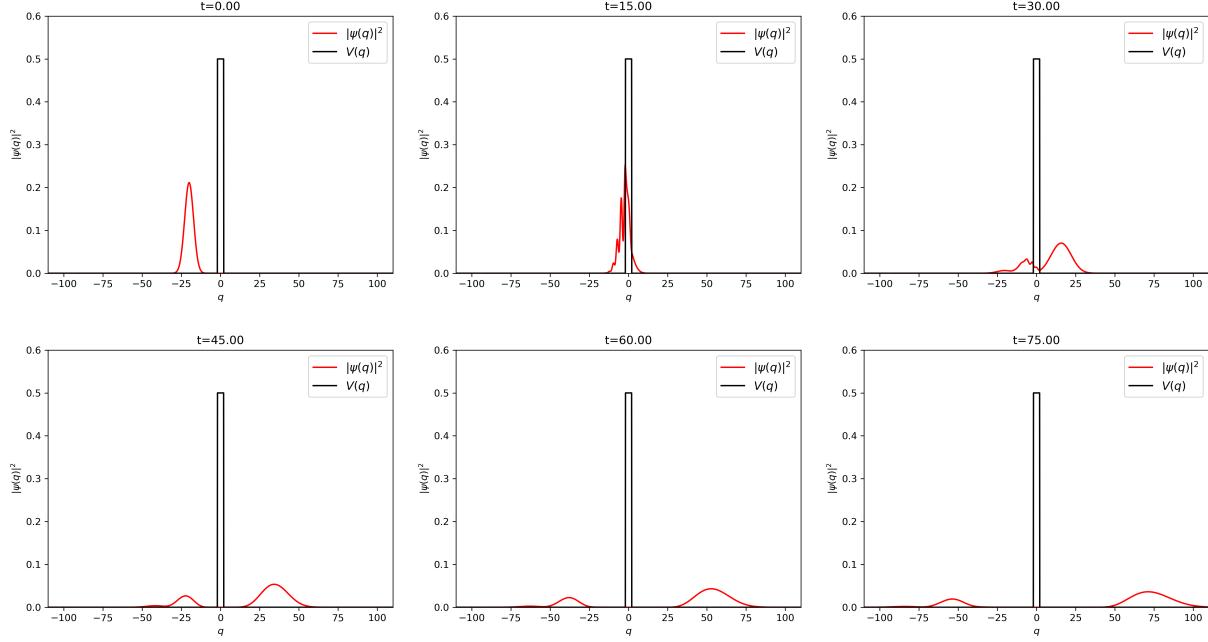


Figure 9: Snapshots of a wave packet with energy $E > V_0$ interacting with a rectangular potential barrier.

Now we consider the case when $\mathbf{E}_n < \mathbf{V}_0$.

In this case, as in the step potential example, we have the same wave functions in region L and R, and that the wave function in region C is a superposition of real growing and decaying exponentials

$$\begin{aligned}\psi_L &= A e^{ik_0 q} + B e^{-ik_0 q} \\ \psi_R &= C e^{ik_0 q} + D e^{-ik_0 q} \\ \psi_C &= G e^{k_- q} + H e^{-k_- q}.\end{aligned}$$

We use the matching conditions at $q = 0$ and $q = a$ to get the four equations

$$A + B = G + H \quad (58)$$

$$ik_0 A - ik_0 B = k_- G - k_- H \quad (59)$$

$$G e^{k_- a} + H e^{-k_- a} = C e^{ik_0 a} \quad (60)$$

$$k_- Ge^{k-a} - k_- He^{-k-a} = ik_0 Ce^{ik_0 a}. \quad (61)$$

Once again, we use that

$$R = r\bar{r} \quad , \quad T = t\bar{t},$$

where $r = \frac{B}{A}$ and $t = \frac{C}{A}$. Now our first mission is to find expressions for $\frac{G}{A}$ and $\frac{H}{A}$. We first divide all of the matching equations above by A to get

$$1 + r = \frac{G}{A} + \frac{H}{A} \quad (62)$$

$$ik_0 - ik_0 r = k_- \frac{G}{A} - k_- \frac{H}{A} \quad (63)$$

$$\frac{G}{A} e^{k-a} + \frac{H}{A} e^{-k-a} = te^{ik_0 a} \quad (64)$$

$$k_- \frac{G}{A} e^{k-a} - k_- \frac{H}{A} e^{-k-a} = ik_0 t e^{ik_0 a}. \quad (65)$$

If we multiply (64) by k_- and add this to (65) we get

$$2k_- \frac{G}{A} e^{k-a} = (ik_0 + k_-) t e^{ik_0 a},$$

which we can rearrange for $\frac{G}{A}$

$$\frac{G}{A} = \frac{k_- + ik_0}{2k_-} t e^{(ik_0 - k_-)a}. \quad (66)$$

Similarly, we can now multiply (64) by k_- again but this time subtract (65) from it and then rearrange for $\frac{H}{A}$ to get

$$\frac{H}{A} = \frac{k_- - ik_0}{2k_-} t e^{(ik_0 + k_-)a}. \quad (67)$$

Now, we can multiply (62) by ik_0 and add it to (63) for

$$2ik_0 = (ik_0 + k_-) \frac{G}{A} + (ik_0 - k_-) \frac{H}{A}.$$

If we sub our equations for $\frac{G}{A}$ from (66) and $\frac{H}{A}$ from (67) into this we get

$$2ik_0 = \frac{t}{2k_-} ((ik_0 + k_-)^2 e^{(ik_0 - k_-)a} - (ik_0 - k_-)^2 e^{(ik_0 + k_-)a}). \quad (68)$$

We can now rearrange (68) and use the Euler form of the hyperbolic trig functions sinh and cosh

$$\sinh(x) = \frac{e^x - e^{-x}}{2}, \quad \cosh(x) = \frac{e^x + e^{-x}}{2}, \quad (69)$$

in order to solve for t

$$\begin{aligned} 2ik_0 &= \frac{te^{ik_0a}}{2k_-} \left(-(k_-^2 - k_0^2)(e^{k_-a} - e^{-k_-a}) + 2ik_0k_-(e^{k_-a} + e^{-k_-a}) \right) \\ \Rightarrow 2ik_0 &= \frac{te^{ik_0a}}{2k_-} \left(2(k_0^2 - k_-^2) \sinh(k_-a) + 4ik_0k_- \cosh(k_-a) \right) \\ \Rightarrow t &= \frac{2ik_0k_-e^{-ik_0a}}{(k_0^2 - k_-^2) \sinh(k_-a) + 2ik_0k_- \cosh(k_-a)}. \end{aligned}$$

This, with some more manipulations, allows us to find the transmission coefficient $T = t\bar{t}$ and the reflection coefficient $R = 1 - T$. We calculate $t\bar{t}$ below, and do some simplifying using the hyperbolic trigonometric identity

$$\sinh^2(x) - \cosh^2(x) = 1. \quad (70)$$

Then,

$$\begin{aligned} T &= t\bar{t} \\ &= \left(\frac{2ik_0k_-e^{-ik_0a}}{(k_0^2 - k_-^2) \sinh(k_-a) + 2ik_0k_- \cosh(k_-a)} \right) \left(\frac{-2ik_0k_-e^{ik_0a}}{(k_0^2 - k_-^2) \sinh(k_-a) - 2ik_0k_- \cosh(k_-a)} \right) \\ &= \frac{4k_0^2k_-^2}{(k_0^2 - k_-^2)^2 \sinh^2(k_-a) + 4k_0^2k_-^2 \cosh^2(k_-a)} \\ &= \frac{4k_0^2k_-^2}{((k_0^2 - k_-^2)^2 + 4k_0^2k_-^2) \sinh^2(k_-a) + 4k_0^2k_-^2} \\ &= \frac{1}{\left(\frac{(k_0^2 - k_-^2)^2}{4k_0^2k_-^2} + 1 \right) \sinh^2(k_-a) + 1} \end{aligned}$$

Now we can simplify the term $\frac{(k_0^2 - k_-^2)^2}{4k_0^2 k_-^2} + 1$ by substituting in $k_0 = \frac{\sqrt{2mE}}{\hbar}$ and $k_- = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$ to get

$$\begin{aligned} \frac{(k_0^2 - k_-^2)^2}{4k_0^2 k_-^2} + 1 &= \frac{k_0^4 - 2k_0^2 k_-^2 + k_-^4}{4k_0^2 k_-^2} + 1 = \frac{k_0^2}{4k_-^2} + \frac{1}{2} + \frac{k_-^2}{4k_0^2} = \frac{E}{4(V_0 - E)} + \frac{1}{2} + \frac{V_0 - E}{4E} \\ &= \frac{(E + (V_0 - E))^2}{4E(V_0 - E)} = \frac{V_0^2}{4E(V_0 - E)}. \end{aligned}$$

Thus we finally have an expression for the transmission and reflection coefficients in terms of E and V_0

$$T = \frac{1}{\frac{V_0^2}{4E(V_0 - E)} \sinh^2(k_- a) + 1}, \quad R = 1 - T = 1 - \frac{1}{\frac{V_0^2}{4E(V_0 - E)} \sinh^2(k_- a) + 1}, \quad (71)$$

We can see some animation snapshots for a rectangular potential when $E < V_0$ in Fig. 10. We can see that the majority of the wave in this case has been reflected back off the barrier, with a small amount of the wave tunnelling through the barrier.

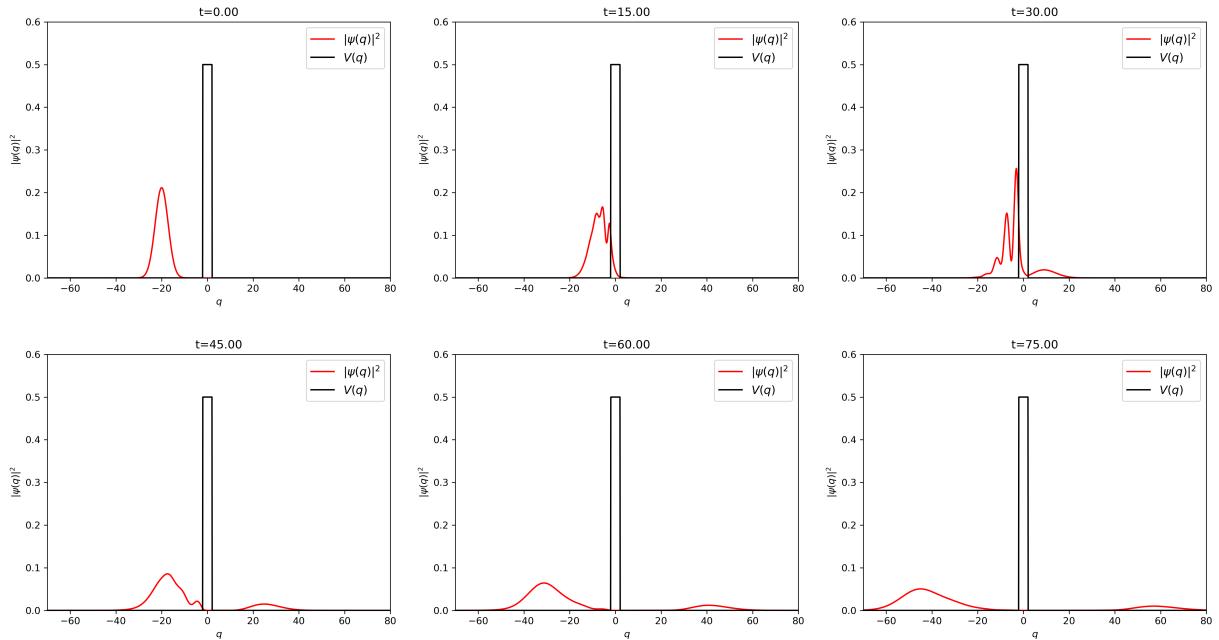


Figure 10: Snapshots of a Gaussian wave packet interacting with a rectangular potential barrier, where the energy of the wave $E < V_0$.

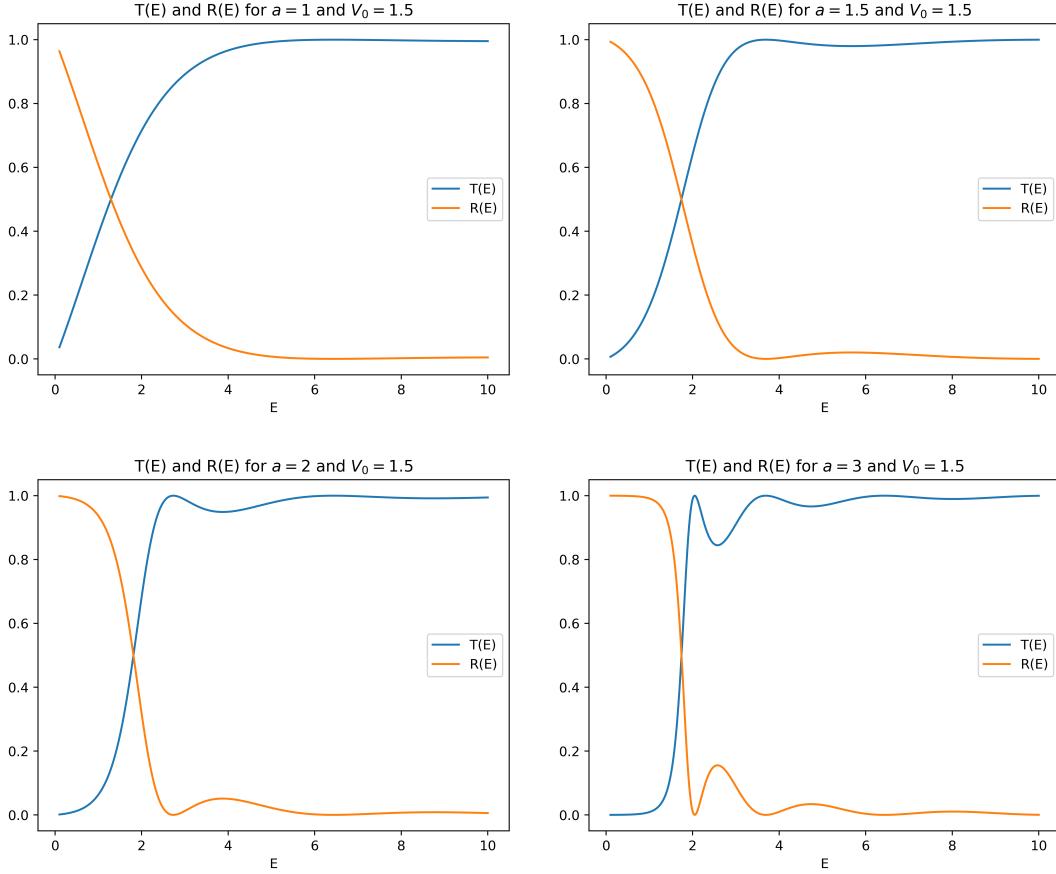


Figure 11: Some graphs of $T(E)$ and $R(E)$ for different barrier widths a .

We have used these equations for R and T in (57) and (71) to plot graphs of them against different energies in Fig.11. Note that we have set $\hbar = 1$ and $m = 1$. As we can see from the graphs in this figure, the reflection and transmission coefficients are equal roughly when $E = V_0 = 1.5$. We will see later in §7 that our coded models behave in a way that correlates with this, where we see that roughly half the wave is transmitted and half is reflected when the energy of the wave equals the peak of the barrier (even with a barrier that is not necessarily rectangular). The reason the graph looks more oscillatory as the width gets bigger is to do with resonance effects. These are not explained here but you can read more on this in chapter 7.6 of [2].

5 Semiclassical Methods

The concepts discussed in this section are available for reference in chapter 15 of [3], chapter 8 of [4], chapter 11 of [5], and finally in chapter 2 and 5.1 of [12].

5.1 WKB Theory

WKB, sometimes called WKBJ, theory is another approach to solving the Schrödinger equation. It was first introduced by Wentzel, Kramers, Brillouin and Jeffreys in 1926 [13] [14] [15] [16]. It is useful in allowing us to find solutions for the wave function in the classically allowed, and importantly, in the classically forbidden regions as well. The WKB approximation is a semi-classical method used to find solutions to second order linear differential equations, and so is used on the Schrödinger equation, specifically when the potential varies slowly. The general idea is that if the potential varies slowly compared to the wavelength ($\lambda = \frac{2\pi\hbar}{p}$), then solutions will locally look like solutions with a constant potential. In the following, we introduce the time independent WKB approximation, and consider some implications of this. Additional time dependent WKB methods are discussed in §8.1.

Time Independent WKB

Start by considering the time independent Schrödinger equation as in (11). Recall from §4, for $E > V(q)$ we can rewrite this as

$$\frac{\partial^2\psi}{\partial q^2} = -\frac{2m(E - V(q))}{\hbar^2}\psi = -\frac{p^2}{\hbar^2}, \quad (72)$$

where $p = \sqrt{2m(E - V(q))}$. Recall from §2.2 that the wave number k is related to p via $k = \frac{p}{\hbar}$ and thus the wave length λ is related to $V(q)$ via $\lambda = \frac{2\pi}{k} = \frac{2\pi\hbar}{p}$.

We then use the following Ansatz

$$\psi(q) = A(q)e^{\frac{i}{\hbar}\phi(q)}, \quad (73)$$

where ϕ is the smoothly varying phase, and A is the amplitude (both of these are real functions). Then, dropping the arguments and using the product rule,

$$\frac{\partial\psi}{\partial q} = A\frac{i}{\hbar}\frac{\partial\phi}{\partial q}e^{\frac{i}{\hbar}\phi} + \frac{\partial A}{\partial q}e^{\frac{i}{\hbar}\phi}$$

and

$$\begin{aligned}\frac{\partial^2 \psi}{\partial q^2} &= A \frac{i}{\hbar} \frac{\partial \phi}{\partial q} \frac{i}{\hbar} \frac{\partial \phi}{\partial q} e^{\frac{i}{\hbar} \phi} + A \frac{i}{\hbar} \frac{\partial^2 \phi}{\partial q^2} e^{\frac{i}{\hbar} \phi} + \frac{\partial A}{\partial q} \frac{i}{\hbar} \frac{\partial \phi}{\partial q} e^{\frac{i}{\hbar} \phi} + \frac{\partial A}{\partial q} \frac{i}{\hbar} \frac{\partial \phi}{\partial q} e^{\frac{i}{\hbar} \phi} + \frac{\partial^2 A}{\partial q^2} e^{\frac{i}{\hbar} \phi} \\ &= e^{\frac{i}{\hbar} \phi} \left(-\frac{1}{\hbar^2} A \left(\frac{\partial \phi}{\partial q} \right)^2 + \frac{i}{\hbar} A \frac{\partial^2 \phi}{\partial q^2} + \frac{2i}{\hbar} \frac{\partial A}{\partial q} \frac{\partial \phi}{\partial q} + \frac{\partial^2 A}{\partial q^2} \right).\end{aligned}\tag{74}$$

Plugging this into the rewritten TISE (72), we have

$$\begin{aligned}-\frac{1}{\hbar^2} A \left(\frac{\partial \phi}{\partial q} \right)^2 + \frac{i}{\hbar} A \frac{\partial^2 \phi}{\partial q^2} + \frac{2i}{\hbar} \frac{\partial A}{\partial q} \frac{\partial \phi}{\partial q} + \frac{\partial^2 A}{\partial q^2} &= -\frac{p^2}{\hbar^2} A \\ \Rightarrow -A \left(\frac{\partial \phi}{\partial q} \right)^2 + i\hbar \frac{\partial^2 \phi}{\partial q^2} + 2i\hbar \frac{\partial A}{\partial q} \frac{\partial \phi}{\partial q} + \hbar^2 \frac{\partial^2 A}{\partial q^2} &= -p^2 A.\end{aligned}$$

We can split this equation into real and imaginary parts

$$\hbar^2 \frac{\partial^2 A}{\partial q^2} - A \left(\frac{\partial \phi}{\partial q} \right)^2 = -p^2 A\tag{75}$$

$$\frac{\partial^2 \phi}{\partial q^2} + 2 \frac{\partial A}{\partial q} \frac{\partial \phi}{\partial q} = 0,\tag{76}$$

and these can be equivalently written, by rearrangement and the product rule, as

$$\hbar^2 \frac{\partial^2 A}{\partial q^2} = A \left(\left(\frac{\partial \phi}{\partial q} \right)^2 - p^2 \right)\tag{77}$$

$$\frac{\partial}{\partial q} \left(A^2 \frac{\partial \phi}{\partial q} \right) = 0.\tag{78}$$

Now, looking at these two equations, (77) cannot be solved easily. However, since we are taking the semiclassical limit ($\hbar \rightarrow 0$), since WKB is a semiclassical approximation method, we know that \hbar is very small, meaning \hbar^2 is even smaller and consequently, this term can be neglected. If we did not take the semiclassical limit, we could assume that the amplitude A varies slowly and then $\frac{\partial^2 A}{\partial q^2}$ would be negligible, allowing it to be set to zero. In either case,

$$\begin{aligned} A \left(\left(\frac{\partial \phi}{\partial q} \right)^2 - p^2 \right) = 0 &\Leftrightarrow \left(\frac{\partial \phi}{\partial q} \right)^2 = p^2 \Leftrightarrow \frac{\partial \phi}{\partial q} = \pm p \\ &\Leftrightarrow \phi(q) = \pm \int p(q) dq + c, \end{aligned}$$

where c is some constant. Note that the relation $\frac{\partial \phi}{\partial q} = p$ links the phase with the classical action as in §2.

Looking at equation (78), this can be solved much more easily

$$A^2 \frac{\partial \phi}{\partial q} = c \Leftrightarrow A^2 = \frac{c}{\mp p} \Leftrightarrow A = \frac{c}{\sqrt{p(q)}},$$

where c has absorbed the constant of integration from the phase, and since $\frac{\partial \phi}{\partial q} = p(q)$.

Finally, we can substitute our equations for $A(q)$ and $\phi(q)$ into the Ansatz (73) and get the solution in the classically allowed region

$$\psi(q) \approx \frac{c}{\sqrt{p(q)}} e^{\pm \frac{i}{\hbar} \int p(q) dq} = \frac{A}{\sqrt{p(q)}} e^{\frac{i}{\hbar} \int p(q) dq} + \frac{B}{\sqrt{p(q)}} e^{-\frac{i}{\hbar} \int p(q) dq}.$$

Note that the constant A here is different from the amplitude $A(q)$.

Now we consider the classically forbidden region, where $E < V(q)$. We can also recall from §4, that the TISE (11) can be rewritten such that

$$\frac{\partial^2 \psi}{\partial q^2} = \frac{2m(V(q) - E)}{\hbar^2} \psi = \frac{p_-^2}{\hbar^2} \psi, \quad (79)$$

where $p_- = \sqrt{2m(V(q) - E)}$.

We can now do similar calculations, by subbing in $\frac{\partial^2 \psi}{\partial q^2}$ from (74) into this rewritten TISE, to get

$$\begin{aligned} -\frac{1}{\hbar^2} A \left(\frac{\partial \phi}{\partial q} \right)^2 + \frac{i}{\hbar} A \frac{\partial^2 \phi}{\partial q^2} + \frac{2i}{\hbar} \frac{\partial A}{\partial q} \frac{\partial \phi}{\partial q} + \frac{\partial^2 A}{\partial q^2} &= \frac{p_-^2}{\hbar^2} A \\ \Rightarrow -A \left(\frac{\partial \phi}{\partial q} \right)^2 + i\hbar A \frac{\partial^2 \phi}{\partial q^2} + 2i\hbar \frac{\partial A}{\partial q} \frac{\partial \phi}{\partial q} + \hbar^2 \frac{\partial^2 A}{\partial q^2} &= p_-^2 A. \end{aligned}$$

We can similarly split this into the real and imaginary parts

$$\hbar^2 \frac{\partial^2 A}{\partial q^2} = A \left(\left(\frac{\partial \phi}{\partial q} \right) + p_-^2 \right) \quad (80)$$

$$\frac{\partial}{\partial q} \left(A^2 \frac{\partial \phi}{\partial q} \right) = 0. \quad (81)$$

Once again, we can solve (81) by assuming $\hbar^2 \frac{\partial^2 A}{\partial q^2} \approx 0$ and we can easily solve (81) to get

$$\begin{aligned} A \left(\left(\frac{\partial \phi}{\partial q} \right)^2 - p_-^2 \right) = 0 &\Leftrightarrow \left(\frac{\partial \phi}{\partial q} \right)^2 = -p_-^2 \Leftrightarrow \frac{\partial \phi}{\partial q} = \pm i p_- \\ &\Leftrightarrow \phi(q) = \pm i \int p_-(q) dq + c \end{aligned}$$

and

$$A^2 \frac{\partial \phi}{\partial q} = c \Leftrightarrow A^2 = \frac{c}{\pm i p_-} \Leftrightarrow A(q) = \frac{c}{\sqrt{p_-(q)}},$$

where the constant c has absorbed the $\frac{1}{\pm i} = \mp i$ term and the constant from integration in $\phi(q)$. Thus, subbing these equations for $A(q)$ and $\phi(q)$ into our Ansatz (73), we get

$$\psi(q) = \frac{c}{\sqrt{p_-(q)}} e^{\pm \frac{1}{\hbar} \int p_-(q) dq} = \frac{C}{\sqrt{p_-(q)}} e^{\frac{1}{\hbar} \int p_-(q) dq} + \frac{D}{\sqrt{p_-(q)}} e^{-\frac{1}{\hbar} \int p_-(q) dq}.$$

5.1.1 Implications

R and T

Consider a simple Gaussian potential as in Fig. 12, where the regions have been split with respect to where the energy of the wave $E = V(q)$ at $a(E)$ and $b(E)$. This is a simple scenario, but the ideas carry over to more complex ones. Recall that for a wave incident from region L we have $\psi_L = A e^{ik(q)q} + B e^{-ik(q)q}$ and $\psi_R = C e^{ik(q)q}$. Now we are able to take the WKB approximation for the wave in the classically forbidden region when $E < V_0$ (between $a < q < b$), and so

$$\psi_C = \frac{C}{\sqrt{p_-(q)}} e^{\frac{1}{\hbar} \int p_-(q) dq} + \frac{D}{\sqrt{p_-(q)}} e^{-\frac{1}{\hbar} \int p_-(q) dq},$$

where we differentiate between the constant C , and the subscript C standing for ‘centre’.

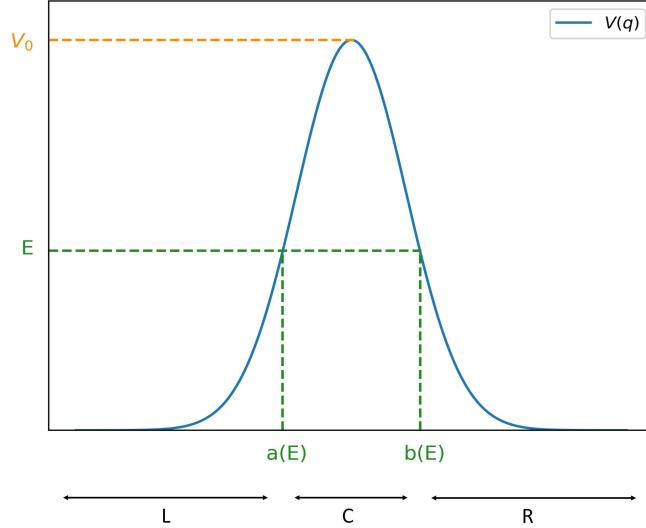


Figure 12: The different regions of a system split with respect to where the kinetic energy of the wave is equal to the potential energy.

Recall that we also had that the transmission coefficient was given by $T = \frac{|C|^2}{|A|^2}$. Now, within the WKB state ψ_C , we have an exponentially increasing and an exponentially decreasing term. If the barrier were very wide, so the probability of transmission is small, we would require that the coefficient in front of the exponentially increasing term to be very small. Then, it would be a good approximation to neglect this term. Thus, the quotient of the coefficients of the incident and transmitted waves is essentially given by the total decrease of the wave in the classically forbidden region, i.e. $\frac{|C|}{|A|} \approx e^{-\frac{1}{\hbar} \int_a^b p_-(q) dq}$. This implies that

$$T = \frac{|C|^2}{|A|^2} \approx e^{-\frac{2}{\hbar} \int_a^b p_-(q) dq}.$$

Alternatively, since the transmission coefficient can be interpreted as the probability of transmission through the barrier, we can also approximate it by the probability that the wave has travelled from a to b and so

$$T \approx |\psi(b)|^2 \approx e^{-\frac{2}{\hbar} \int_a^b p_-(q) dq}.$$

Finally, we can also calculate the reflection coefficient, since $R + T = 1$ and so

$$R = 1 - T \approx 1 - e^{-\frac{2}{\hbar} \int_a^b p_-(q) dq}.$$

We include a more rigorous proof of this idea in §5.3.

Limitations

An important fact in WKB theory, is that the approximation breaks down close to the turning points (e.g. close to a and b) where $E = V(q)$. This is due to the fact that $p = p_- = 0$ when $E = V(q)$ and so the amplitude terms $A(q)$ which involve \sqrt{p} and $\sqrt{p_-}$ in the denominator, go to infinity. This means we cannot match the wave functions over the classically allowed and forbidden regions at the turning points as we have done before. We can get around this however, by using Airy functions near the turning points to approximate the wave function solutions. We can match the asymptotic expansions of the Airy functions to the WKB approximations at these points. We cover this in more detail in §5.3.

5.2 Airy Functions for Linear Potential

Since the WKB approximation breaks down near the potential barrier, in this section we consider how to solve the Schrödinger equation when a state is close to it. Before we begin, we introduce the Airy equation and the Airy functions. The Airy equation, also called the Stokes equation, is a second order differential equation given by

$$\frac{\partial^2 y}{\partial q^2} = qy.$$

This equation looks simple but it is actually very complicated and cannot be solved explicitly. It has two linearly independent solutions, the Airy function of the first kind, $\text{Ai}(q)$ and the Airy function of the second kind, $\text{Bi}(q)$. We define the Ai as

$$\text{Ai}(q) = \frac{1}{\pi} \int_0^\infty \cos \left(\frac{t^3}{3} + qt \right) dt, \quad (82)$$

and Bi is defined as

$$\text{Bi}(q) = \frac{1}{\pi} \int_0^\infty e^{\frac{t^3}{3} + qt} + \sin \left(\frac{t^3}{3} + qt \right) dt. \quad (83)$$

We can see these functions plotted in Fig. 13.

As a wave with a given energy approaches a potential barrier, we can model the barrier as a linear potential. We can find this potential by Taylor expanding $V(q)$ around the point where the energy and potential are equal, at $q = a$. Then we have that $V(q) = V(a) + V'(a)(q - a) + \mathcal{O}((q - a)^2) = E + V'(a)(q - a)$. Note that the dash indicates a differential with respect to position q . This can also be seen since the linear potential will be the tangent to $V(q)$ at a , and then we can solve the equation for the straight line $V(q) = V'(a)q + c$ at $V(a) = E$. This all works until we get to the top of the barrier, where

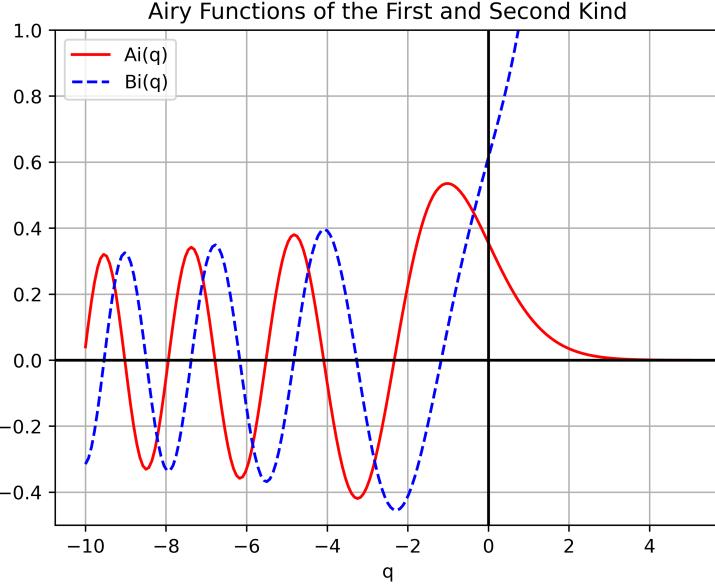


Figure 13: Here we have plotted Airy functions of the first kind, $Ai(q)$, and the second kind, $Bi(q)$.

the tangent is horizontal. We do not deal with this case in this paper, but you can read further on the topic in §5.3 of [17].

Moving on, we consider the TISE with a potential of this form, giving us

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial q^2} + V'(a)(q - a)\psi = 0. \quad (84)$$

We can make a substitution of

$$u := (q - a) \left(\frac{2mV'(a)}{\hbar^2} \right)^{\frac{1}{3}}, \quad (85)$$

which yields the TISE as an Airy function of the form

$$\frac{\partial^2 \psi}{\partial u^2} = u\psi.$$

We can show this rigorously by Fourier and inverse Fourier transforming the Schrödinger equation in order to solve it. The TISE for a linear potential above (84) can be rewritten using the position operator $\hat{q} = q$ and the momentum operator $\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial q}$ from §2.2 to get

$$\frac{\hat{p}^2}{2m}\psi + V'(a)(\hat{q} - a)\psi = \frac{\hat{p}^2}{2m}\psi + V'(a)\hat{q}\psi - V'(a)a\psi. \quad (86)$$

Then this can be Fourier transformed to become

$$\frac{p^2}{2m}\tilde{\psi} + V'(a)i\hbar\frac{\partial\tilde{\psi}}{\partial p} - V'(a)a\tilde{\psi} = 0.$$

Proof. As we have proved earlier in lemma 2.5, the Fourier transform of $\psi(q)$ is given by $\tilde{\psi}(p) = \langle p|\psi \rangle$. Also, from §2.2.1 recall that

$$\psi_p = |p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}pq}$$

is the eigenfunction of the momentum operator. So, $\tilde{\psi}(p) = \langle \psi_p | \psi \rangle = p\tilde{\psi}(p)$. Then, we have that

$$\langle \psi_p | \hat{p} | \psi \rangle = \langle \hat{p} \psi_p | \psi \rangle = p \langle \psi_p | \psi \rangle = p\tilde{\psi}(p),$$

since \hat{p} is self adjoint, and p is real. Thus the application of \hat{p} leads to multiplication by p .

Next, note that

$$\frac{\partial}{\partial p}\psi_p = \frac{i}{\hbar}\frac{q}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}pq},$$

so then,

$$\langle \psi_p | \hat{q} | \psi \rangle = \langle \hat{q} \psi_p | \psi \rangle = \langle \frac{q}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}pq} | \psi \rangle = \langle \frac{\hbar}{i}\frac{\partial}{\partial p}\psi_p | \psi \rangle = -\frac{\hbar}{i}\frac{\partial}{\partial p}\langle \psi_p | \psi \rangle = -\frac{\hbar}{i}\frac{\partial}{\partial p}\tilde{\psi}(p).$$

Thus, the application of \hat{q} turns into $i\hbar\frac{\partial}{\partial p}$. We can insert these into the rewritten TISE with a linear potential (86) to obtain the result. \square

Now we have the Fourier transformed TISE for a linear potential, we can rearrange it to get $\tilde{\psi}$ using the fact that $\frac{\partial}{\partial x} \ln(f(x)) = \frac{f'(x)}{f(x)}$.

$$\begin{aligned}
& \left(\frac{p^2}{2m} - V'(a)a \right) \tilde{\psi} + i\hbar V'(a) \frac{\partial \tilde{\psi}}{\partial p} = 0 \\
\Rightarrow & \frac{\frac{\partial \tilde{\psi}}{\partial p}}{\tilde{\psi}} = \frac{i}{V'(a)\hbar} \left(\frac{p^2}{2m} - V'(a)a \right) \\
\Rightarrow & \frac{\partial}{\partial p} \ln(\tilde{\psi}) = \frac{i}{V'(a)\hbar} \left(\frac{p^2}{2m} - V'(a)a \right) \\
\Rightarrow & \ln(\tilde{\psi}) = \frac{i}{V'(a)\hbar} \int \frac{p^2}{2m} - V'(a)a dp \\
\Rightarrow & \ln(\tilde{\psi}) = \frac{i}{V'(a)\hbar} \left(\frac{p^3}{6m} - V'(a)ap \right) + c \\
\Rightarrow & \tilde{\psi} = ce^{\frac{i}{V'(a)\hbar} \left(\frac{p^3}{6m} - V'(a)ap \right)}.
\end{aligned}$$

Now we can iFT back using (16) to get

$$\psi = \frac{c}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} e^{\frac{i}{V'(a)\hbar} \left(\frac{p^3}{6m} - V'(a)ap \right)} e^{\frac{i}{\hbar} pq}.$$

We show this is of Airy form by doing some manipulations

$$\begin{aligned}
\psi &= \frac{c}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} e^{\frac{i}{V'(a)\hbar} \left(\frac{p^3}{6m} + V'(a)(q-a)p \right)} \\
&= \frac{c}{\sqrt{2\pi\hbar}} \left(\int_0^{+\infty} e^{\frac{i}{V'(a)\hbar} \left(\frac{p^3}{6m} + V'(a)(q-a)p \right)} dp + \int_{-\infty}^0 e^{\frac{i}{V'(a)\hbar} \left(\frac{p^3}{6m} + V'(a)(q-a)p \right)} dp \right) \\
&= \frac{c}{\sqrt{2\pi\hbar}} \left(\int_0^{+\infty} e^{\frac{i}{V'(a)\hbar} \left(\frac{p^3}{6m} + V'(a)(q-a)p \right)} dp - \int_0^{-\infty} e^{\frac{i}{V'(a)\hbar} \left(\frac{p^3}{6m} + V'(a)(q-a)p \right)} dp \right),
\end{aligned}$$

where we have switched the integration limits in the second integral. Now we can also make the substitution $p \rightarrow -p$ in the second integral to get

$$\begin{aligned}
\psi &= \frac{c}{\sqrt{2\pi\hbar}} \left(\int_0^{+\infty} e^{\frac{i}{V'(a)\hbar} \left(\frac{p^3}{6m} + V'(a)(q-a)p \right)} dp + \int_0^{+\infty} e^{-\frac{i}{V'(a)\hbar} \left(\frac{p^3}{6m} + V'(a)(q-a)p \right)} dp \right) \\
&= \frac{c}{\sqrt{2\pi\hbar}} \int_0^{+\infty} e^{\frac{i}{V'(a)\hbar} \left(\frac{p^3}{6m} + V'(a)(q-a)p \right)} + e^{-\frac{i}{V'(a)\hbar} \left(\frac{p^3}{6m} + V'(a)(q-a)p \right)} dp \\
&= \frac{c}{\sqrt{2\pi\hbar}} \int_0^{+\infty} 2 \cos\left(\frac{1}{V'(a)\hbar} \left(\frac{p^3}{6m} + V'(a)(q-a)p \right)\right) dp \\
&= \frac{2c}{\sqrt{2\pi\hbar}} \int_0^{+\infty} \cos\left(\frac{p^3}{6mV'(a)\hbar} + \frac{(q-a)p}{\hbar}\right) dp,
\end{aligned}$$

where we have used the fact that $\cos(x) = \frac{1}{2}(e^{ix} + e^{-ix})$ from (55). Finally, to show this is of an Airy form, we make the substitution $p \rightarrow \gamma p$ where $\gamma > 0$ to get

$$\psi = \frac{2c\gamma}{\sqrt{2\pi\hbar}} \int_0^{+\infty} \cos\left(\frac{\gamma^3 p^3}{6mV'(a)\hbar} + \frac{(q-a)\gamma p}{\hbar}\right) dp.$$

Thus we want that $\frac{\gamma^3}{2mV'(a)\hbar} = 1 \Leftrightarrow \gamma = (2mV'(a)\hbar)^{\frac{1}{3}}$ in order for this to be an Airy function. This means that

$$\psi = \frac{2c\gamma}{\sqrt{2\pi\hbar}} \frac{\pi}{\pi} \int_0^{+\infty} \cos\left(\frac{p^3}{3} + (q-a) \left(\frac{2mV'(a)}{\hbar}\right)^{\frac{1}{3}} p\right) dp = \alpha \text{Ai}(u),$$

where $u = (q-a) \left(\frac{2mV'(a)}{\hbar}\right)^{\frac{1}{3}}$ as mentioned earlier, and where α has absorbed most of the constants in front of the integral. This is only one solution however, but we know since the Schrödinger equation is a second order differential, that there must be two linearly independent solutions, with the general solution being a linear combination of the two. Thus we have shown, with the substitution of u as in (85), that the solution is a superposition of the Airy functions

$$\psi = \alpha \text{Ai}(u) + \beta \text{Bi}(u),$$

and that the TISE in this case, is an Airy equation.

Summarising, close to a potential barrier when most potentials are roughly linear, the wave acts like an Airy function. Looking at Fig. 13, this means the incoming / reflected waves (in the backwards negative direction) are a superposition of oscillations, and the transmitted waves (in the forwards positive direction), are a linear combination of exponentially decaying and exponentially growing functions. Having said that, with further calculations

(see [18]), we can show that this combination is dominated by Ai since the coefficient β in front of Bi is so small that it is negligible. Thus the transmitted wave will decay - the forward transmission here represents the phenomenon of quantum tunnelling. From my coded animations using the split operator method, we can see how the waves act like an Airy function close to the barrier in Fig. 14 when comparing it to Fig. 13.

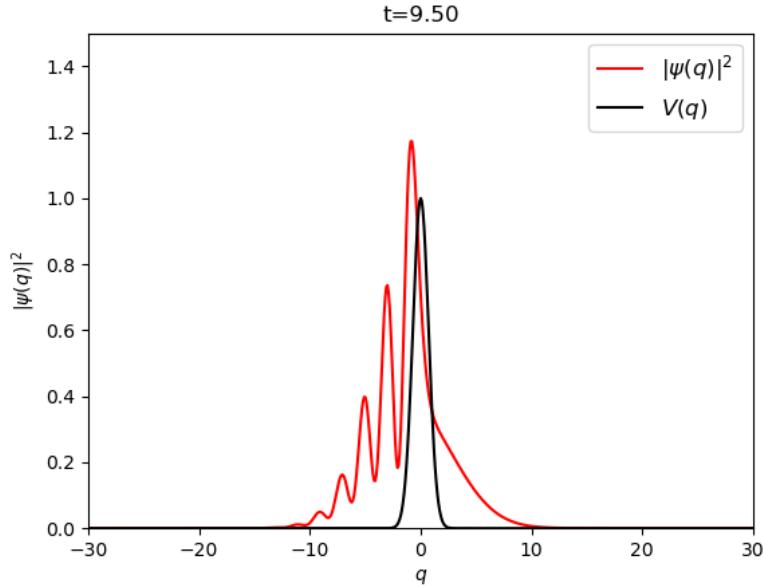


Figure 14: Pictured is a snapshot of an initially Gaussian wave packet interacting with a Gaussian potential barrier at a certain time.

Asymptotic Expansions of Airy Functions

So far we have the integral form of the Airy function of the first kind from (82)

$$\text{Ai}(q) = \frac{1}{\pi} \int_0^\infty \cos \left(\frac{t^3}{3} + qt \right) dt,$$

and the integral form of the Airy function of the second kind from (83)

$$\text{Bi}(q) = \frac{1}{\pi} \int_0^\infty e^{-\frac{t^3}{3} + qt} + \sin \left(\frac{t^3}{3} - qt \right) dt.$$

Now we are interested in the asymptotic expansions of $\text{Ai}(q)$ and $\text{Bi}(q)$ (see chapter 8.3 of [4], chapter 15.5 of [3] and chapter 11.1 of [5] for full details). It is possible to show through deformation of the contour of integration (a method from complex analysis) and

by applying the method of steepest descent to $\text{Ai}(q)$ in (82), that we can get the asymptotic expansion of $\text{Ai}(q)$ as $q \rightarrow +\infty$. We can also show through the stationary phase approximation, that we can get the asymptotic expansion of $\text{Ai}(q)$ as $q \rightarrow -\infty$. These Asymptotic expansions of $\text{Ai}(q)$ are given by

$$\text{Ai}(q) \approx \begin{cases} \frac{1}{2\sqrt{\pi}q^{\frac{1}{4}}} e^{-\frac{2}{3}q^{\frac{3}{2}}} & q \rightarrow +\infty \\ \frac{1}{\sqrt{\pi}(-q)^{\frac{1}{4}}} \sin\left(\frac{2}{3}(-q)^{\frac{3}{2}} + \frac{\pi}{4}\right) & q \rightarrow -\infty . \end{cases}$$

Similarly, we can get the asymptotic expansions of $\text{Bi}(q)$ which are given by

$$\text{Bi}(q) \approx \begin{cases} \frac{1}{\sqrt{\pi}q^{\frac{1}{4}}} e^{\frac{2}{3}q^{\frac{3}{2}}} & q \rightarrow +\infty \\ \frac{1}{\sqrt{\pi}(-q)^{\frac{1}{4}}} \cos\left(\frac{2}{3}(-q)^{\frac{3}{2}} + \frac{\pi}{4}\right) & q \rightarrow -\infty . \end{cases}$$

We can see the asymptotic expansions of Ai and Bi plotted against their actual Airy functions in Fig. 15.

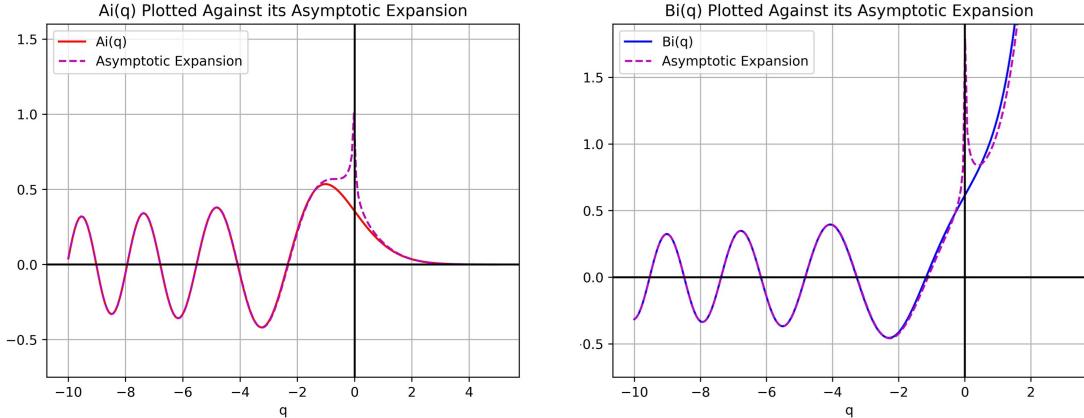


Figure 15: The Airy functions of the first and second kind (solid lines) plotted against their asymptotic expansions (dashed lines).

5.3 Connecting WKB and Airy Functions

In this section, we aim to make a connection between the WKB states and the Airy functions close to the barrier. We have shown in §5.2 that close to the turning points, the potential can be thought of as linear and the solution looks like a linear combination of Ai and Bi (defined in (82) and (83) respectively). We call this solution the patching wave function ψ_P . In order to connect the patching solutions and the WKB solutions, we consider a region of the system such that we are close enough to the barrier that it can be

thought of as linear and ψ_P is valid, but far enough away that the WKB approximation, ψ_{WKB} , is still valid. Think of a situation with a simple Gaussian potential as we have before - like in Fig. 12. In this scenario, we have the turning points at a and b , so looking at either side of each turning point, there are four matching equations. We work these out going from left to right.

Turning point at a

We start by considering the turning point at $q = a$. This situation is visualised in Fig. 16.

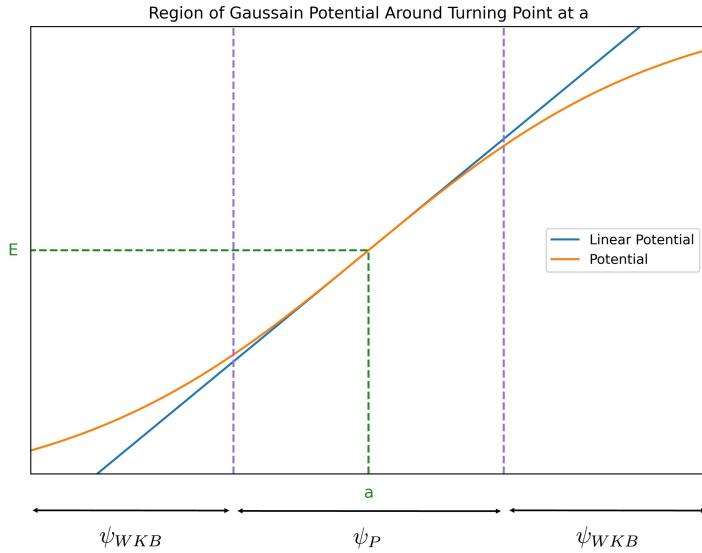


Figure 16: A zoomed in section of the potential at a , where the WKB and patching sections have been indicated.

Close to the turning point, we consider the potential to be linear and so it is of the form $V(q) = V(a) + V'(a)(q - a) = E + V'(a)(q - a)$. We can see this just by the fact that the gradient is $V'(a)$ and the line goes through E at $q = a$. But, we can also see this by Taylor expanding the potential around $q = a$ to the first order.

Left side of a

We first consider the left hand side of $q = a$, since this is where $E > V(q)$.

$$\psi_{WKB}^L$$

Recall from §5.1 that when $E > V(q)$ we have the WKB formula

$$\psi_{WKB}^L = \frac{A}{\sqrt{p(q)}} e^{\frac{i}{\hbar} \int_q^a p(q') dq'} + \frac{B}{\sqrt{p(q)}} e^{-\frac{i}{\hbar} \int_q^a p(q') dq'}.$$

Since $E > V(q)$, and using the equation for the linear potential above, means that close to the turning point at a , the momentum function is given by

$$p(q) = \sqrt{2m(E - V(q))} = \sqrt{2m(E - E - V'(a)(q - a))} = \sqrt{2mV'(a)(a - q)}.$$

Therefore,

$$\begin{aligned} \pm \frac{i}{\hbar} \int_q^a p(q') dq' &= \pm \frac{i}{\hbar} \int_q^a \sqrt{2mV'(a)(a - q')} dq' = \pm \frac{i}{\hbar} \sqrt{2mV'(a)} \int_q^a (a - q')^{\frac{1}{2}} dq' \\ &= \mp \frac{i}{\hbar} \frac{2}{3} \sqrt{2mV'(a)} \left[(a - q')^{\frac{3}{2}} \right]_q^a = \pm \frac{i}{\hbar} \frac{2}{3} \sqrt{2mV'(a)} (a - q)^{\frac{3}{2}}. \end{aligned}$$

Using our new form of $p(q)$, our WKB state becomes

$$\psi_{WKB}^L = \frac{A}{\sqrt{p(q)}} e^{\frac{i}{\hbar} \frac{2}{3} \sqrt{2mV'(a)} (a - q)^{\frac{3}{2}}} + \frac{B}{\sqrt{p(q)}} e^{-\frac{i}{\hbar} \frac{2}{3} \sqrt{2mV'(a)} (a - q)^{\frac{3}{2}}}.$$

Recall from §5.2 when we set $u := \left(\frac{2mV'(a)}{\hbar^2} \right)^{\frac{1}{3}} (q - a)$ in (85). Then notice we have that,

$$(-u)^{\frac{3}{2}} = \frac{1}{\hbar} \sqrt{2mV'(a)} (a - q)^{\frac{3}{2}},$$

and $\sqrt{p(q)} = (2mV'(a)(a - q))^{\frac{1}{4}}$ and $(-u)^{\frac{1}{4}} = \frac{(2mV'(a))^{\frac{1}{12}}}{\hbar^{\frac{1}{6}}} (a - q)^{\frac{1}{4}}$, which implies that

$$\sqrt{p(q)} = (2m\hbar V'(a))^{\frac{1}{6}} (-u)^{\frac{1}{4}}.$$

So, the WKB state becomes

$$\psi_{WKB}^L = \frac{A}{(2m\hbar V'(a))^{\frac{1}{6}} (-u)^{\frac{1}{4}}} e^{i \frac{2}{3} (-u)^{\frac{3}{2}}} + \frac{B}{(2m\hbar V'(a))^{\frac{1}{6}} (-u)^{\frac{1}{4}}} e^{-i \frac{2}{3} (-u)^{\frac{3}{2}}}. \quad (87)$$

ψ_P^L

Recall further from §5.2, that with a linear potential, the TISE is of the form of an Airy equation $f''(q) = qf(q)$, which have general solutions of the form $f(q) = \alpha Ai(q) + \beta Bi(q)$. We call this Airy solution the patching solution ψ_P . We consider the TISE (11) and use the Ansatz $\psi_P(q) = f(\gamma(q - a))$. So $\psi'_P(q) = \gamma f'(\gamma(q - a))$ and $\psi''_P(q) = \gamma^2 f''(\gamma(q - a))$, where a dash indicates the derivative with respect to position q . Then, since the Airy equation implies $f''(q) = qf(q)$ we have that $\psi''_P(q) = \gamma^2 f''(\gamma(q - a)) = \gamma^3 (q - a) f(\gamma(q - a)) = \gamma^3 (q - a) \psi_P(q)$. We want to match this to the TISE

$$-\frac{\hbar^2}{2m} \psi''_P(q) + V(q) \psi_P(q) = E \psi(q) \Leftrightarrow -\frac{\hbar^2}{2m} \psi''_P(q) + V'(a)(q - a) \psi_P(q) = 0.$$

We can do this by rearranging the equation for $\psi_P''(q)$ and multiplying it by $-\frac{\hbar^2}{2m}$

$$\psi_P''(q) - \gamma^3(q-a)\psi_P(q) = 0 \Leftrightarrow -\frac{\hbar^2}{2m}\psi_P''(q) + \frac{\hbar^2}{2m}\gamma^3(q-a)\psi_P(q) = 0.$$

Therefore we have to match $V'(a) = \frac{\hbar^2}{2m}\gamma^3$ and thus $\gamma = \left(\frac{2mV'(a)}{\hbar^2}\right)^{\frac{1}{3}}$.

So we now essentially have the patching solution since $\psi_P(q) = f(\gamma(q-a)) = \alpha Ai(\gamma(q-a)) + \beta Bi(\gamma(q-a))$, thus close to the turning point at a , we have

$$\psi_P = \alpha Ai\left(\left(\frac{2mV'(a)}{\hbar^2}\right)^{\frac{1}{3}}(q-a)\right) + \beta Bi\left(\left(\frac{2mV'(a)}{\hbar^2}\right)^{\frac{1}{3}}(q-a)\right).$$

Using again from (85) the substitution $u := \left(\frac{2mV'(a)}{\hbar^2}\right)^{\frac{1}{3}}(q-a)$ we have the same result from §5.2, specifically,

$$\psi_P = \alpha Ai(u) + \beta Bi(u).$$

We also recall the asymptotic Airy expansions from §5.2

$$Ai(u) \approx \begin{cases} \frac{1}{2\sqrt{\pi}u^{\frac{1}{4}}} e^{-\frac{2}{3}u^{\frac{3}{2}}} & u \rightarrow +\infty \\ \frac{1}{\sqrt{\pi}(-u)^{\frac{1}{4}}} \sin\left(\frac{2}{3}(-u)^{\frac{3}{2}} + \frac{\pi}{4}\right) & u \rightarrow -\infty \end{cases}$$

and

$$Bi(u) \approx \begin{cases} \frac{1}{\sqrt{\pi}u^{\frac{1}{4}}} e^{\frac{2}{3}u^{\frac{3}{2}}} & u \rightarrow +\infty \\ \frac{1}{\sqrt{\pi}(-u)^{\frac{1}{4}}} \cos\left(\frac{2}{3}(-u)^{\frac{3}{2}} + \frac{\pi}{4}\right) & u \rightarrow -\infty. \end{cases}$$

For ψ_P^L we expect the Airy function to be approximated by $u \rightarrow -\infty$. Then, we can asymptotically expand this solution to get

$$\psi_P^L = \frac{\alpha}{\sqrt{\pi}(-u)^{\frac{1}{4}}} \sin\left(\frac{2}{3}(-u)^{\frac{3}{2}} + \frac{\pi}{4}\right) + \frac{\beta}{\sqrt{\pi}(-u)^{\frac{1}{4}}} \cos\left(\frac{2}{3}(-u)^{\frac{3}{2}} + \frac{\pi}{4}\right). \quad (88)$$

We can expand this equation out using the Euler forms of the trig functions from (55) to get

$$\begin{aligned}
\psi_P^L &= \frac{\alpha}{\sqrt{\pi}(-u)^{\frac{1}{4}}} \left(\frac{e^{i\frac{2}{3}(-u)^{\frac{3}{2}}+i\frac{\pi}{4}} - e^{-i\frac{2}{3}(-u)^{\frac{3}{2}}-i\frac{\pi}{4}}}{2i} \right) + \frac{\beta}{\sqrt{\pi}(-u)^{\frac{1}{4}}} \left(\frac{e^{i\frac{2}{3}(u)^{\frac{3}{2}}+i\frac{\pi}{4}} + e^{-i\frac{2}{3}(-u)^{\frac{3}{2}}-i\frac{\pi}{4}}}{2} \right) \\
&= \frac{\beta - i\alpha}{2\sqrt{\pi}(-u)^{\frac{1}{4}}} e^{i\frac{2}{3}(-u)^{\frac{3}{2}}} e^{i\frac{\pi}{4}} + \frac{\beta + i\alpha}{2\sqrt{\pi}(-u)^{\frac{1}{4}}} e^{-i\frac{2}{3}(-u)^{\frac{3}{2}}} e^{-i\frac{\pi}{4}} \\
&= \frac{(\beta - i\alpha)(1+i)}{2\sqrt{2\pi}(-u)^{\frac{1}{4}}} e^{i\frac{2}{3}(-u)^{\frac{3}{2}}} + \frac{(\beta + i\alpha)(1-i)}{2\sqrt{2\pi}(-u)^{\frac{1}{4}}} e^{-i\frac{2}{3}(-u)^{\frac{3}{2}}} \\
&= \frac{(1-i)\alpha + (1+i)\beta}{2\sqrt{2\pi}(-u)^{\frac{1}{4}}} e^{i\frac{2}{3}(-u)^{\frac{3}{2}}} + \frac{(1+i)\alpha + (1-i)\beta}{2\sqrt{2\pi}(-u)^{\frac{1}{4}}} e^{-i\frac{2}{3}(-u)^{\frac{3}{2}}},
\end{aligned}$$

where we have used the fact that

$$e^{i\theta} = \cos(\theta) + i \sin(\theta) \quad (89)$$

and thus $e^{i\frac{\pi}{4}} = \cos\left(\frac{\pi}{4}\right) + i \sin\left(\frac{\pi}{4}\right) = \frac{1}{\sqrt{2}}(1+i)$ and $e^{-i\frac{\pi}{4}} = \cos\left(-\frac{\pi}{4}\right) + i \sin\left(-\frac{\pi}{4}\right) = \frac{1}{\sqrt{2}}(1-i)$.

We can now match ψ_{WKB}^L (87) and ψ_P^L (88) to get our first set of matching equations

$$\frac{A}{(2m\hbar V'(a))^{\frac{1}{6}}} = \frac{(1-i)\alpha + (1+i)\beta}{2\sqrt{2\pi}} \quad (90)$$

$$\frac{B}{(2m\hbar V'(a))^{\frac{1}{6}}} = \frac{(1+i)\alpha + (1-i)\beta}{2\sqrt{2\pi}}. \quad (91)$$

Right side of a

For the right side of the turning point at $q = a$ where $E < V(q)$, we use the same ideas as for the left side of the turning point.

$$\psi_P^{C,L}$$

Since we are moving from left to right, the next solution to consider would be the patching solution on the other side of a . As we did before, we can use the Airy solution to the TISE

$$\psi_P^{C,L} = \alpha Ai(u) + \beta Bi(u),$$

but this time we use the asymptotic expansions when $u \rightarrow +\infty$ so

$$\psi_P^{C,L} = \frac{\alpha}{2\sqrt{\pi}u^{\frac{1}{4}}} e^{-\frac{2}{3}u^{\frac{3}{2}}} + \frac{\beta}{\sqrt{\pi}u^{\frac{1}{4}}} e^{\frac{2}{3}u^{\frac{3}{2}}}. \quad (92)$$

$$\psi_{\text{WKB}}^{\text{C,L}}$$

Next, we consider the WKB state in the forbidden region close to $q = a$. Recall that here the WKB state is given by

$$\psi_{WKB}^{C,L} = \frac{E}{\sqrt{p_-(q)}} e^{\frac{1}{\hbar} \int_a^q p_-(q') dq'} + \frac{F}{\sqrt{p_-(q)}} e^{-\frac{1}{\hbar} \int_a^q p_-(q') dq'}.$$

We have again that $V(q) = E + V'(a)(q - a)$ and so

$$p_-(q) = \sqrt{2m(V(q) - E)} = \sqrt{2mV'(a)(q - a)},$$

and thus

$$\begin{aligned} \pm \frac{1}{\hbar} \int_a^q p_-(q') dq' &= \pm \frac{1}{\hbar} \int_a^q \sqrt{2mV'(a)(q' - a)} dq' = \pm \frac{1}{\hbar} \sqrt{2mV'(a)} \int_a^q (q' - a)^{\frac{1}{2}} dq' \\ &= \pm \frac{1}{\hbar} \frac{2}{3} \sqrt{2mV'(a)} \left[(q' - a)^{\frac{3}{2}} \right]_a^q = \pm \frac{1}{\hbar} \frac{2}{3} \sqrt{2mV'(a)} (q - a)^{\frac{3}{2}}. \end{aligned}$$

So the WKB state to the right of the first turning point at a is

$$\psi_{WKB}^{C,L} = \frac{E}{\sqrt{p_-(q)}} e^{\frac{1}{\hbar} \frac{2}{3} \sqrt{2mV'(a)} (q - a)^{\frac{3}{2}}} + \frac{F}{\sqrt{p_-(q)}} e^{-\frac{1}{\hbar} \frac{2}{3} \sqrt{2mV'(a)} (q - a)^{\frac{3}{2}}}.$$

Using the change of variable $u := \left(\frac{2mV'(a)}{\hbar^2} \right)^{\frac{1}{3}} (q - a)$ again, we have

$$\psi_{WKB}^{C,L} = \frac{E}{(2m\hbar V'(a))^{\frac{1}{6}} u^{\frac{1}{4}}} e^{\frac{2}{3} u^{\frac{3}{2}}} + \frac{F}{(2m\hbar V'(a))^{\frac{1}{6}} u^{\frac{1}{4}}} e^{-\frac{2}{3} u^{\frac{3}{2}}}. \quad (93)$$

Thus comparing $\psi_{WKB}^{C,L}$ (93) with $\psi_P^{C,L}$ (92) we have our second set of matching equations

$$\frac{E}{(2m\hbar V'(a))^{\frac{1}{6}}} = \frac{\beta}{\sqrt{\pi}} \quad (94)$$

$$\frac{F}{(2m\hbar V'(a))^{\frac{1}{6}}} = \frac{\alpha}{2\sqrt{\pi}}. \quad (95)$$

Turning point at b

Now we can look at the turning point at $q = b$. This situation is visualised in Fig. 17.

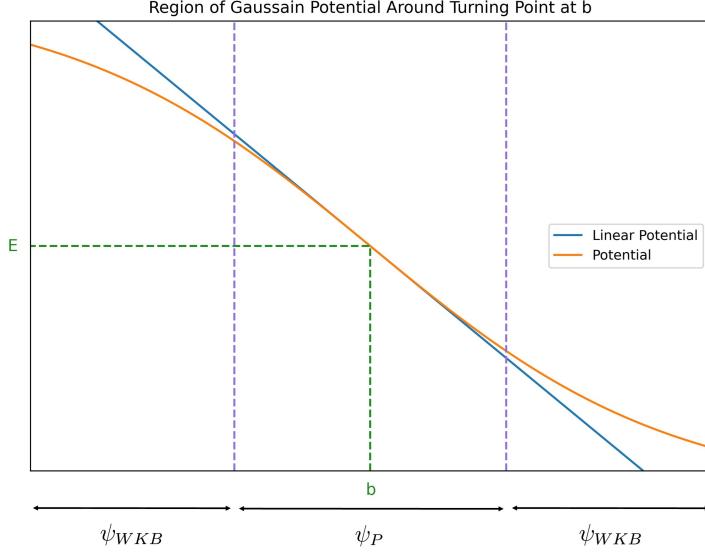


Figure 17: A zoomed in section of the potential at b , where the WKB and patching sections have been indicated.

Left side of b

On the left side of this turning point, we are in the classically forbidden region where $E < V(q)$. This means, using the same reasoning as for the turning point at a , we can approximate the potential in the region of this turning point as a linear potential. This is similarly given by $V(q) \approx E + V'(b)(q - b)$, which is the first order Taylor expansion of the potential around $q = b$.

$$\psi_{WKB}^{C,R}$$

We use the same WKB state from before for the centre region

$$\psi_{WKB}^{C,R} = \frac{E}{\sqrt{p_-(q)}} e^{\frac{1}{\hbar} \int_a^q p_-(q') dq'} + \frac{F}{\sqrt{p_-(q)}} e^{-\frac{1}{\hbar} \int_a^q p_-(q') dq'}$$

but this time we assume q is close to b , and so

$$\psi_{WKB}^{C,R} = \frac{E}{\sqrt{p_-(q)}} e^{\frac{1}{\hbar} \int_a^b p_-(q) dq - \int_q^b p_-(q') dq'} + \frac{F}{\sqrt{p_-(q)}} e^{-\frac{1}{\hbar} \int_a^b p_-(q) dq + \int_q^b p_-(q') dq'}.$$

Now, when q is close to b , the momentum function is given by

$$p_-(q) = \sqrt{2m(V(q) - E)} = \sqrt{2m(E + V'(b)(q - b) - E)} = \sqrt{2mV'(b)(q - b)},$$

so we have that

$$\begin{aligned} \pm \frac{1}{\hbar} \int_q^b p_-(q') dq' &= \pm \frac{1}{\hbar} \int_q^b \sqrt{2mV'(b)(q'-b)} dq' = \pm \frac{1}{\hbar} \sqrt{2mV'(b)} \int_q^b (q'-b)^{\frac{1}{2}} dq' \\ &= \pm \frac{1}{\hbar} \frac{2}{3} \sqrt{2mV'(b)} \left[(q'-b)^{\frac{3}{2}} \right]_q^b = \mp \frac{1}{\hbar} \frac{2}{3} \sqrt{2mV'(b)} (q-b)^{\frac{3}{2}}. \end{aligned}$$

Then, on the left side of b the state becomes

$$\psi_{WKB}^{C,R} = \frac{E}{\sqrt{p_-(q)}} e^{\frac{1}{\hbar} \int_a^b p_-(q) dq + \frac{1}{\hbar} \frac{2}{3} \sqrt{2mV'(b)} (q-b)^{\frac{3}{2}}} + \frac{F}{\sqrt{p_-(q)}} e^{-\frac{1}{\hbar} \int_a^b p_-(q) dq - \frac{1}{\hbar} \frac{2}{3} \sqrt{2mV'(b)} (q-b)^{\frac{3}{2}}}.$$

Now in a similar way as we did for u , we can define

$$v := \left(\frac{2mV'(b)}{\hbar^2} \right)^{\frac{1}{3}} (q-b). \quad (96)$$

Then, notice that

$$v^{\frac{3}{2}} = \frac{1}{\hbar} \sqrt{2mV'(b)} (q-b)^{\frac{3}{2}},$$

and further, $v^{\frac{1}{4}} = \frac{(2mV'(b))^{\frac{1}{12}}}{\hbar^{\frac{1}{6}}} (q-b)^{\frac{1}{4}}$, so since $\sqrt{p_-(q)} = (2mV'(b)(q-b))^{\frac{1}{4}}$, we have that

$$\sqrt{p_-(q)} = (2m\hbar V'(b))^{\frac{1}{6}} v^{\frac{1}{4}}.$$

Thus,

$$\psi_{WKB}^{C,R} = \frac{E}{(2m\hbar V'(b))^{\frac{1}{6}} v^{\frac{1}{4}}} e^{\frac{1}{\hbar} \int_a^b p_-(q) dq} e^{\frac{2}{3} v^{\frac{3}{2}}} + \frac{F}{(2m\hbar V'(b))^{\frac{1}{6}} v^{\frac{1}{4}}} e^{-\frac{1}{\hbar} \int_a^b p_-(q) dq} e^{-\frac{2}{3} v^{\frac{3}{2}}} \quad (97)$$

$$\psi_{\mathbf{P}}^{\mathbf{C},\mathbf{R}}$$

We can now argue in a similar way as we did for the turning point at a , and show that close to the turning point at b , the wave function is given by

$$\psi_P = \gamma Ai(v) + \delta Bi(v).$$

On the left of the barrier, we are in the classically forbidden region so we take the asymptotic limits as $v \rightarrow +\infty$ and the patching solution becomes

$$\psi_P^{C,R} = \frac{\gamma}{2\sqrt{\pi}v^{\frac{1}{4}}} e^{-\frac{2}{3}v^{\frac{3}{2}}} + \frac{\delta}{\sqrt{\pi}v^{\frac{1}{4}}} e^{\frac{2}{3}v^{\frac{3}{2}}}. \quad (98)$$

Now we can match $\psi_{WKB}^{C,R}$ (97) and $\psi_P^{C,R}$ (98) giving us our third set of matching equations

$$\frac{E}{(2m\hbar V'(b))^{\frac{1}{6}}} e^{\frac{1}{\hbar} \int_a^b p_-(q) dq} = \frac{\delta}{\sqrt{\pi}} \quad (99)$$

$$\frac{F}{(2m\hbar V'(b))^{\frac{1}{6}}} e^{-\frac{1}{\hbar} \int_a^b p_-(q) dq} = \frac{\gamma}{2\sqrt{\pi}}. \quad (100)$$

Right side of b

On the right side of this turning point, we are in the classically allowed region where $E > V(q)$.

$$\psi_P^R$$

Since we are in the classically allowed region here, we take the asymptotic expansions of the Airy functions as $v \rightarrow -\infty$, and the patching solution becomes

$$\psi_P^R = \frac{\gamma}{\sqrt{\pi}(-v)^{\frac{1}{4}}} \sin\left(\frac{2}{3}(-v)^{\frac{3}{2}} + \frac{\pi}{4}\right) + \frac{\delta}{\sqrt{\pi}(-v)^{\frac{1}{4}}} \cos\left(\frac{2}{3}(-v)^{\frac{3}{2}} + \frac{\pi}{4}\right). \quad (101)$$

We can now expand sin and cos out in terms of exponentials from (55), so

$$\begin{aligned} \psi_P^R &= \frac{\gamma}{\sqrt{\pi}(-v)^{\frac{1}{4}}} \left(\frac{e^{i\frac{2}{3}(-v)^{\frac{3}{2}}+i\frac{\pi}{4}} - e^{-i\frac{2}{3}(-v)^{\frac{3}{2}}-i\frac{\pi}{4}}}{2i} \right) + \frac{\delta}{\sqrt{\pi}(-v)^{\frac{1}{4}}} \left(\frac{e^{i\frac{2}{3}(-v)^{\frac{3}{2}}+i\frac{\pi}{4}} + e^{-i\frac{2}{3}(-v)^{\frac{3}{2}}-i\frac{\pi}{4}}}{2} \right) \\ &= \frac{\delta - i\gamma}{2\sqrt{\pi}(-v)^{\frac{1}{4}}} e^{i\frac{2}{3}(-v)^{\frac{3}{2}}} e^{i\frac{\pi}{4}} + \frac{\delta + i\gamma}{2\sqrt{\pi}(-v)^{\frac{1}{4}}} e^{-i\frac{2}{3}(-v)^{\frac{3}{2}}} e^{-i\frac{\pi}{4}} \\ &= \frac{(\delta - i\gamma)(1+i)}{2\sqrt{2\pi}(-v)^{\frac{1}{4}}} e^{i\frac{2}{3}(-v)^{\frac{3}{2}}} + \frac{(\delta + i\gamma)(1-i)}{2\sqrt{2\pi}(-v)^{\frac{1}{4}}} e^{-i\frac{2}{3}(-v)^{\frac{3}{2}}} \\ &= \frac{(1-i)\gamma + (1+i)\delta}{2\sqrt{2\pi}(-v)^{\frac{1}{4}}} e^{i\frac{2}{3}(-v)^{\frac{3}{2}}} + \frac{(1+i)\gamma + (1-i)\delta}{2\sqrt{2\pi}(-v)^{\frac{1}{4}}} e^{-i\frac{2}{3}(-v)^{\frac{3}{2}}}, \end{aligned}$$

where we have used (89) again for the fact that $e^{i\frac{\pi}{4}} = \frac{1}{\sqrt{2}}(1+i)$ and $e^{-i\frac{\pi}{4}} = \frac{1}{\sqrt{2}}(1-i)$.

$$\psi_{WKB}^R$$

Here the WKB state is generally given by

$$\psi_{WKB}^R = \frac{C}{\sqrt{p(q)}} e^{\frac{i}{\hbar} \int_b^q p(q') dq'} + \frac{D}{\sqrt{p(q)}} e^{-\frac{i}{\hbar} \int_b^q p(q') dq'},$$

and since in the classically allowed region $E > V(q)$, and using the equation for the linear potential close to b , we have that

$$p(q) = \sqrt{2m(E - V(q))} = \sqrt{2m(E - E - V'(b)(q - b))} = \sqrt{2mV'(b)(b - q)}.$$

Thus,

$$\begin{aligned} \pm \frac{i}{\hbar} \int_b^q p(q') dq' &= \pm \frac{i}{\hbar} \int_b^q \sqrt{2mV'(b)(b - q')} dq' = \pm \frac{i}{\hbar} \sqrt{2mV'(b)} \int_b^q (b - q')^{\frac{1}{2}} \\ &= \pm \frac{i}{\hbar} \sqrt{2mV'(b)} \frac{2}{3} \left[(b - q')^{\frac{3}{2}} \right]_b^q = \pm \frac{i}{\hbar} \frac{2}{3} \sqrt{2mV'(b)} (b - q)^{\frac{3}{2}}, \end{aligned}$$

and so the WKB state on the right side of this turning point at b is

$$\psi_{WKB}^R = \frac{C}{\sqrt{p(q)}} e^{\frac{i}{\hbar} \frac{2}{3} \sqrt{2mV'(b)} (b - q)^{\frac{3}{2}}} + \frac{D}{\sqrt{p(q)}} e^{-\frac{i}{\hbar} \frac{2}{3} \sqrt{2mV'(b)} (b - q)^{\frac{3}{2}}}.$$

Now recalling our definition (96), $v := \left(\frac{2mV'(b)}{\hbar^2}\right)^{\frac{1}{3}} (q - b)$, notice that

$$(-v)^{\frac{3}{2}} = \frac{1}{\hbar} \sqrt{2mV'(b)} (b - q)^{\frac{3}{2}},$$

and $(-v)^{\frac{1}{4}} = \frac{(2mV'(b))^{\frac{1}{12}}}{\hbar^{\frac{1}{6}}} (b - q)^{\frac{1}{4}}$. Since $\sqrt{p(q)} = (2mV'(b)(b - q))^{\frac{1}{4}}$ we therefore have that

$$\sqrt{p(q)} = (2m\hbar V'(b))^{\frac{1}{6}} (-v)^{\frac{1}{4}}.$$

Thus our state can be written,

$$\psi_{WKB}^R = \frac{C}{(2m\hbar V'(b))^{\frac{1}{6}} (-v)^{\frac{1}{4}}} e^{i\frac{2}{3}(-v)^{\frac{3}{2}}} + \frac{D}{(2m\hbar V'(b))^{\frac{1}{6}} (-v)^{\frac{1}{4}}} e^{-i\frac{2}{3}(-v)^{\frac{3}{2}}}. \quad (102)$$

Now, we are in a position to compare the coefficients of ψ_{WKB}^R (102) and ψ_P^R (101) to get our final set of matching equations

$$\frac{C}{(2m\hbar V'(b))^{\frac{1}{6}}} = \frac{(1-i)\gamma + (1+i)\delta}{2\sqrt{2\pi}} \quad (103)$$

$$\frac{D}{(2m\hbar V'(b))^{\frac{1}{6}}} = \frac{(1+i)\gamma + (1-i)\delta}{2\sqrt{2\pi}}. \quad (104)$$

Combining the matching equations

After all of this, we have 4 different sets of matching equations for each side of the turning points. We use these to find the transfer matrix M relating the state in region L where $q < a$, and the state in region R where $q > b$. We find M by finding the transfer matrix between each sub region and successively multiplying them together. So if we go from left to right, $\psi_{WKB}^L = M_I \psi_P^L$ and $\psi_P^L = M_{II} \psi_{WKB}^{C,L}$ and $\psi_{WKB}^{C,R} = M_{III} \psi_P^R$ and $\psi_P^R = M_{IV} \psi_{WKB}^R$. Then,

$$\begin{bmatrix} A \\ B \end{bmatrix} = M_I \begin{bmatrix} \alpha \\ \beta \end{bmatrix}, \quad \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = M_{II} \begin{bmatrix} E \\ F \end{bmatrix}, \quad \begin{bmatrix} E \\ F \end{bmatrix} = M_{III} \begin{bmatrix} \gamma \\ \delta \end{bmatrix}, \quad \begin{bmatrix} \gamma \\ \delta \end{bmatrix} = M_{IV} \begin{bmatrix} C \\ D \end{bmatrix}.$$

So, we can subsequently multiply all these matrices together to get the transfer matrix between ψ_{WKB}^L and ψ_{WKB}^R and thus

$$\begin{bmatrix} A \\ B \end{bmatrix} = M_I M_{II} M_{III} M_{IV} \begin{bmatrix} C \\ D \end{bmatrix}.$$

But before we can do this, we need to work out what M_I , M_{II} , M_{III} and M_{IV} are. First we consider M_I by recalling equations (90) and (91). We have that

$$\begin{bmatrix} A \\ B \end{bmatrix} = M_I \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \Rightarrow \begin{bmatrix} A \\ B \end{bmatrix} = \frac{(2m\hbar V'(a))^{\frac{1}{6}}}{2\sqrt{2\pi}} \begin{bmatrix} 1-i & 1+i \\ 1+i & 1-i \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix},$$

thus

$$M_I = \frac{(2m\hbar V'(a))^{\frac{1}{6}}}{2\sqrt{2\pi}} \begin{bmatrix} 1-i & 1+i \\ 1+i & 1-i \end{bmatrix}. \quad (105)$$

Next we can find M_{II} by considering equation (94) and (95). So,

$$\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = M_{II} \begin{bmatrix} E \\ F \end{bmatrix} \Rightarrow \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \frac{\sqrt{\pi}}{(2m\hbar V'(a))^{\frac{1}{6}}} \begin{bmatrix} 0 & 2 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} E \\ F \end{bmatrix},$$

and thus,

$$M_{II} = \frac{\sqrt{\pi}}{(2m\hbar V'(a))^{\frac{1}{6}}} \begin{bmatrix} 0 & 2 \\ 1 & 0 \end{bmatrix}. \quad (106)$$

Next we can work out M_{III} by considering equations (99) and (100) so

$$\begin{bmatrix} E \\ F \end{bmatrix} = M_{III} \begin{bmatrix} \gamma \\ \delta \end{bmatrix} \Rightarrow \begin{bmatrix} E \\ F \end{bmatrix} = \frac{(2m\hbar V'(b))^{\frac{1}{6}}}{\sqrt{\pi}} \begin{bmatrix} 0 & e^{-\frac{1}{\hbar} \int_a^b p_-(q)dq} \\ \frac{1}{2}e^{\frac{1}{\hbar} \int_a^b p_-(q)dq} & 0 \end{bmatrix} \begin{bmatrix} \gamma \\ \delta \end{bmatrix},$$

and therefore

$$M_{III} = \frac{(2m\hbar V'(b))^{\frac{1}{6}}}{\sqrt{\pi}} \begin{bmatrix} 0 & e^{-\frac{1}{\hbar} \int_a^b p_-(q)dq} \\ \frac{1}{2}e^{\frac{1}{\hbar} \int_a^b p_-(q)dq} & 0 \end{bmatrix}. \quad (107)$$

Finally, we can find M_{IV} by looking at the equations (103) and (104), so

$$\begin{bmatrix} \gamma \\ \delta \end{bmatrix} = M_{IV} \begin{bmatrix} C \\ D \end{bmatrix} \Rightarrow \begin{bmatrix} C \\ D \end{bmatrix} = M_{IV}^{-1} \begin{bmatrix} \gamma \\ \delta \end{bmatrix} \Rightarrow \begin{bmatrix} C \\ D \end{bmatrix} = \frac{(2m\hbar V'(b))^{\frac{1}{6}}}{2\sqrt{2\pi}} \begin{bmatrix} 1-i & 1+i \\ 1+i & 1-i \end{bmatrix}.$$

Thus, using the fact that the inverse of a 2×2 matrix is given by

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix},$$

since

$$M_{IV}^{-1} = \frac{(2m\hbar V'(b))^{\frac{1}{6}}}{2\sqrt{2\pi}} \begin{bmatrix} 1-i & 1+i \\ 1+i & 1-i \end{bmatrix},$$

we have that

$$M_{IV} = \frac{\sqrt{\pi}}{\sqrt{2}(2m\hbar V'(b))^{\frac{1}{6}}} \begin{bmatrix} 1+i & 1-i \\ 1-i & 1+i \end{bmatrix}, \quad (108)$$

after doing some simple algebraic manipulations.

Now we can finally multiply all these matrices together to obtain the transfer matrix between the left and right regions since

$$\begin{bmatrix} A \\ B \end{bmatrix} = M_I M_{II} M_{III} M_{IV} \begin{bmatrix} C \\ D \end{bmatrix} = M \begin{bmatrix} C \\ D \end{bmatrix}.$$

Recalling the matrices we have worked out for M_I , M_{II} , M_{III} and M_{IV} in (105), (106), (107), (108) respectively, notice that almost all of the prefactors cancel out, except for a factor of $\frac{1}{4}$. Then we have

$$\begin{aligned} M &= \frac{1}{4} \begin{bmatrix} 1-i & 1+i \\ 1+i & 1-i \end{bmatrix} \begin{bmatrix} 0 & 2 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & e^{-\frac{1}{\hbar} \int_a^b p_-(q)dq} \\ \frac{1}{2} e^{\frac{1}{\hbar} \int_a^b p_-(q)dq} & 0 \end{bmatrix} \begin{bmatrix} 1+i & 1-i \\ 1-i & 1+i \end{bmatrix} \\ &= \frac{1}{4} \begin{bmatrix} 1+i & 1-i \\ 1-i & 1+i \end{bmatrix} \begin{bmatrix} e^{\frac{1}{\hbar} \int_a^b p_-(q)dq} & 0 \\ 0 & e^{-\frac{1}{\hbar} \int_a^b p_-(q)dq} \end{bmatrix} \begin{bmatrix} 1+i & 1-i \\ 1-i & 1+i \end{bmatrix} \\ &= \frac{1}{4} \begin{bmatrix} 1-i & 1+i \\ 1+i & 1-i \end{bmatrix} \begin{bmatrix} (1+i)e^{\frac{1}{\hbar} \int_a^b p_-(q)dq} & (1-i)e^{\frac{1}{\hbar} \int_a^b p_-(q)dq} \\ (1-i)e^{-\frac{1}{\hbar} \int_a^b p_-(q)dq} & (1+i)e^{-\frac{1}{\hbar} \int_a^b p_-(q)dq} \end{bmatrix} \\ &= \frac{1}{2} \begin{bmatrix} e^{\frac{1}{\hbar} \int_a^b p_-(q)dq} + e^{-\frac{1}{\hbar} \int_a^b p_-(q)dq} & -ie^{\frac{1}{\hbar} \int_a^b p_-(q)dq} + ie^{-\frac{1}{\hbar} \int_a^b p_-(q)dq} \\ ie^{\frac{1}{\hbar} \int_a^b p_-(q)dq} - ie^{-\frac{1}{\hbar} \int_a^b p_-(q)dq} & e^{\frac{1}{\hbar} \int_a^b p_-(q)dq} + e^{-\frac{1}{\hbar} \int_a^b p_-(q)dq} \end{bmatrix}. \end{aligned}$$

Now we have M , but were not finished just yet! From M , we recall from §4.2 that we can find the scattering matrix S from M as in (40)

$$S = \frac{1}{M_{22}} \begin{bmatrix} -M_{21} & 1 \\ \det(M) & M_{12} \end{bmatrix}.$$

We have

$$\begin{aligned} \det(M) &= \frac{1}{4} \left(e^{\frac{1}{\hbar} \int_a^b p_-(q)dq} + e^{-\frac{1}{\hbar} \int_a^b p_-(q)dq} \right)^2 + \frac{1}{4} \left(ie^{\frac{1}{\hbar} \int_a^b p_-(q)dq} - ie^{-\frac{1}{\hbar} \int_a^b p_-(q)dq} \right)^2 \\ &= \frac{1}{4} \left(e^{\frac{2}{\hbar} \int_a^b p_-(q)dq} + 2 + e^{-\frac{2}{\hbar} \int_a^b p_-(q)dq} - e^{\frac{2}{\hbar} \int_a^b p_-(q)dq} + 2 - e^{-\frac{2}{\hbar} \int_a^b p_-(q)dq} \right) \\ &= 1, \end{aligned}$$

and this gives us that

$$S = \frac{1}{e^{\frac{1}{\hbar} \int_a^b p_-(q)dq} + e^{-\frac{1}{\hbar} \int_a^b p_-(q)dq}} \begin{bmatrix} ie^{-\frac{1}{\hbar} \int_a^b p_-(q)dq} - ie^{\frac{1}{\hbar} \int_a^b p_-(q)dq} & 1 \\ 1 & ie^{-\frac{1}{\hbar} \int_a^b p_-(q)dq} - ie^{\frac{1}{\hbar} \int_a^b p_-(q)dq} \end{bmatrix}.$$

Recall further from §4.2, that the transmission coefficient T (for an incident wave from the left) is related to the S -matrix such that $T = |S_{21}|^2$, therefore we have that

$$\begin{aligned} T &= \frac{1}{|e^{\frac{1}{\hbar} \int_a^b p_-(q)dq} + e^{-\frac{1}{\hbar} \int_a^b p_-(q)dq}|^2} \\ &= \frac{e^{-\frac{2}{\hbar} \int_a^b p_-(q)dq}}{|1 + e^{-\frac{2}{\hbar} \int_a^b p_-(q)dq}|^2} \end{aligned}$$

Now, if we consider Taylor expanding $f(x) = \frac{1}{|1+x|^2}$ around $x = 0$, we have that $f(x) = 1 - 2x + \mathcal{O}(x^2)$, then subbing in $e^{-\frac{2}{\hbar} \int_a^b p_-(q)dq}$ in place of x , we get that

$$T = e^{-\frac{2}{\hbar} \int_a^b p_-(q)dq} + \mathcal{O}(e^{-\frac{4}{\hbar} \int_a^b p_-(q)dq}) \approx e^{-\frac{2}{\hbar} \int_a^b p_-(q)dq}$$

and

$$R = 1 - e^{-\frac{2}{\hbar} \int_a^b p_-(q)dq} + \mathcal{O}(e^{-\frac{4}{\hbar} \int_a^b p_-(q)dq}) \approx 1 - e^{-\frac{2}{\hbar} \int_a^b p_-(q)dq}.$$

This is exactly what we said R and T would look like back in §5.1.1.

Top of the Barrier

As we mentioned briefly earlier, these methods only work when the potential can be approximated as linear but not horizontal, i.e. we have no method for the top of a barrier when the first derivative is zero. For this situation, we cite an equation for R and T from [17]

$$T(E) = \frac{1}{1 + e^{-\frac{2\pi}{\hbar} \frac{E-V_0}{\lambda}}} \tag{109}$$

and

$$R(E) = 1 - \frac{1}{1 + e^{-\frac{2\pi}{\hbar} \frac{E-V_0}{\lambda}}} = \frac{e^{-\frac{2\pi}{\hbar} \frac{E-V_0}{\lambda}}}{1 + e^{-\frac{2\pi}{\hbar} \frac{E-V_0}{\lambda}}}. \tag{110}$$

This is for a parabolic barrier $V = V_0 - \frac{1}{2}V''(q_0)(q - q_0)^2$, and $\lambda = \sqrt{\frac{V''(q_0)}{m}}$ and $V'(q_0) = 0$. Here, q_0 is where the peak of the barrier is centred.

Below in Fig. 18, we can see a plot of the reflection and transmission coefficients for a single Gaussian potential, given by the equations in (109) and (110). We have set $\hbar = m = 1$ in this case. This looks exactly how we would expect it to, and it also looks similar to the graphs for R and T seen for the case with a rectangular potential in §4.3.1.

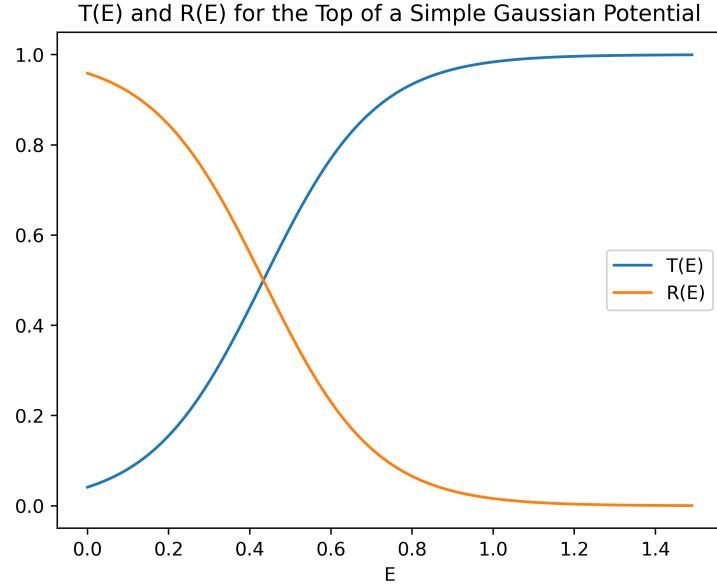


Figure 18: Graph of reflection and transmission coefficients for varying wave energies, when interacting with a Gaussian potential barrier. These were calculated from the equations in (109) and (110).

6 The Wigner Function

For references in this section, see chapter 5 of [2] and chapter 6.4 of [19].

The Wigner Function

We introduced the idea of phase space at the beginning of this project in §2, and the idea carries on throughout the sections with the Fourier and inverse Fourier transforms (15), (16). In this section, we introduce a convenient tool for visualising wave functions in phase space - the Wigner function, first introduced by Eugene Wigner [20]. Plotting in phase space allows us to see the motion of a state in both position and momentum simultaneously - we have seen something like this in §2 where we plotted classical energy level sets in phase space in Fig. 1. An important aspect of the Wigner function is that it is a quasi-probability distribution in phase space, so it behaves similarly to a probability distribution, however it does not satisfy all the conventional properties, namely, it can take on negative values. We define the Wigner function, or Wigner transform, of a wave function $\psi(q)$ as

$$W(q, p) := \frac{1}{\pi\hbar} \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}2py} \psi(q-y)\bar{\psi}(q+y) dy. \quad (111)$$

Making a change of variable, $y \rightarrow \frac{y}{2}$, this can be rewritten in the form

$$W(q, p) := \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}y} \psi(q - \frac{y}{2})\bar{\psi}(q + \frac{y}{2}) dy, \quad (112)$$

which corresponds to a Fourier transform (15) of $\psi(q - \frac{y}{2})\bar{\psi}(q + \frac{y}{2})$ in y .

The Wigner transform of a wave function can give us its probability distribution in position and momentum via the following lemma.

Lemma 6.1.

$$\int W(q, p) dp = |\psi(q)|^2 \quad , \quad \int W(q, p) dq = |\tilde{\psi}(p)|^2.$$

Proof. Recall the definition of the Dirac delta function in (20), then inserting the definition from (112)

$$\begin{aligned} \int W(q, p) dp &= \frac{1}{2\pi\hbar} \int \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}py} \psi(q - \frac{y}{2})\bar{\psi}(q + \frac{y}{2}) dy dp = \int_{-\infty}^{+\infty} \delta(y) \psi(q - \frac{y}{2})\bar{\psi}(q + \frac{y}{2}) dy \\ &= \int_{-\infty}^{+\infty} \delta(y) \psi(q)\bar{\psi}(q) dy = \psi(q)\bar{\psi}(q) = |\psi(q)|^2, \end{aligned}$$

using an alternative definition of the Dirac delta function from (18). A similar proof holds for $\tilde{\psi}(p)$. \square

Some final interesting properties of the Wigner function are firstly, that Wigner functions of Gaussians are also Gaussians (see [19], §8.5). Secondly, in Wigner transforms of superpositions of multiple states, we see interference effects between them [21]. This is a well known phenomenon, and is partly why the Wigner function is not entirely like a probability distribution, since these interference regions take on negative values.

6.1 Examples

Using the Fourier-like definition of the Wigner function in (112), I was able to code and visualise it in plots and animations in Python, using similar techniques to those mentioned in §3.1. This is detailed further in Appendix 10.2. From this we can see some of the properties of the Wigner transform mentioned above.

Cat State

In quantum mechanics, the cat state is a superposition of two Gaussian states. In the following example, we can clearly see properties of the Wigner function, including the fact that the Wigner transform of a Gaussian is too a Gaussian, as well as the interference effects seen between two superposed states. Below in Fig. 19, we see the superposition of two initially Gaussian waves at opposing positions with opposite momenta - one is centred at $q = -25$ moving towards the right, and the other is centred at $q = 25$ moving towards the left.

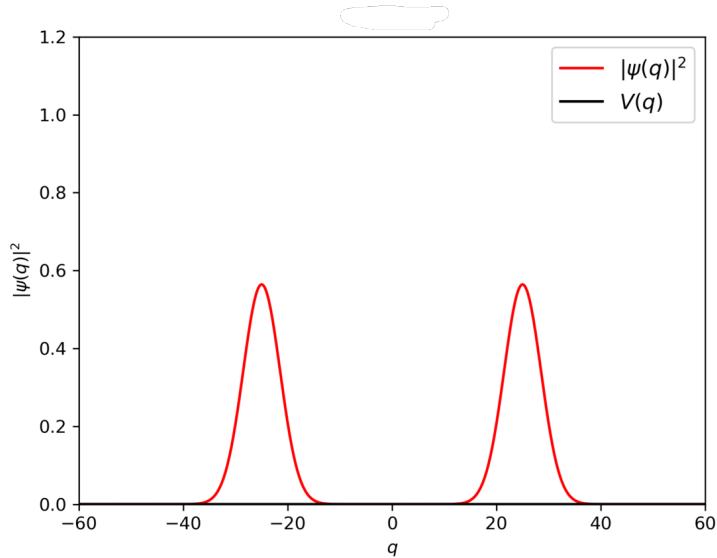


Figure 19: We show the plotted wave function of a cat state - in this case two equal Gaussian waves centred at opposing positions.

Since we are plotting a function in three dimensions, the Wigner plot can be visualised by a 3D surface plot, or alternatively a density plot. In Fig. 20, we can see a 3D surface plot of the cat state pictured in Fig. 19. In the phase space plot, its easy to see both the difference in position on the q -axis, as well as the differing momenta on the p -axis. A benefit of this 3D visualisation is that we can clearly see that the two Gaussian waves correspond to Gaussian waves in phase space. We can also easily see the interference effects between the waves in the centre of the plot and how they reach double the height of the coherent states in both the positive and negative directions.

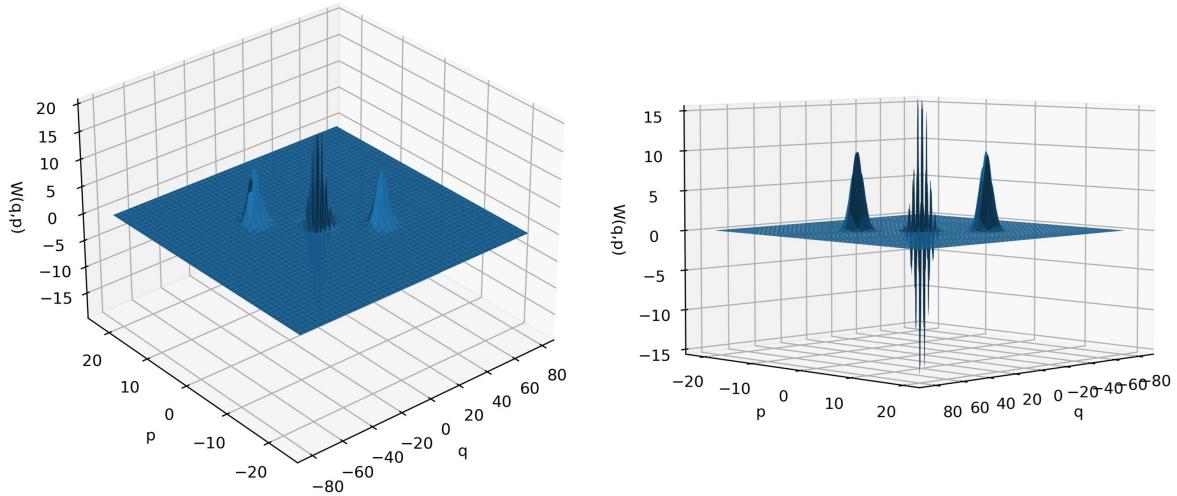


Figure 20: Two surface plots of the Wigner transform of the cat state in Fig. 19, displayed at different viewing angles.

We compare these numerical results with an explicit solution of the Wigner transform of a cat state, from example 2.8.1 in [22]. From this, we can cite the following: define a superposition of two coherent states centred symmetrically as

$$\psi := \frac{1}{\sqrt{2}}\psi_{\mathbf{y}_1} + \frac{1}{\sqrt{2}}\psi_{\mathbf{y}_2},$$

where the subscripts denote the states initial centres and momentum, i.e. $\mathbf{y}_1 = (q_1, p_1)$ and $\mathbf{y}_2 = (q_2, p_2)$. Then the Wigner function of such a superposition is given by

$$\rho(\mathbf{x}) = \frac{1}{2}\rho_{\mathbf{y}_1}(\mathbf{x}) + \frac{1}{2}\rho_{\mathbf{y}_2}(\mathbf{x}) + \frac{e^{\frac{i}{\hbar}\alpha}}{2}e^{\frac{i}{\hbar}\delta_{\mathbf{y}} \cdot (q - \bar{y})}\rho_{\bar{\mathbf{y}}}(q) + \frac{e^{-\frac{i}{\hbar}\alpha}}{2}e^{-\frac{i}{\hbar}\delta_{\mathbf{y}} \cdot (\mathbf{x} - \bar{\mathbf{y}})}\rho_{\bar{\mathbf{y}}}(\mathbf{x}),$$

where

$$\rho_{\mathbf{y}}(\mathbf{x}) = 2^n e^{-\frac{i}{\hbar}|\mathbf{x}-\mathbf{y}|^2}$$

and

$$\bar{\mathbf{y}} = \frac{1}{2}(\mathbf{y}_1 + \mathbf{y}_2) \quad , \quad \delta_{\mathbf{y}} = \mathbf{y}_2 - \mathbf{y}_1 \quad , \quad \alpha = \frac{1}{2}\bar{\mathbf{y}} \cdot \begin{bmatrix} 0 & I \\ 0 & 0 \end{bmatrix} \delta_{\mathbf{y}}.$$

In this notation, we have that $\mathbf{x} = (q, p)$, and $\rho(\mathbf{x})$ is the Wigner function. From these equations, we can see a 3D plot of a generic cat state in Fig. 21.

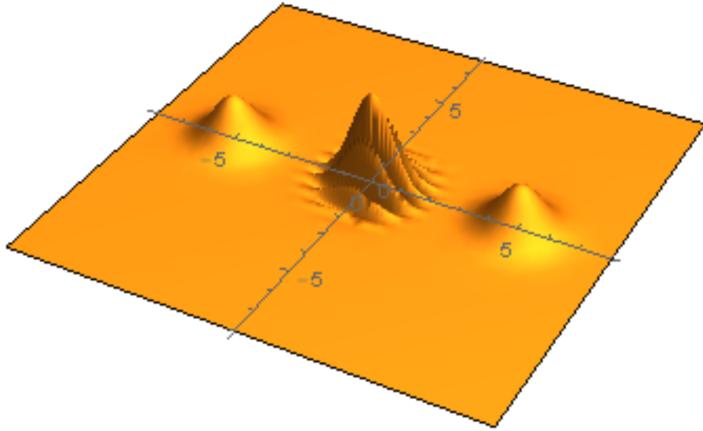


Figure 21: A 3D plot of a cat state from example 2.8.1 in [22].

We can see from the image above, that our numerical results coincide with the analytical solutions provided in [22].

Moving on, in the following figures 22 and 23, we show our numerically generated snapshots of the evolution of the cat state shown above in figures 19 and 20. This time, when plotting the Wigner function, we use a density plot rather than a 3D plot, and we will in general use density Wigner plots for the remainder of the paper due to time constraints on generating surface plots for many frames. In these density plots in Fig. 23, we see how the waves pass through each other, as they do in the corresponding snapshots from Fig. 19 with equal and opposite momenta. We can also see how they return localised states after interacting, with a broader range in position. The stripes between the waves indicate the interference effects seen between states that we mentioned earlier.

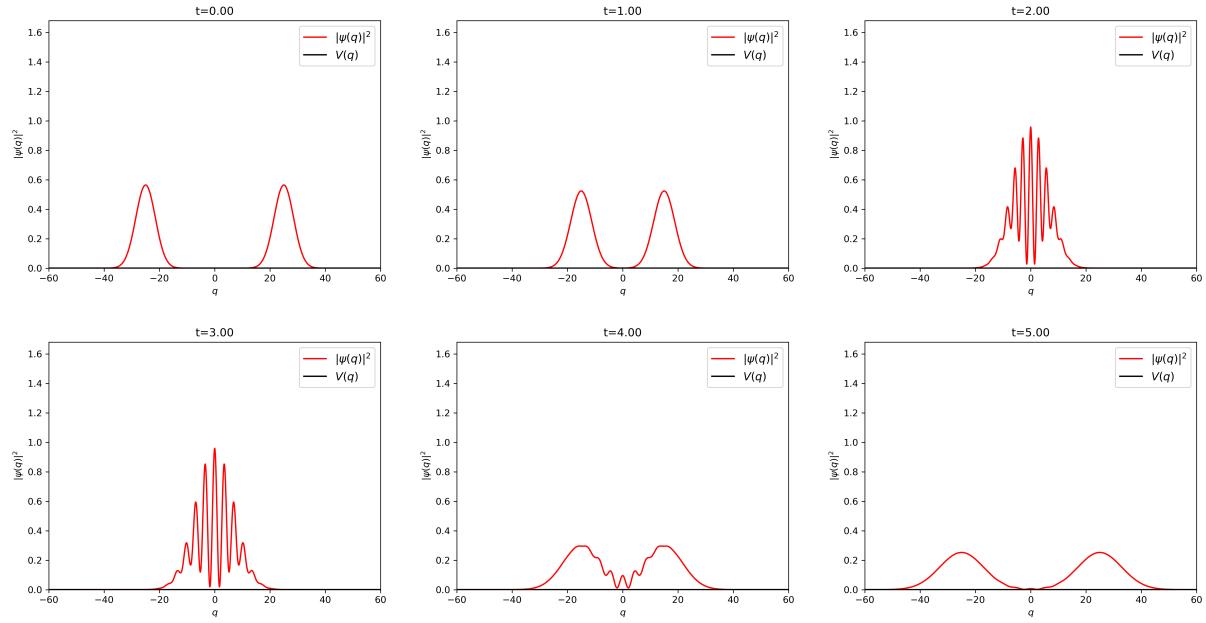


Figure 22: Snapshots of the evolution of the wave function of the cat state pictured above in Fig. 19 and Fig. 20.

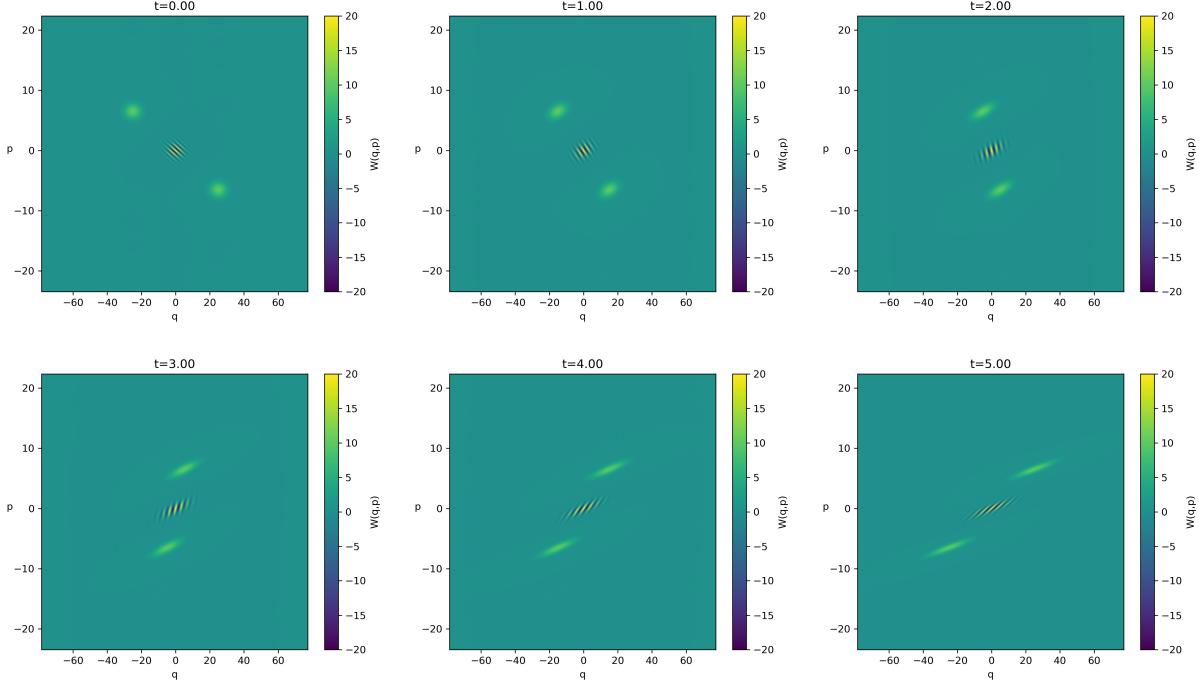


Figure 23: The corresponding Wigner function evolution of Fig. 22, visualised using a density plot.

Step Potential

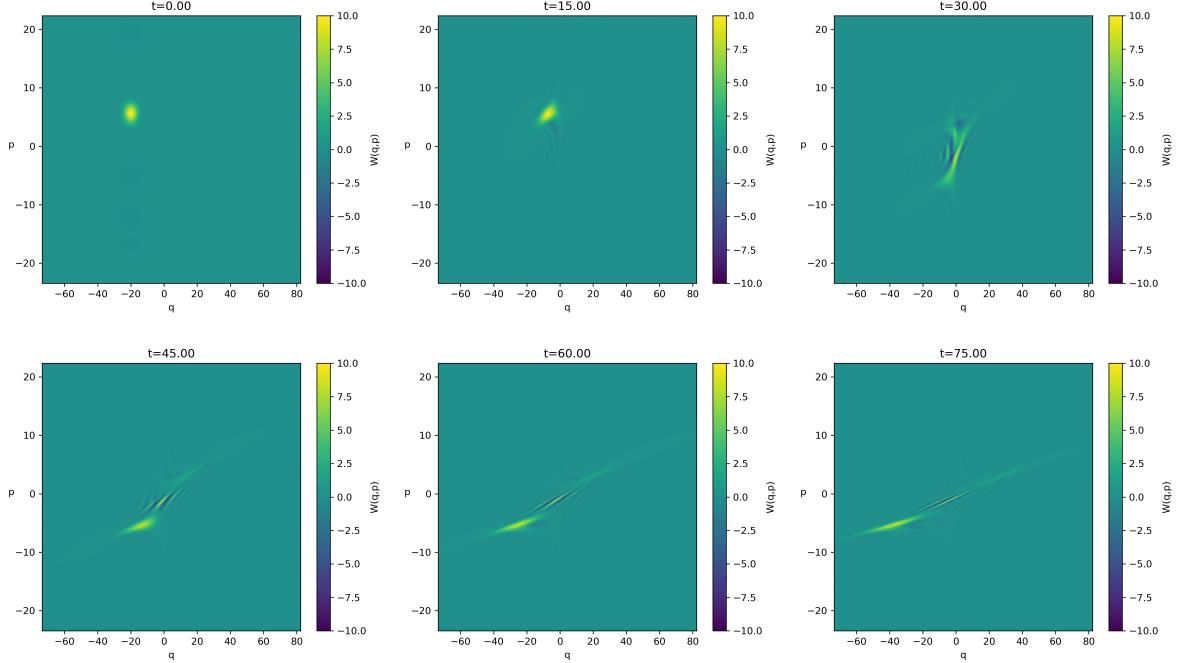


Figure 24: Wigner function snapshots for a step potential when $E < V_0$.

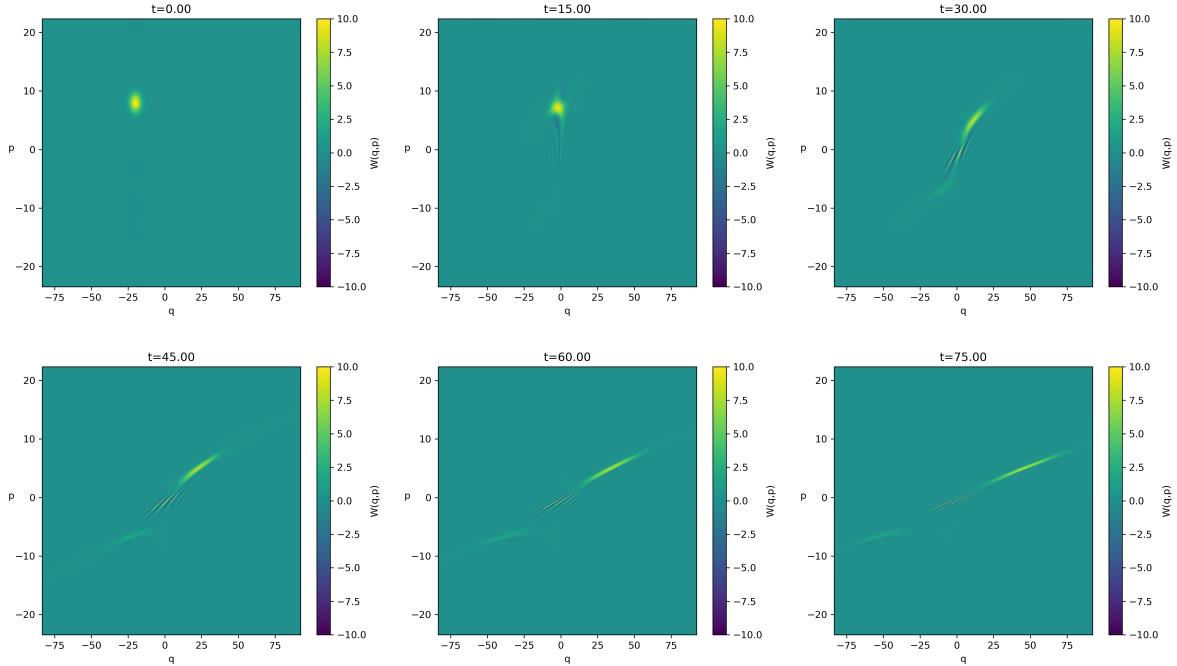


Figure 25: Wigner function snapshots for a step potential when $E > V_0$.

Above we show the Wigner snapshots of a state interacting with a step potential with a height of V_0 . These snapshots correspond to the wave function snapshots from §4.3.1, in figures 5 and 7. Now, Fig. 24 shows the case when the energy of the wave $E < V_0$, and Fig. 25 shows the case when $E > V_0$.

We can see from the intensity of the colour of the wave, how more or less of it gets reflected or transmitted depending on its energy. We also see some interesting wave splitting at the barrier, as well as interference effects between the resulting waves similar to the ones seen in Fig. 23. The wave splitting effects are covered in slightly more detail in §7. However, it is interesting to note that the wave has not fully split in the last frame in Fig. 24, and this is because it never does. If we recall the corresponding example from §4.3.1, the reflection coefficient is always 1 when $E < V_0$, so eventually, all of the wave will get reflected back.

Rectangular Potential

Below we see some snapshots of the Wigner functions of a state interacting with a rectangular potential. This barrier also has a height of V_0 , but this time it has finite length. The plots correspond to the wave function snapshots seen in Figures 9 and 10 back in §4.3.1.

We see that the snapshots look fairly similar to the Wigner snapshots for a step potential above, as when the energy of the wave $E < V_0$ in Fig. 26, more of the wave is reflected, and in Fig. 27 where $E > V_0$, more of the wave is transmitted. This corresponds to the graph for R and T we saw in Fig. 11, and we will also see a similar graph generated for this scenario using numerical methods at the beginning of the next section in Fig. 28. Even though these images are similar to the ones for a step potential, there are slight differences, for example the states are more localised after interaction. This makes sense since the barrier is finite this time, and so the interaction does not last as long.

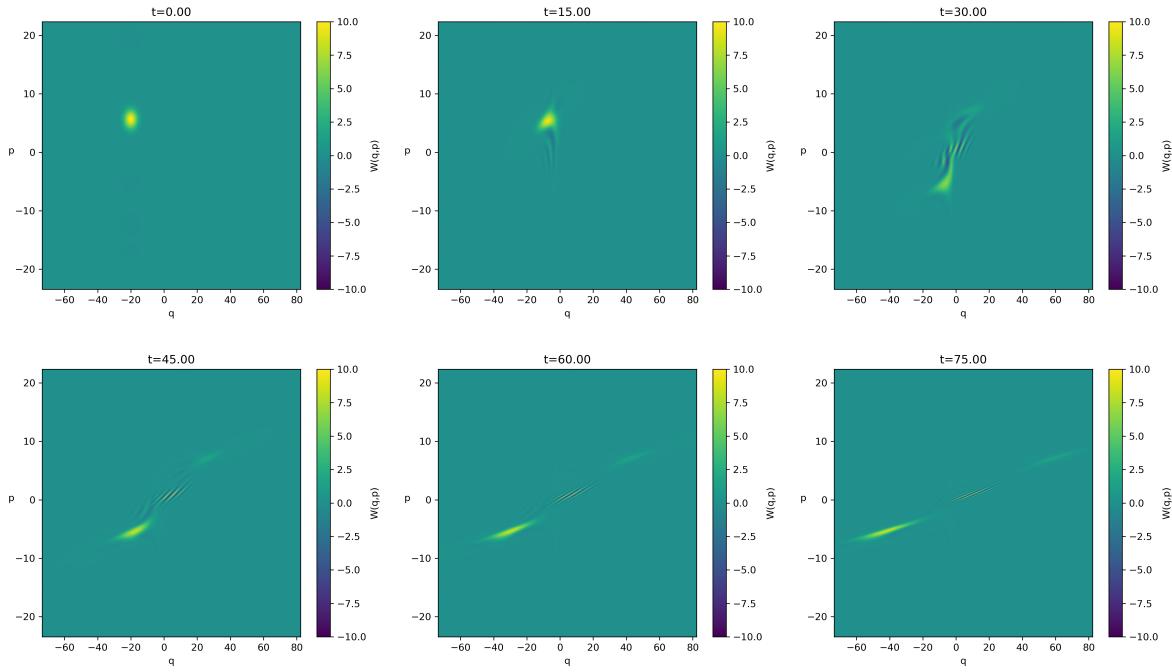


Figure 26: Wigner snapshots for a rectangular potential, where $E < V_0$.

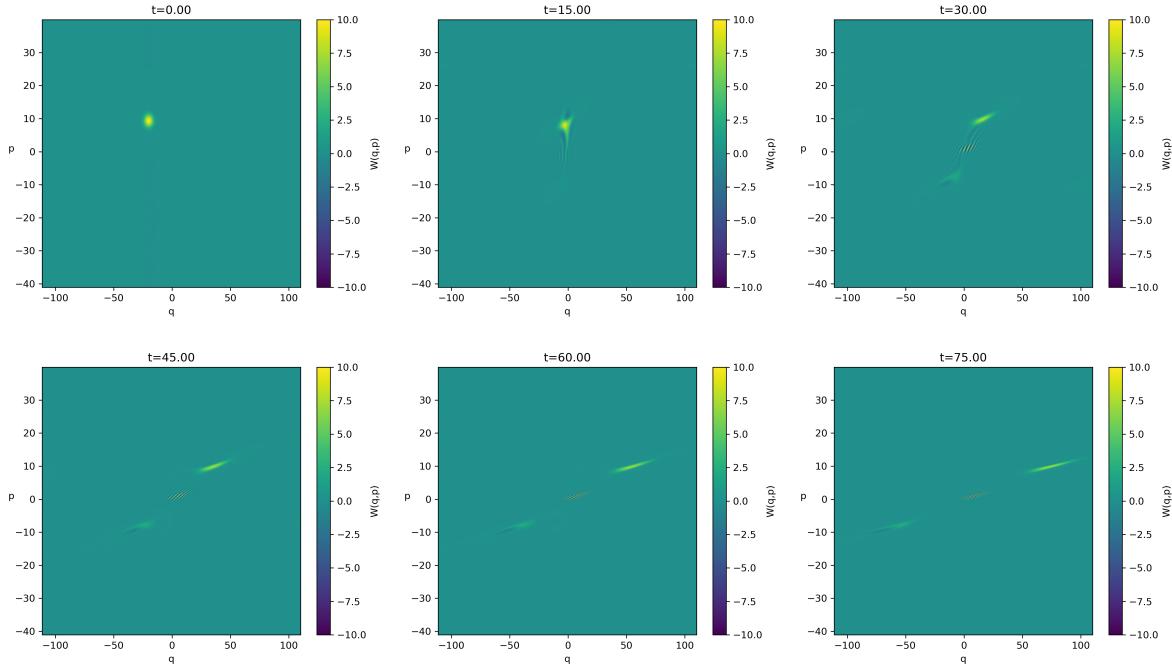


Figure 27: Wigner snapshots for a rectangular potential, where $E > V_0$.

7 Animation Analyses

In the examples below, we will look at different scenarios of an initially Gaussian wave packet interacting with different potential barriers. We have animated these scenarios using the ideas from §3.1 and the code is shown explicitly in the Appendix 10.1. We also look at the Wigner functions for each example using the code from Appendix 10.2. Finally, we look at graphs for the reflection and transmission coefficients using code shown in Appendix 10.3. The idea behind this is to simply integrate the modulus squared of the wave functions on either side of the barrier at a large enough time, so that the wave interaction with the potential is complete. This works, since our initial wave packets are normalised to integrate to 1.

Example - rectangular potential

We saw at the end of the last section, some Wigner snapshots for a finite rectangular potential, corresponding to the scenario we showed in Figures 9 and 10 in §4.3.1. Recall that in this section, we also plotted the reflection and transmission coefficients in Fig. 11, using analytical methods. Using Fig. 28, we can compare the graph for R and T generated by the numerical methods mentioned above, and notice how it coincides very closely with the first graph in Fig. 11.

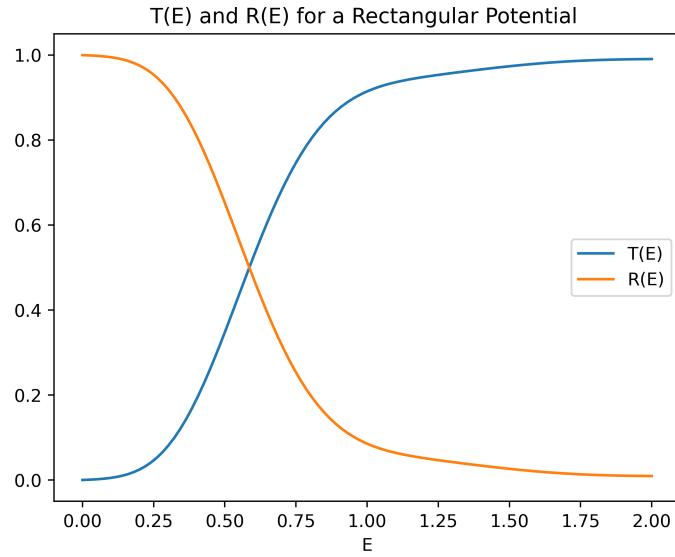


Figure 28: The plots for the reflection and transmission coefficients for a rectangular potential like the one in Fig. 9 and Fig. 10.

We do not however see perturbations in this graph like we do in the graphs for wider barriers in Fig. 11. This could be because the barrier in this example is not wide enough (and the wave not localised enough) for these effects to emerge. This can also be explained, using the fact that the code calculates $|\psi_R|^2$ and $|\psi_T|^2$ for R and T respectively. Recalling theorem 4.1 in §4, we know that to calculate this, we multiply the reflection and transmission coefficients by some ‘envelope’ function $|A|^2$, which is localised around some k_0 , and this acts as a smoothing window for R and T .

In the following, we go through various scenarios of wave packets interacting with varying barriers, and we start off with a simple situation where a wave interacts with a single Gaussian potential. After that, we see how ideas from this scenario will combine when we deal with different double potential barriers, and finally we look at what happens when a wave is in potential wells.

7.1 Single Gaussian Potential

In the following figures, we have an initially Gaussian wave packet with varying energies sent from an initial position centred at $q = -20$, to the right travelling towards a single Gaussian potential barrier, centred at $q = 0$. We have discussed a scenario similar to this before in §4.3.1 and §6 with a rectangular, rather than Gaussian, barrier and the findings agree.

From the wave function figures in 29, 32 and 34, we can clearly see how an initially wave packet moves and scatters when interacting with the barrier. We see that the transmitted wave looks like the original wave packet with a smaller amplitude (on the right of the barrier), and how the reflected wave interferes with itself in the oscillations (on the left of the barrier). We can also see that for large enough times however, the resulting waves return to a nice looking Gaussian wave packet - like a damped version of the original. This is what is theorised would happen with scattering theory. More of the wave gets reflected when $E < V_0$, and more gets transmitted when $E > V_0$, and in both cases, there is still small amounts of transmission and reflected respectively. This is also in agreement with what we saw in scattering theory in §4.

$E < V_0$

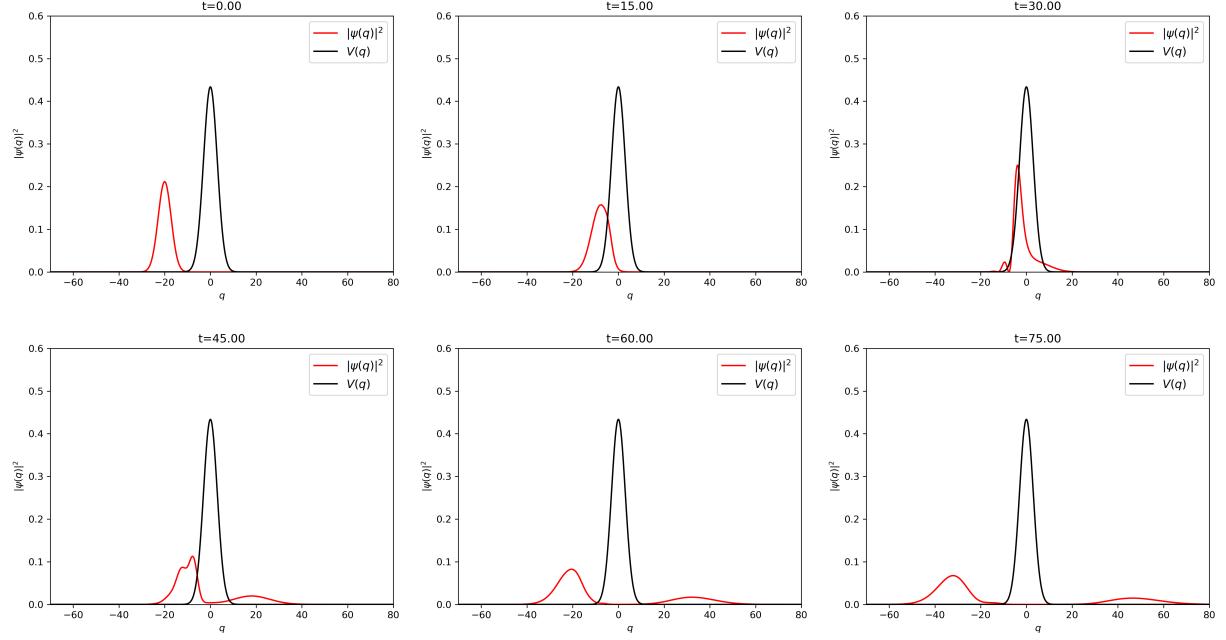


Figure 29: Wave function snapshots for a single Gaussian potential when $E < V_0$.

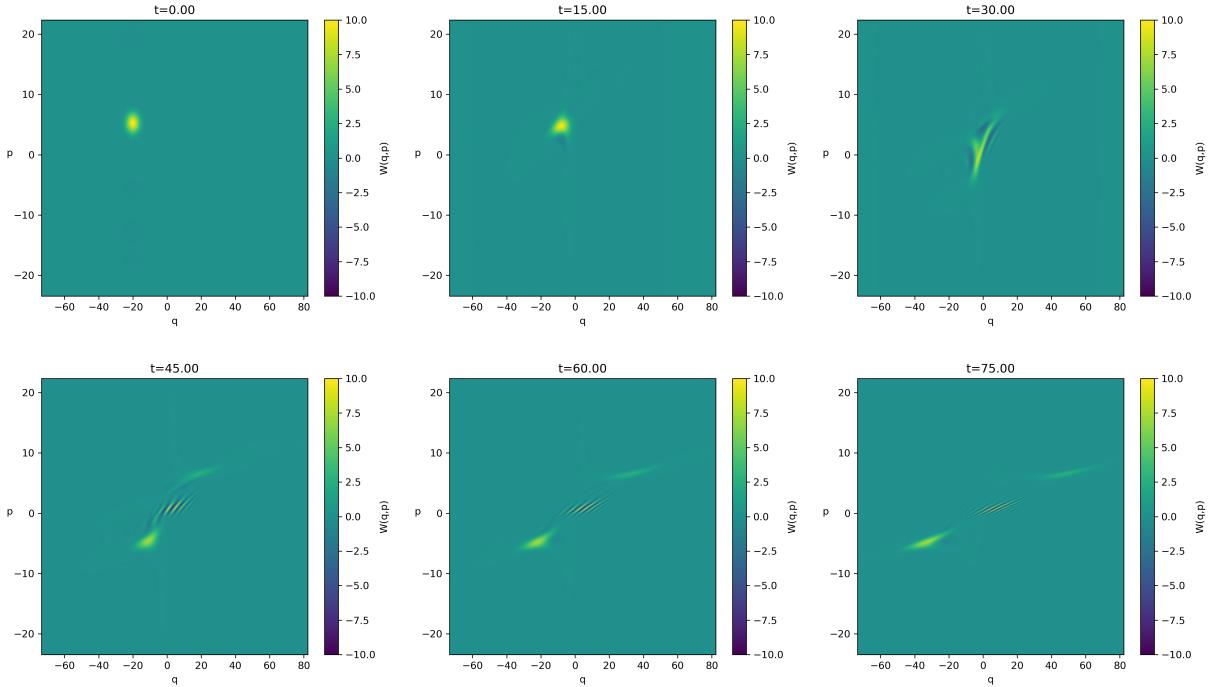


Figure 30: Wigner function snapshots for a single Gaussian potential when $E < V_0$.

$$\mathbf{E} = \mathbf{V}_0$$

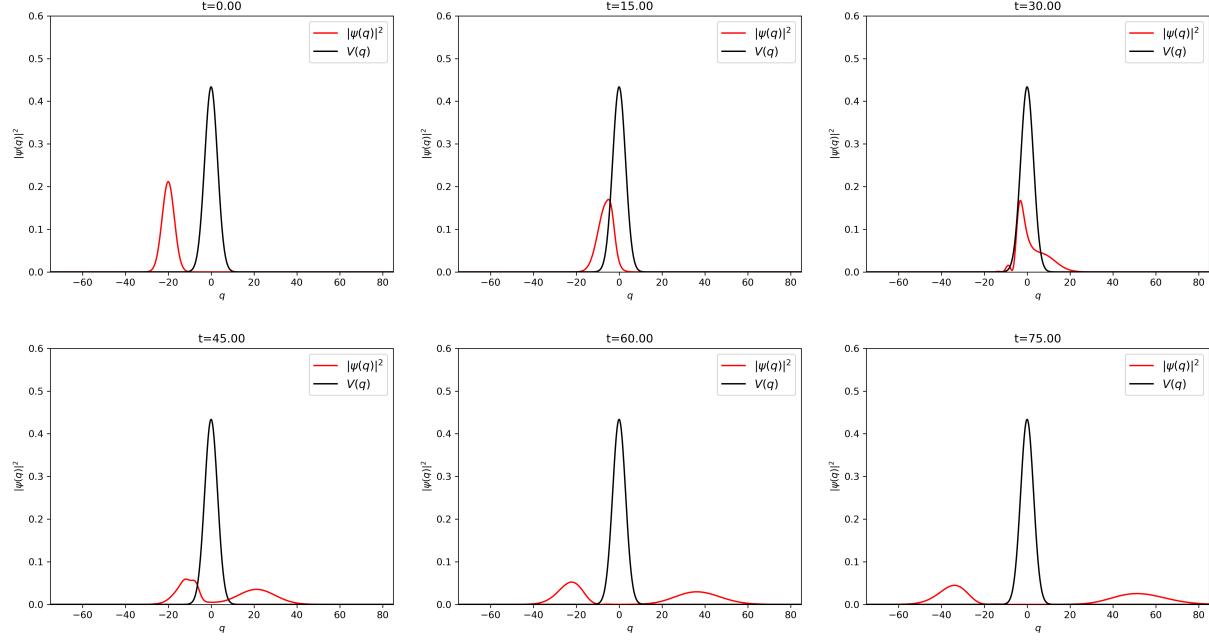


Figure 31: Wave function snapshots for a single Gaussian potential when $E = V_0$.

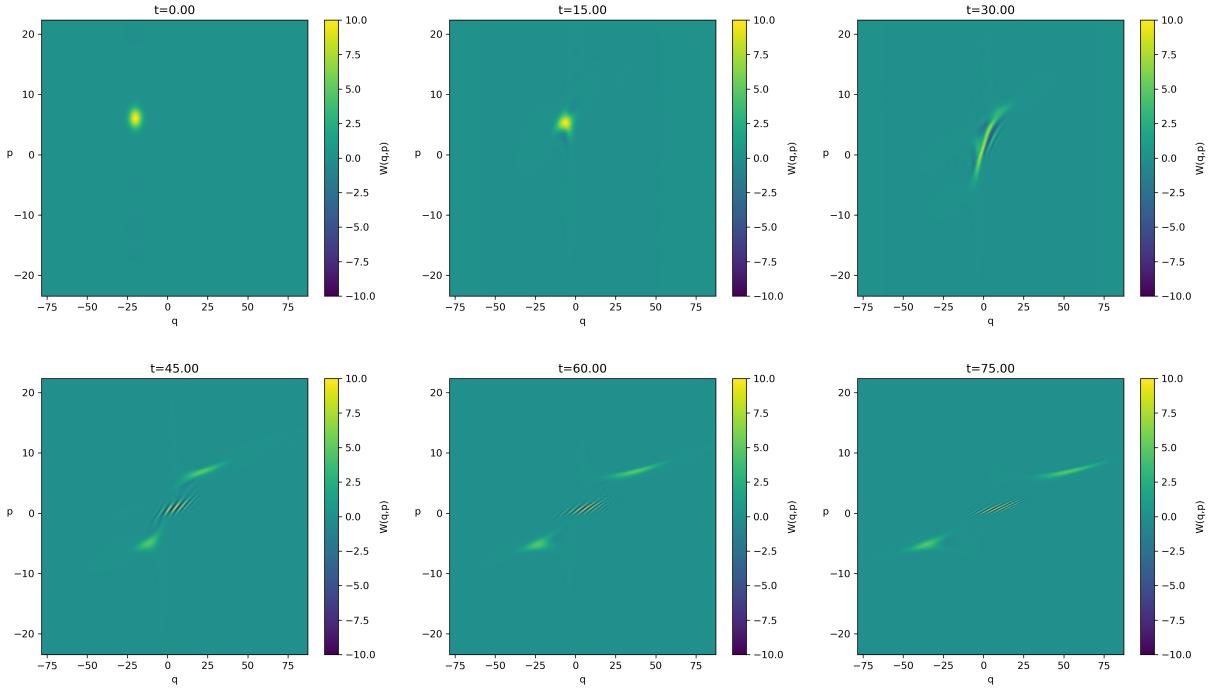


Figure 32: Wigner function snapshots for a single Gaussian potential when $E = V_0$.

$E > V_0$

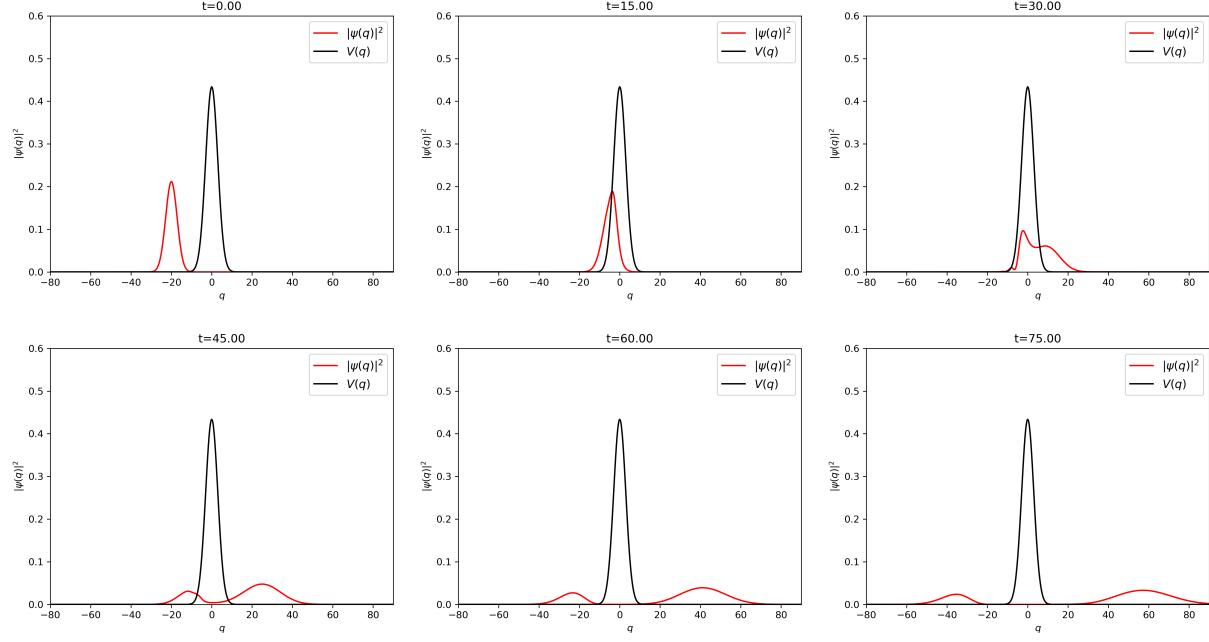


Figure 33: Wave function snapshots for a single Gaussian potential when $E > V_0$.

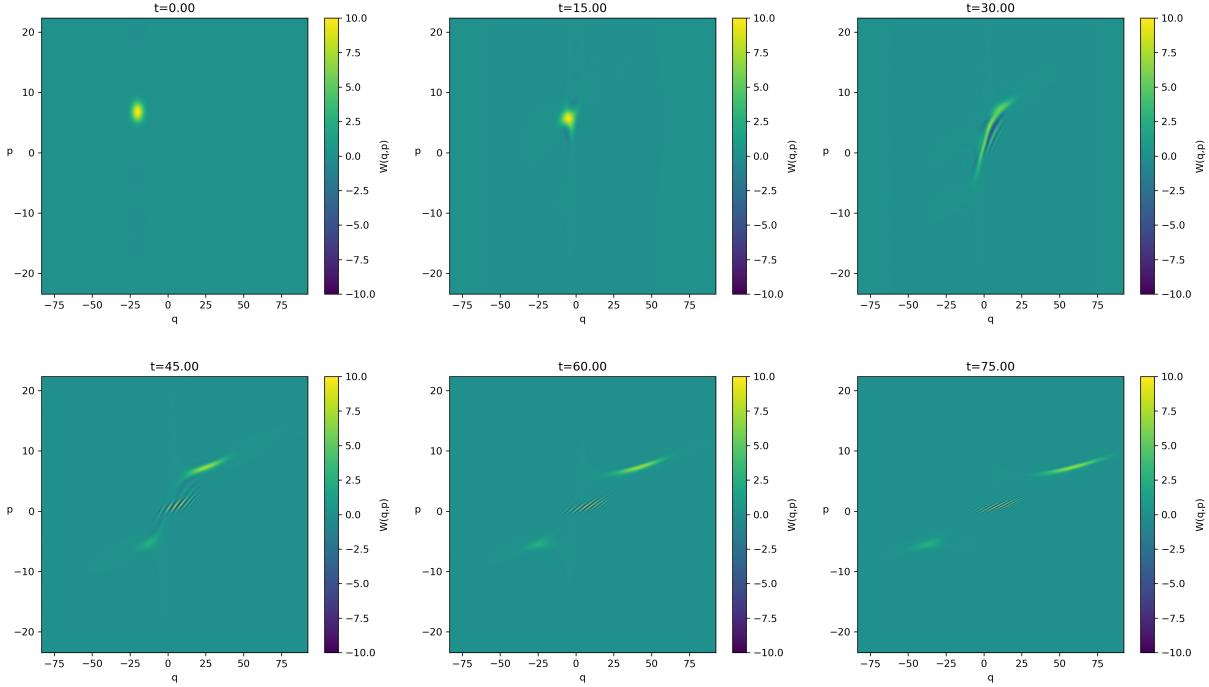


Figure 34: Wigner function snapshots for a single Gaussian potential when $E > V_0$.

Discussion

In the above pictures, we have seen three scenarios of a wave packet interacting with a single Gaussian barrier through the lens of the wave function and the Wigner function. Classically, if $E < V_0$, where V_0 is the maximum potential of the barrier, the particle will wholly be reflected back, and if $E > V_0$, the particle will completely pass over the barrier. As we have discussed in §4 however, in the quantum case, there is a small chance a particle can tunnel through a barrier even if it does not have enough energy to overcome it classically, which we see from the last frames in Fig. 29. We also see that even when a particle has a higher energy than the potential barrier, there is still a small chance of reflection, as we can see from the last frames in Fig. 33. These animations, and the graph generated for R and T from them (in Fig. 35), coincide with our results for the transmission and reflection coefficients in both §4 and §5. We recall Fig. 18, which is an analytically generated graph for R and T for the exact same potential barrier as in this example. The graphs entirely agree, which is reassuring.

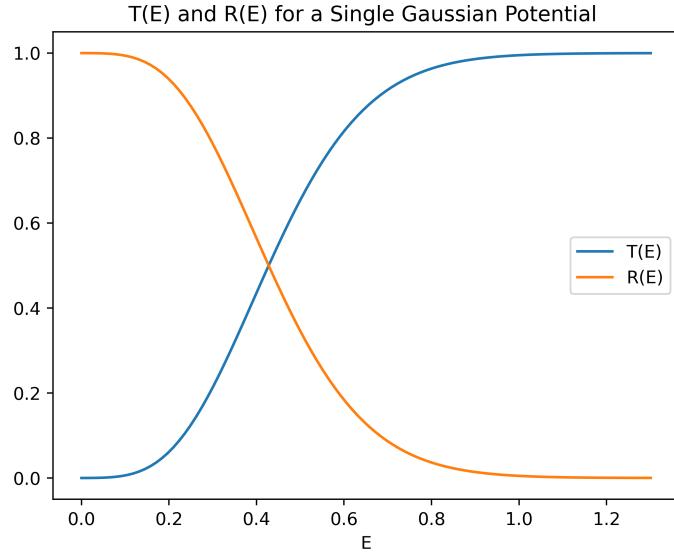


Figure 35: The reflection and transmission coefficients for varying wave energies E , when interacting with a single Gaussian potential.

The Wigner snapshots show further information about the interactions. We can still see, from the intensity of the colours, how more or less of the wave is transmitted as the energy changes, but from the position of these spots, we can see not only where they are in position space, but also with what momentum they are travelling. In all scenarios, we start off with a localised wave in the first frame, with a relatively small variation in position and momentum. During the interaction, we can see this localised wave stretch out and split in two. This process has very interesting theoretical explanations that are beyond the

scope of this paper, but they are mentioned in §8 and you can read more in [23]. After these interactions, in the final frames of Figures 30, 32 and 34, we see that the wave has completely split into two. These separate wave packets are still fairly localised, but with broader position ranges. Finally, we can also see the interference patterns between the split waves, a phenomenon introduced in §6.

7.2 Double Gaussian Potential

In the following, we see how the ideas from the single Gaussian potential in §7.1 combine for more than one barrier. We expect for double barriers, to see the stretching and splitting effects twice, once at each barrier. We consider first the scenario where the heights of the barriers are equal. This is a simple case, since the same thing is expected at each barrier, since the maximum potentials and energy of the wave will not change. Next, we consider the case where the first barrier is smaller than the second. This is more complicated situation, and slightly more interesting, since we expect to see different thing at each barrier depending on its maximum.

7.2.1 Equal Heights

In the following figures, we have an initially Gaussian wave packet with varying energies sent from an initial position centred at $q = -40$. They all have positive momentum and so are travelling to the right towards a potential composed of two Gaussians centred at $q = -20$ and $q = 20$. These barriers both have the same maximum potential at V_0 . At each interaction with the two barriers, we would expect to see something similar to what we saw in §7.1 for a single barrier. This means we expect the wave function to split once at the first barrier, and then again at the second barrier, with varying amounts of the wave being reflected and transmitted past each of them.

$E < V_0$

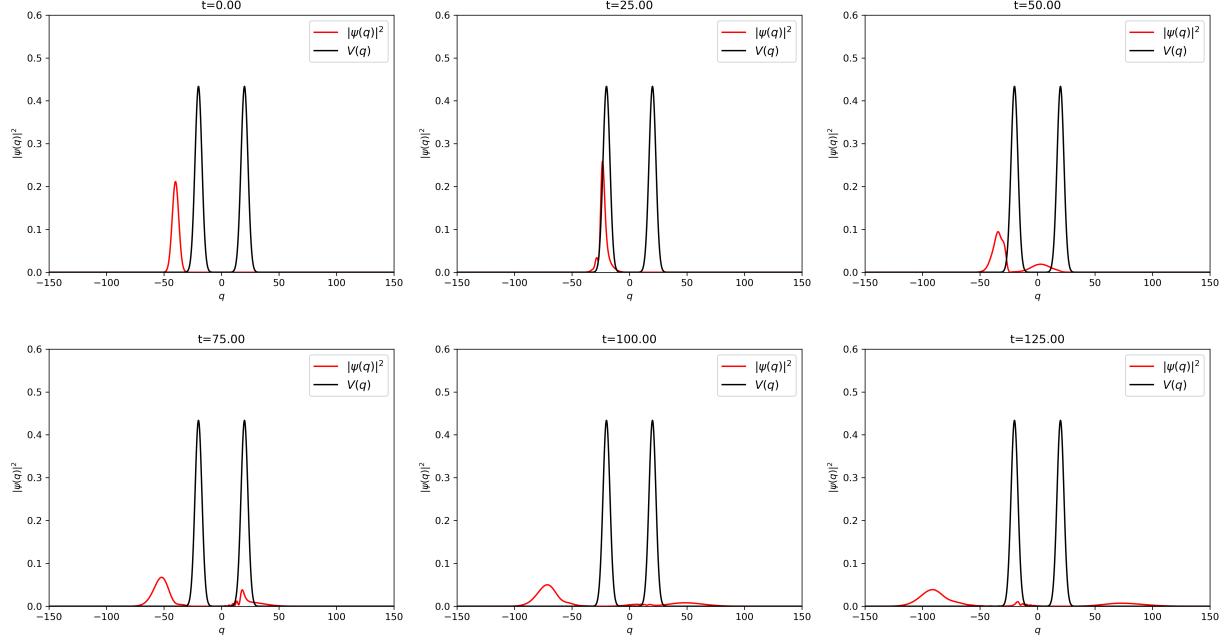


Figure 36: Wave snapshots for an equal double Gaussian barrier when $E < V_0$.

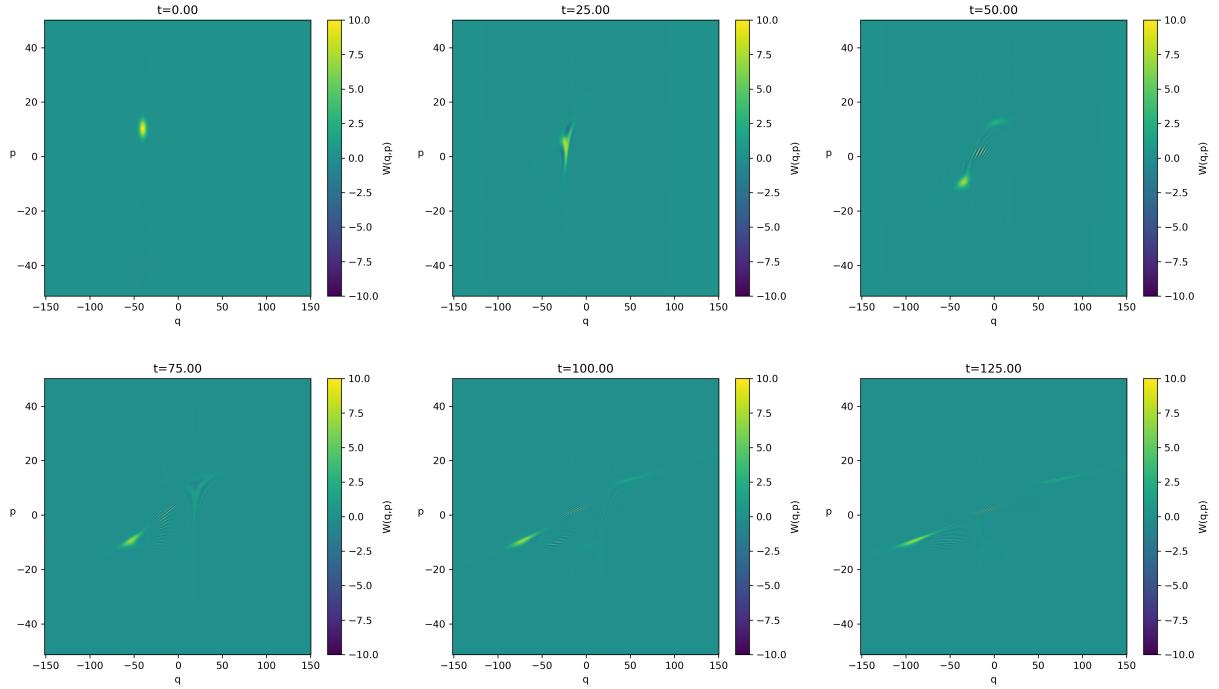


Figure 37: Wigner snapshots for an equal double Gaussian barrier when $E < V_0$.

$$\mathbf{E} = \mathbf{V}_0$$

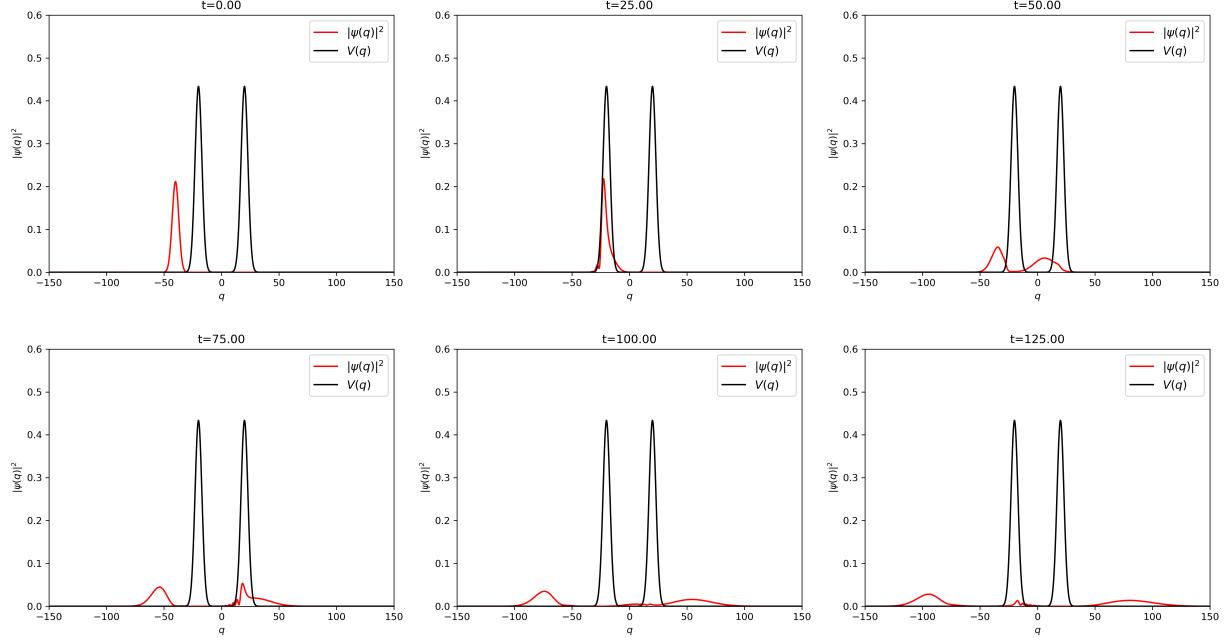


Figure 38: Wave snapshots for an equal double Gaussian potential when $E = V_0$.

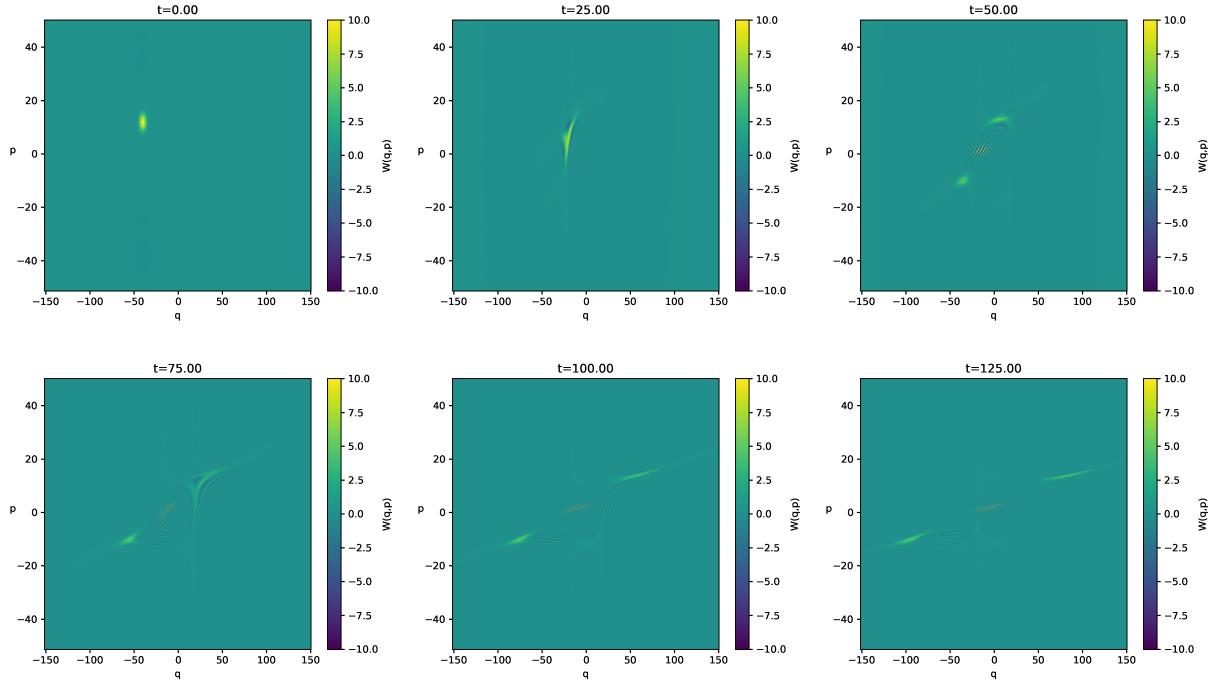


Figure 39: Wigner snapshots for an equal double Gaussian potential when $E = V_0$.

$$E > V_0$$

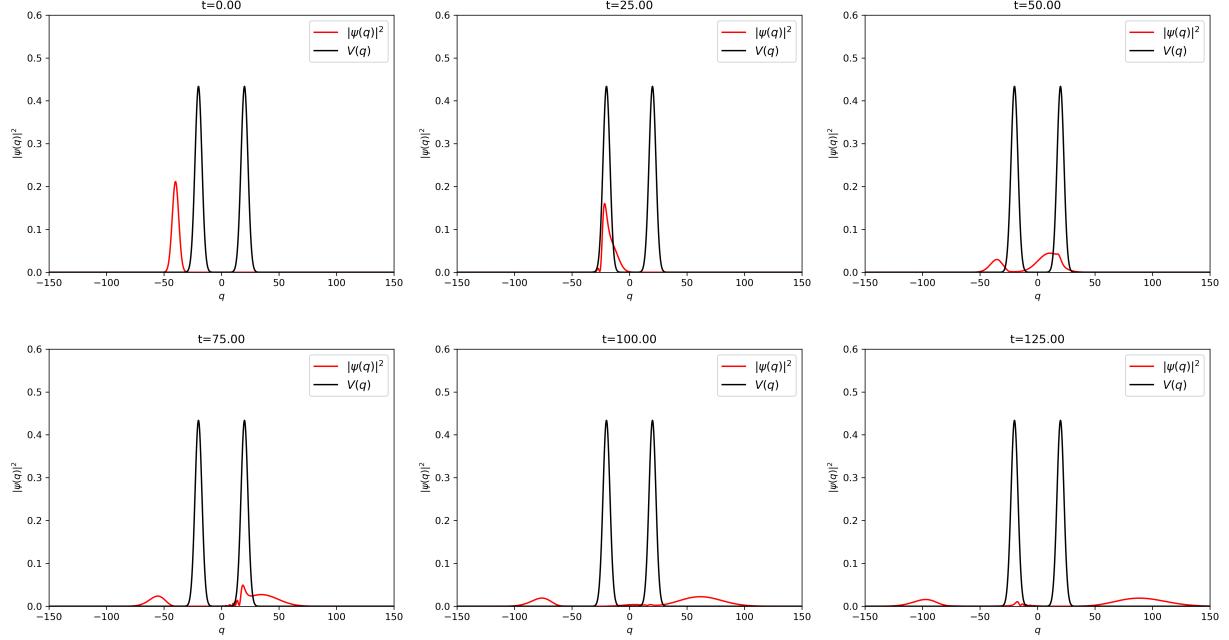


Figure 40: Wave snapshots for an equal double Gaussian barrier when $E > V_0$.

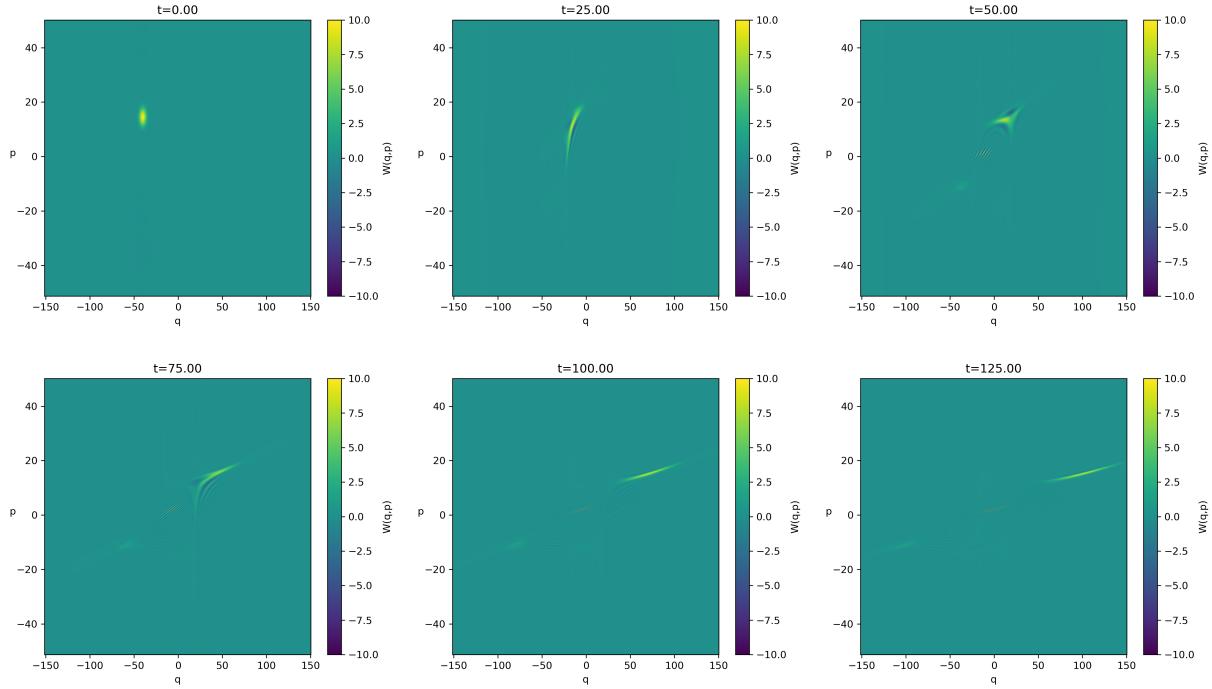


Figure 41: Wigner snapshots for an equal double Gaussian barrier when $E > V_0$.

Discussion

As expected, from the wave function plots and the Wigner plots, the state gets split in two at each barrier. Similarly to the case with a single barrier, when $E < V_0$, most of the wave is reflected with a small amount of transmission as can be seen in Fig. 36. When $E > V_0$, there is more transmission with less of the wave function reflected, as can be seen in Fig. 40. This behaviour also means we see similar plots for the reflection and transmission coefficients in Fig. 42.

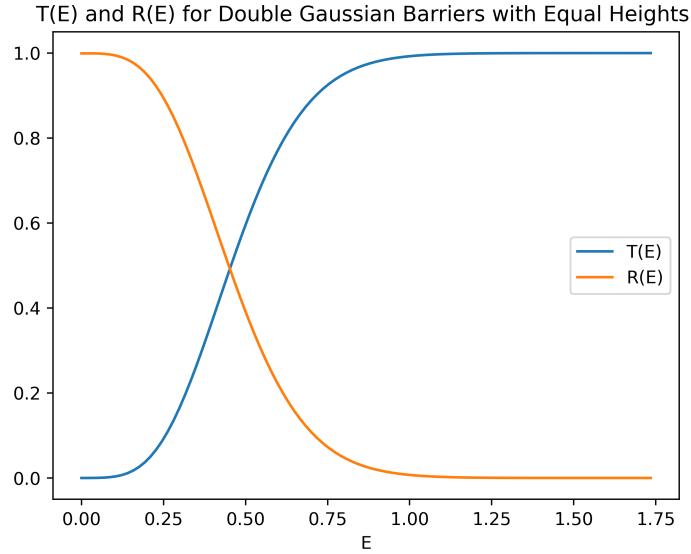


Figure 42: Plots of R and T for a double barrier with equal peaks.

What is fairly interesting are the plots of the Wigner functions in Figures 37, 39 and 41. We can see the same stretching and splitting effects as before (and the resulting interference patterns) at the first barrier, but then we see it happen again at the second barrier. We see this most prominently in Fig. 41, since more of the original wave function reaches the second barrier. This double splitting results in the wave function eventually being in three parts, which can be seen in the later frames. Here, we see two of the (leftmost) parts have a negative momentum as they have both been reflected, and the rightmost part has a positive momentum as its been transmitted past both barriers. This also results in more complicated interference effects as they appear between each pair of wave functions, so we see three regions of interference that are equidistant from each pair of yellow spots.

7.2.2 Unequal Heights

In the following figures we have an identical situation as in §7.2.1, besides the fact that the barriers have different peaks - the first is lower with a height of V_0 , and the second is higher with a height of V_1 .

$E < V_0$

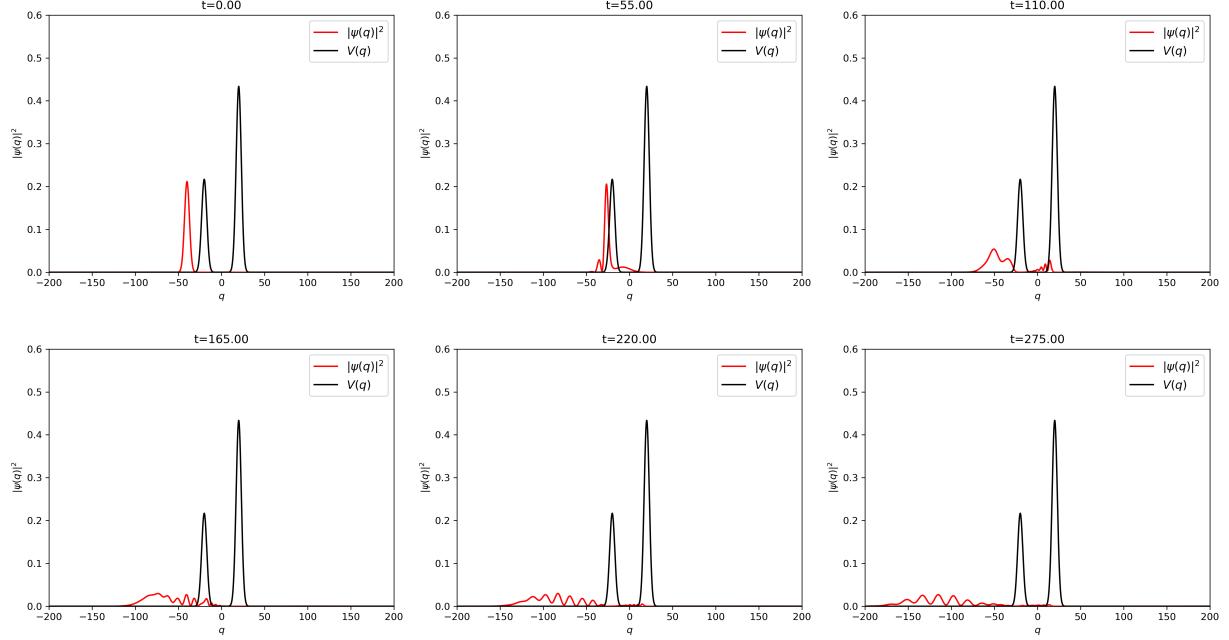


Figure 43: Wave function snapshots where its energy is smaller than the lower peak.

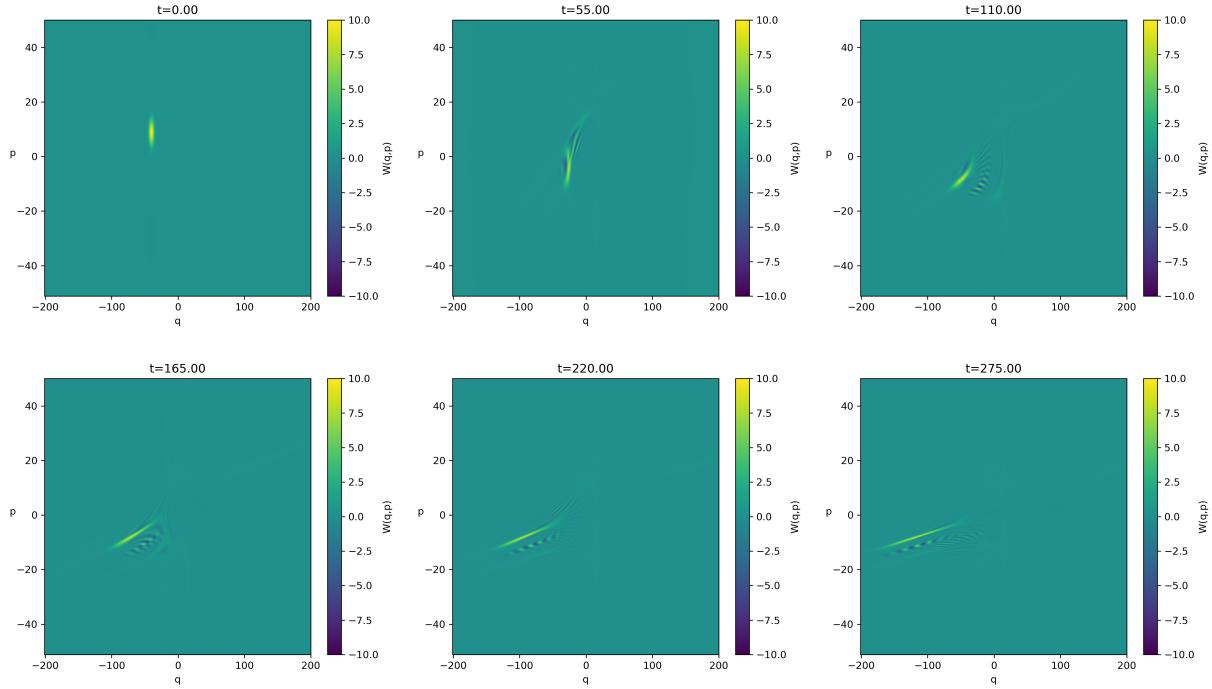


Figure 44: Wigner function snapshots for an unequal double barrier where $E < V_0$.

$$V_0 < E < V_1$$

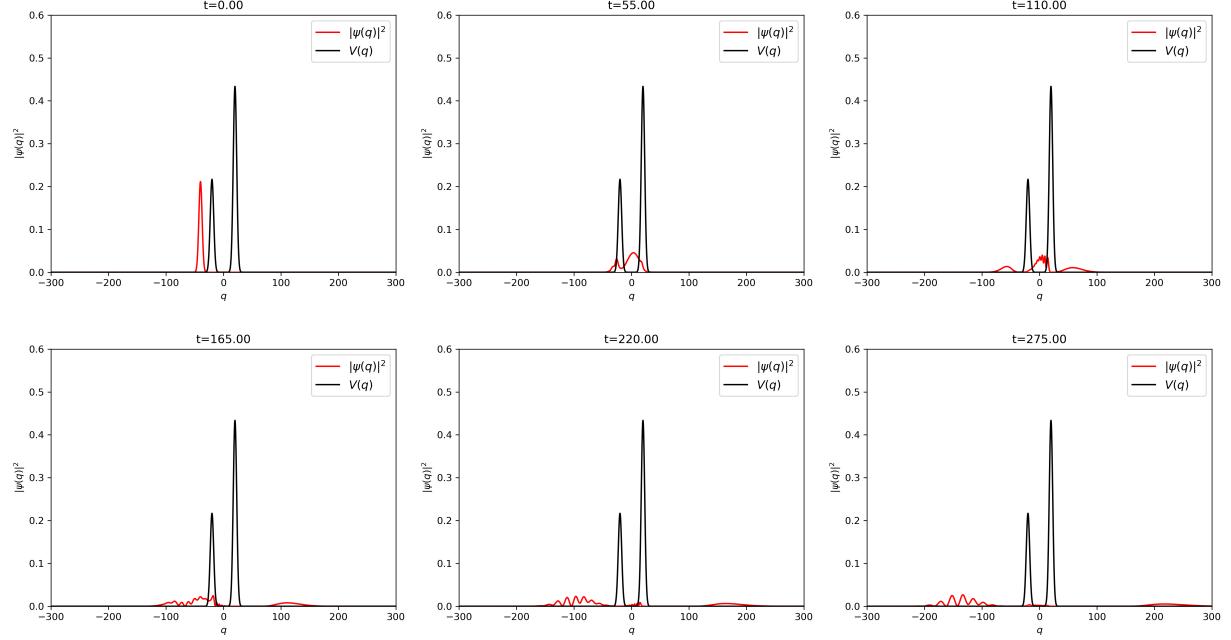


Figure 45: Wave function snapshots where its energy is between the potential peaks.

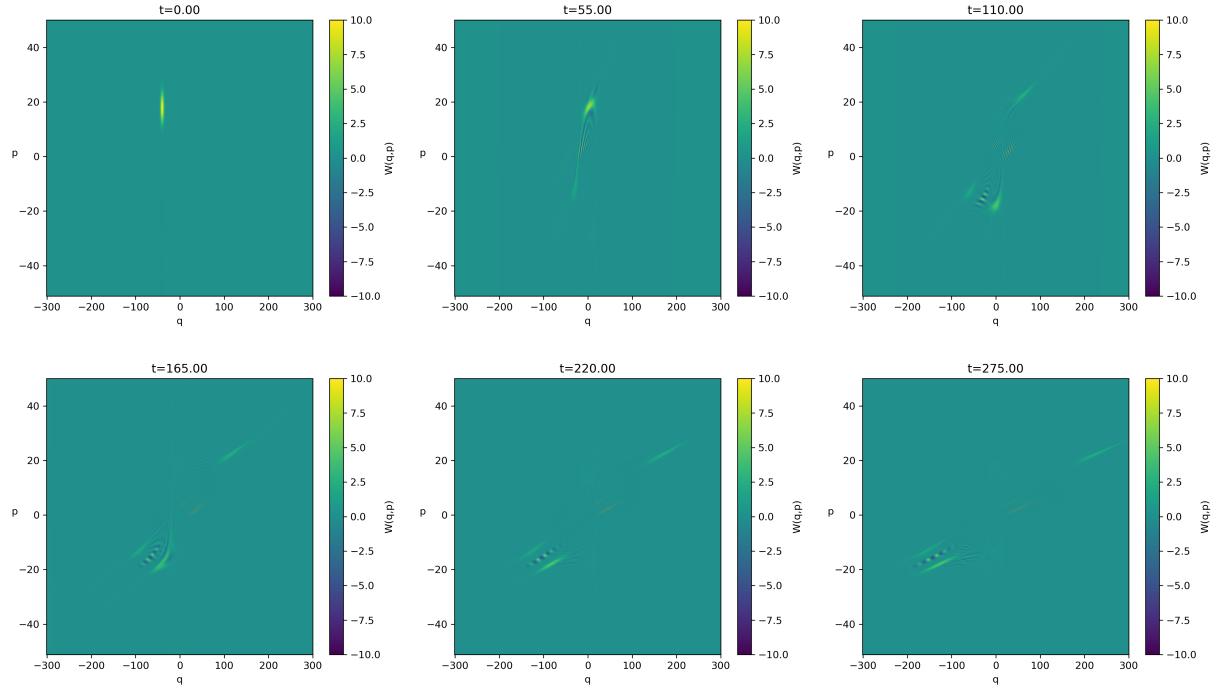


Figure 46: Wigner function snapshots for an unequal double barrier, where $V_0 < E < V_1$.

$E > V_1$

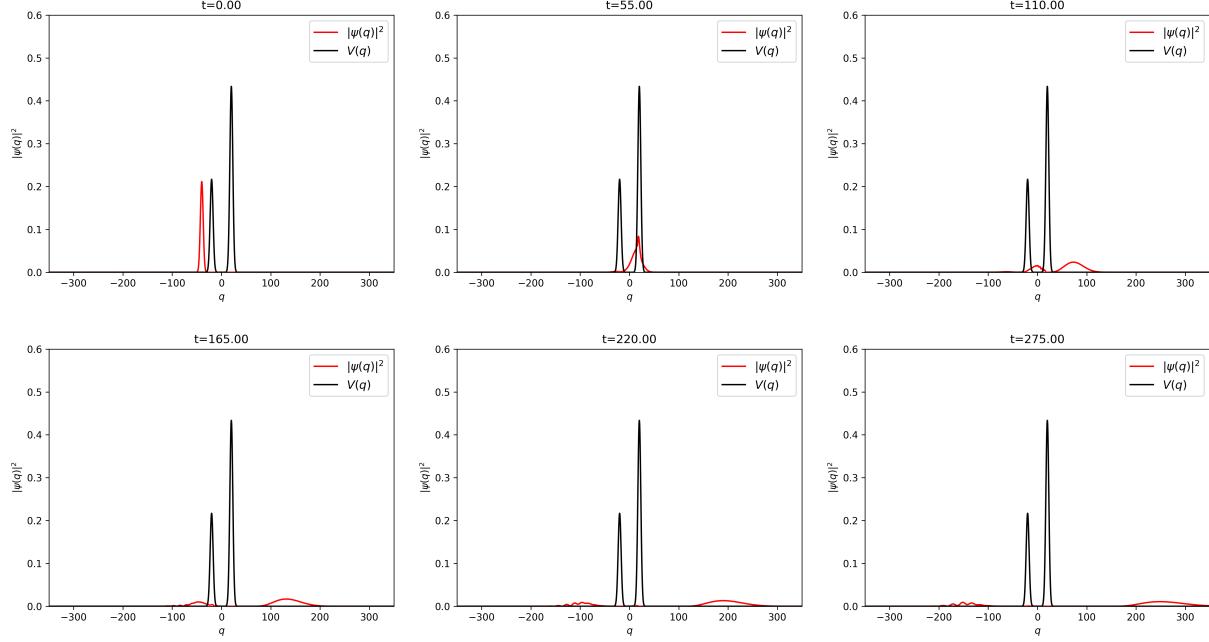


Figure 47: Wave function snapshots where $E > V_1$.

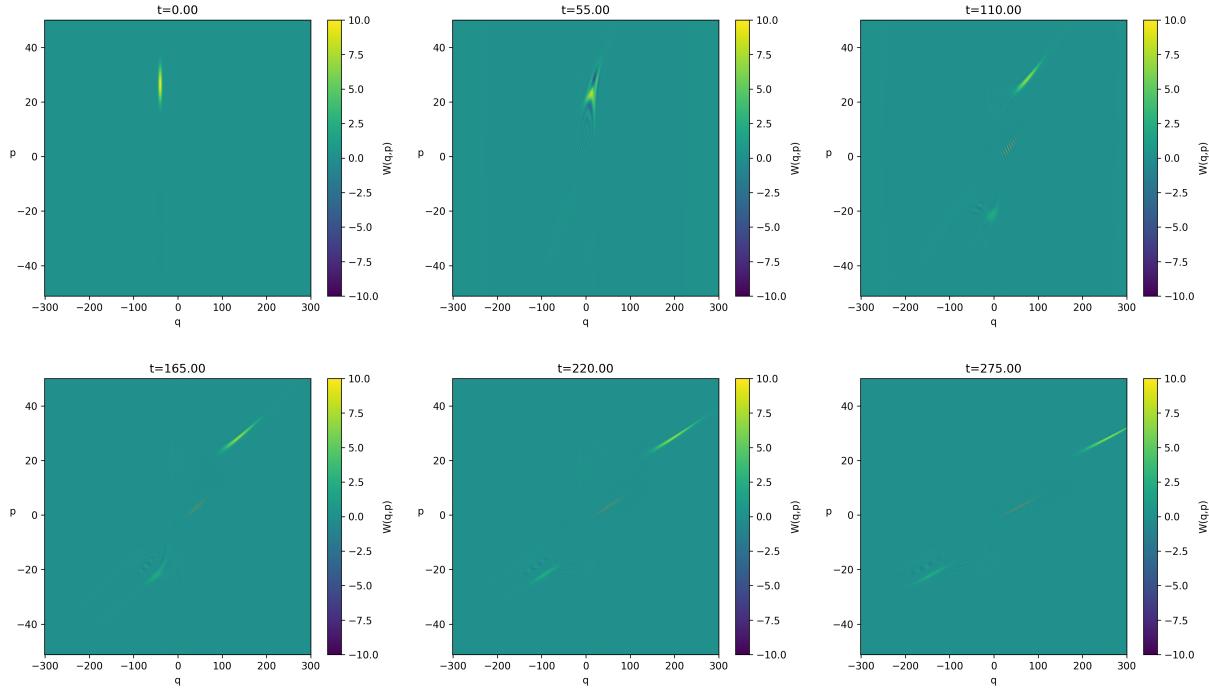


Figure 48: Wigner snapshots for an unequal double barrier where $E > V_1$.

Discussion

Looking at figures 43, 45 and 47, we can see that this situation is similar to, although a bit more interesting than for equal double barriers. Since we have different amounts of reflection and transmission at each barrier, we see oscillatory wave-let structures in the reflected waves due to interference. It is still interesting that these look roughly Gaussian when combined however, so one might expect that they return to a nice looking Gaussian for a large enough t . We can see from Fig. 48, that since the energy is larger than the first barrier, the part that is reflected off the second barrier does not get stuck inside the well. In figure 43 however, since the energy of the wave is much lower than the second barrier, none (or negligible amounts) of the wave gets transmitted through this, and it all eventually gets transmitted back past the first barrier. This scenario is particularly interesting, since we see small wavelet formations of decreasing amplitudes. You could explain these wavelets by considering that the wave in between the potentials oscillates back and forth between them, and while it can't get through the right side, a small amount can be transmitted back through the left side. You can see that these wavelets decrease in amplitude, as less of the wave remains in between the barriers as time goes on. We see something similar happen when the energy is between the barrier, $V_0 < E < V_1$ too.

In Fig. 49, we see the resulting numerical plots for R and T . As one would expect, this looks like the other graphs from the examples above, since more of the wave is transmitted when its energy increases.

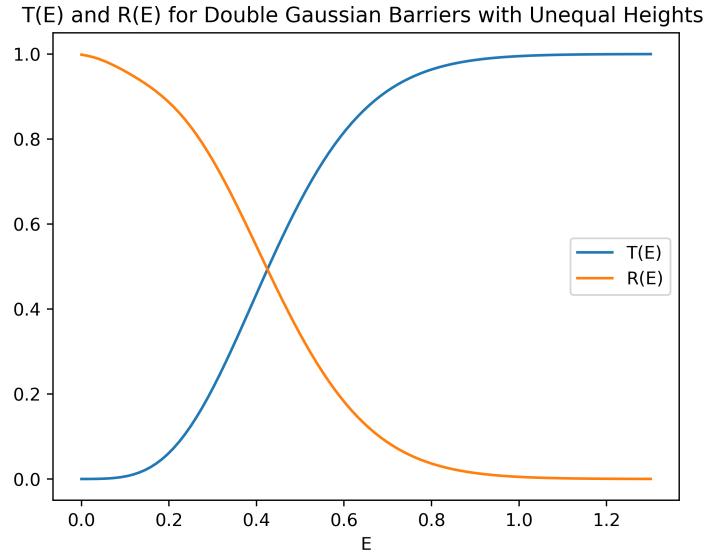


Figure 49: Plots for R and T for an initially Gaussian wave packet interacting with a double barrier - the first peak being smaller than the second.

What we described of the wave function plots above agrees with what we see in the Wigner plots in figures 44, 46 and 48. Just as we saw in the case for equal double barriers, the incoming wave splits at the first barrier, and the resulting transmission splits again at the second barrier. The Wigner plots look interesting due to this, with multiple interference regions between the separate wave forms. This can be seen most clearly in Fig. 46.

Finally, we note how the reflected waveform in the Wigner plot in Fig. 44 when $E < V_0$, compared to the wave forms in the following Wigner plots. This can be explained by the fact that none (or a negligible amount) of the wave is able to pass through the second barrier since the energy of the wave is much smaller than V_1 . This means that all of the wave is eventually reflected back to the left, and thus the wave becomes more spread out due to interaction time. We have discussed a similar thing happening with the Wigner plot in the context of a step potential when the energy of the wave $E < V_0$ in Fig. 24.

7.3 Potential Wells

In the next two examples, we consider potential wells - this is when a wave begins between two barriers. We consider the same combinations of barriers as in the previous section, i.e. one example where the two barriers have equal heights in figures 50 and 51, and one where they have unequal heights in figure 52 and 53. We also only consider the case when the energy of the wave is below the height of the barrier, since this is a more interesting setting to contemplate.

In the first example, the height of the barriers are equal to V_0 , and the energy of the wave is given by $\frac{1}{2}V_0$. In the second example, the height of the smaller barrier is V_0 , while the height of the second barrier is V_1 . We also set the energy of the wave in this case to be $\frac{1}{2}V_0$, thus in both examples, the wave does not have enough energy to overcome any of the barriers, classically speaking. We will see some interesting wave behaviours, as well as some impressive Wigner density plots.

Equal Well

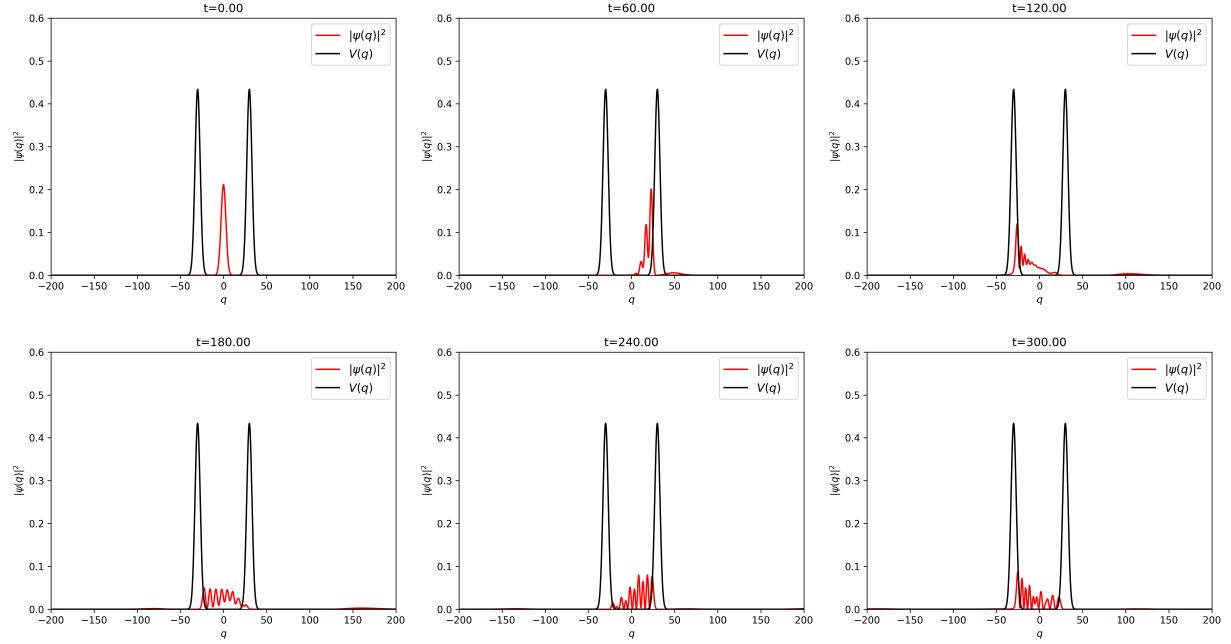


Figure 50: A wave evolving in a well with equal barrier heights.

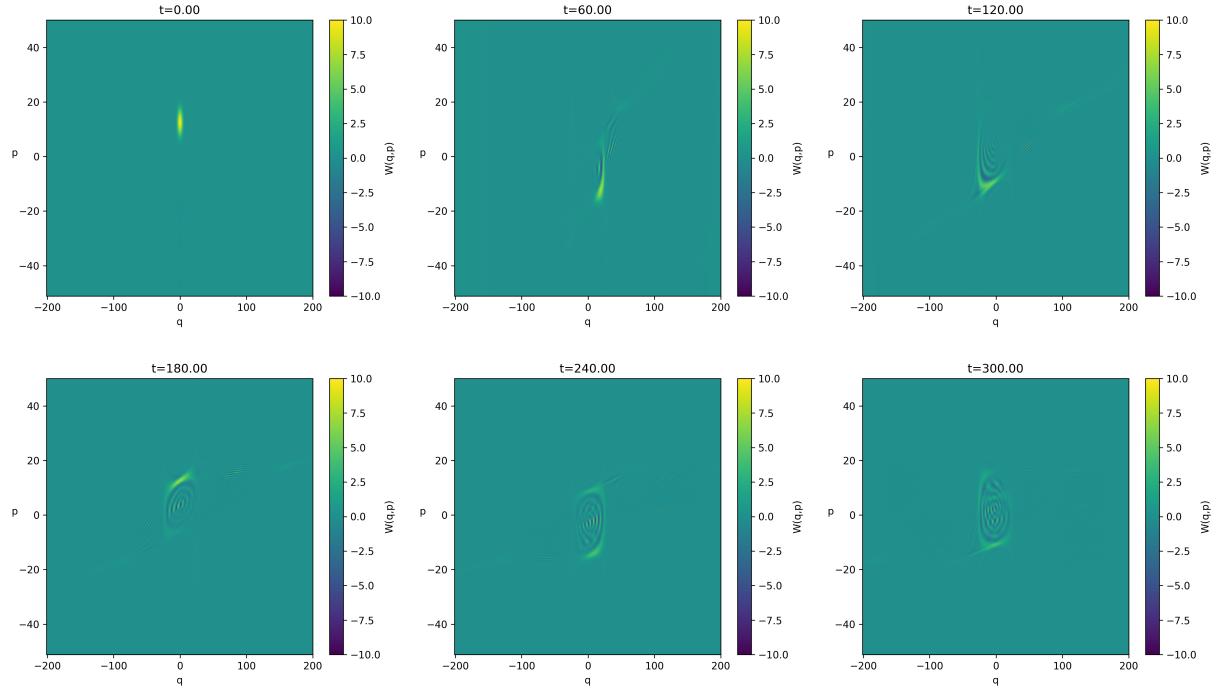


Figure 51: The Wigner plots of a wave evolving in a well with equal barriers.

Unequal Well

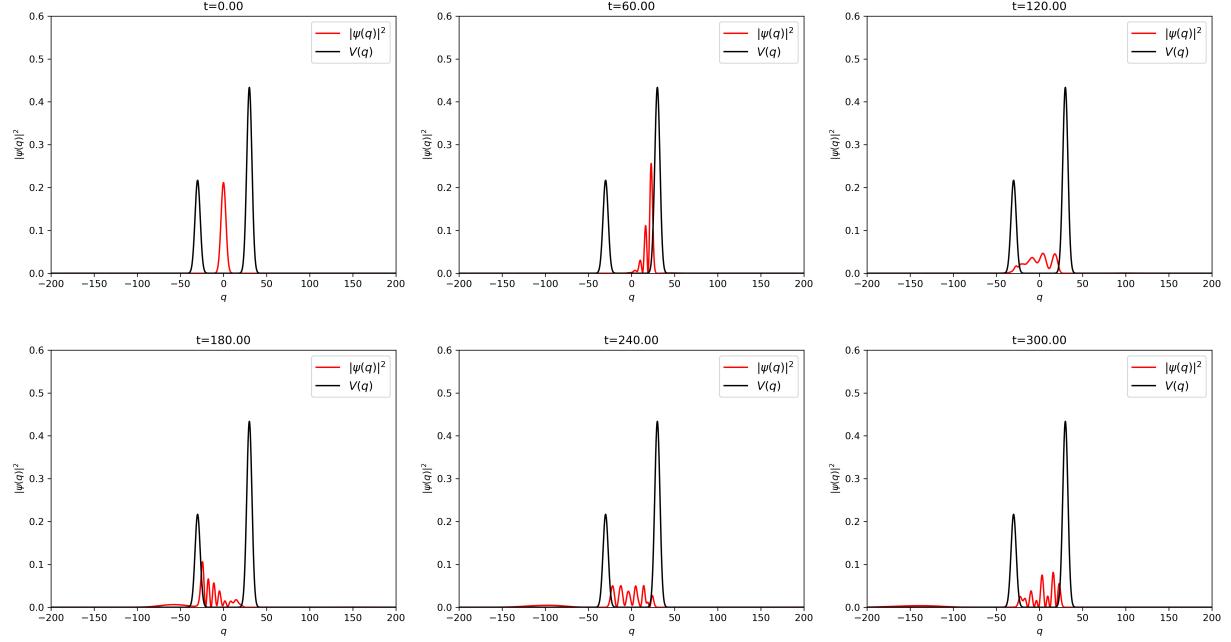


Figure 52: A wave evolving in a well with unequal barrier heights.

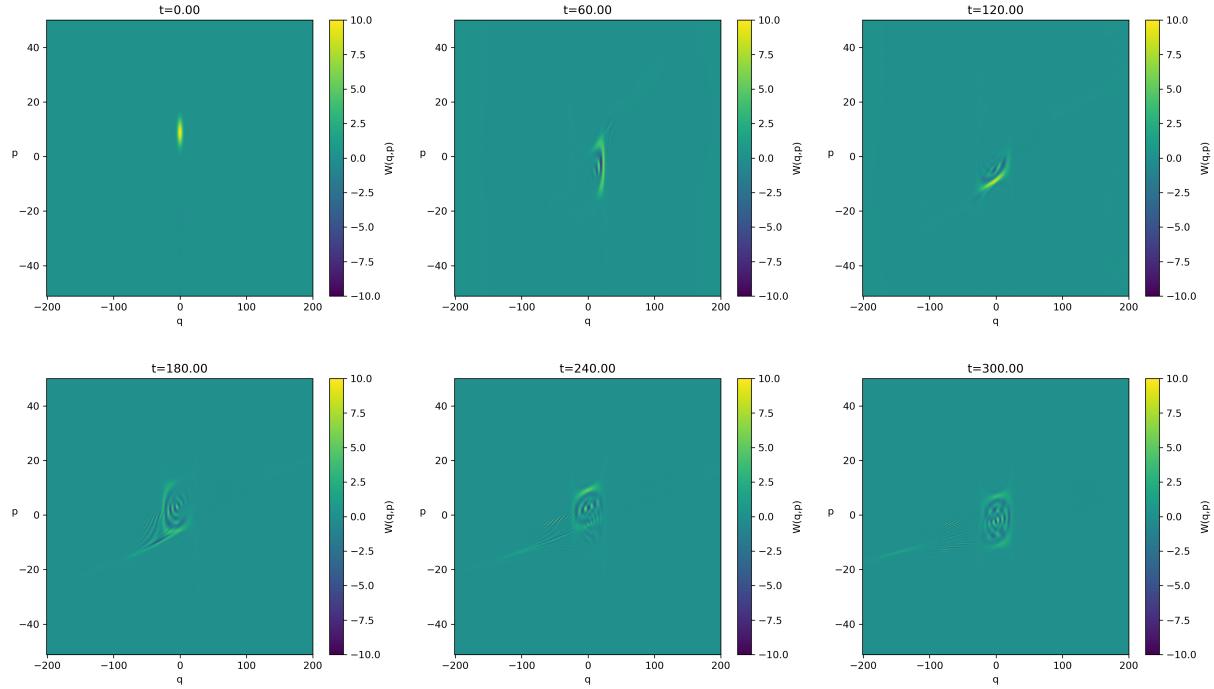


Figure 53: The Wigner plots of a wave evolving in a well with unequal barriers.

Discussion

In the above wave function snapshots, we can see how the state in the wave oscillates back and forth, being reflected off of each barrier. This is slightly more prominent in Fig. 50, since there is an equal amount of reflection at each side, compared to Fig. 52, where there is more transmission when interacting with the smaller barrier. We also see the wave in the well get progressively more oscillatory as time goes on, and this is due to the interference effects between the reflected and transmitted parts of the wave after each interaction. In all the simulations, we have set $\hbar = 1$, however if we were to decrease \hbar , then the wave packets inside the well would stay localised for longer.

The Wigner functions in these examples are especially appealing. In both scenarios, we see nice concentric ring-like structures in the well, which are strikingly similar to Wigner plots you would see for resonance states in bounded potentials (see [24]). These rings tend to do stay perfectly concentric however, and this is due to ‘leakage’ through the barriers at either side, in other words small amounts of the wave are tunneling through the barriers each time the state interacts with them. This would not happen if we were to extend the barrier heights to infinity, and in this case we would expect the concentric rings to remain through time. This is backed up by the fact that the circular patterns are less clear in Fig. 53, with the unequal well, since the amount of tunneling through the left (smaller) barrier is much higher than the amount occurring through the right barrier.

8 Further Topics

In this section we touch on some further ideas that could be explored and built upon with more time. We specifically focus on adapting the WKB approximation introduced in §5.1, and approaching it from a time dependent perspective. For the topics covered, please see chapter 2.4 of [12], as well as [23] and [25].

8.1 Time Dependent WKB

We have seen in §5.1 that the time independent WKB method has very useful implications in areas of quantum mechanics including scattering theory. We now develop some basic WKB theory in the time dependent case, as well as some extensions on the method, which can be applied to more complex scenarios.

Basic Approach

We start off by considering the TISE as in (13),

$$i\hbar \frac{\partial}{\partial t} \psi(q, t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} \psi(q, t) + V(q)\psi(q, t). \quad (113)$$

We use the following Ansatz

$$\psi(q, t) = A(q, t) e^{\frac{i}{\hbar} \phi(q, t)}, \quad (114)$$

where A is the amplitude and ϕ is the phase. These are both real functions and we assume that they vary slowly as in the time independent case. However the i in the exponent means that the wave oscillates, and combined with $\frac{1}{\hbar}$ where \hbar is small, means that the wave oscillates rapidly and this is why the wavelength λ varies faster.

We sub this Ansatz into the Schrödinger equation to get out second order linear differential equation to apply the WKB method to, and we drop the arguments (q, t) for simplicity. First we need to compute

$$\frac{\partial \psi}{\partial q} = A \frac{i}{\hbar} \frac{\partial \phi}{\partial q} e^{\frac{i}{\hbar} \phi} + \frac{\partial A}{\partial q} e^{\frac{i}{\hbar} \phi}$$

and,

$$\begin{aligned} \frac{\partial^2 \psi}{\partial q^2} &= \frac{i}{\hbar} A \frac{\partial \phi}{\partial q} \frac{\partial \phi}{\partial q} \frac{i}{\hbar} e^{\frac{i}{\hbar} \phi} + \frac{i}{\hbar} A \frac{\partial}{\partial q} \left(\frac{\partial \phi}{\partial q} \right) e^{\frac{i}{\hbar} \phi} + \frac{\partial A}{\partial q} \frac{i}{\hbar} \frac{\partial \phi}{\partial q} e^{\frac{i}{\hbar} \phi} + \frac{\partial}{\partial q} \left(\frac{\partial A}{\partial q} \right) e^{\frac{i}{\hbar} \phi} + \frac{i}{\hbar} \frac{\partial A}{\partial q} \frac{\partial \phi}{\partial q} e^{\frac{i}{\hbar} \phi} \\ &= e^{\frac{i}{\hbar} \phi} \left(-\frac{1}{\hbar^2} A \left(\frac{\partial \phi}{\partial q} \right)^2 + \frac{i}{\hbar} A \frac{\partial^2 \phi}{\partial q^2} + \frac{2i}{\hbar} \frac{\partial A}{\partial q} \frac{\partial \phi}{\partial q} + \frac{\partial^2 A}{\partial q^2} \right). \end{aligned}$$

Then, plugging $\frac{\partial^2 \psi}{\partial q^2}$ into (113), we get

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \left(A e^{\frac{i}{\hbar}\phi} \right) &= -\frac{\hbar^2}{2m} e^{\frac{i}{\hbar}\phi} \left(-\frac{1}{\hbar^2} A \left(\frac{\partial \phi}{\partial q} \right)^2 + \frac{i}{\hbar} A \frac{\partial^2 \phi}{\partial q^2} + \frac{2i}{\hbar} \frac{\partial A}{\partial q} \frac{\partial \phi}{\partial q} + \frac{\partial^2 A}{\partial q^2} \right) + V \left(A e^{\frac{i}{\hbar}\phi} \right) \\ \Rightarrow i\hbar \left(A \frac{i}{\hbar} \frac{\partial \phi}{\partial t} e^{\frac{i}{\hbar}\phi} \right) &= \frac{1}{2m} e^{\frac{i}{\hbar}\phi} \left(A \left(\frac{\partial \phi}{\partial q} \right)^2 - i\hbar A \frac{\partial^2 \phi}{\partial q^2} - 2i\hbar \frac{\partial A}{\partial q} \frac{\partial \phi}{\partial q} - \hbar^2 \frac{\partial^2 A}{\partial q^2} \right) + V A e^{\frac{i}{\hbar}\phi} \\ \Rightarrow -A \frac{\partial \phi}{\partial t} e^{\frac{i}{\hbar}\phi} + i\hbar \frac{\partial A}{\partial t} e^{\frac{i}{\hbar}\phi} &= e^{\frac{i}{\hbar}\phi} \left(\frac{1}{2m} A \left(\frac{\partial \phi}{\partial q} \right)^2 + V A \right) \hbar^0 - \frac{i}{2m} e^{\frac{i}{\hbar}\phi} \left(A \frac{\partial^2 \phi}{\partial q^2} + 2 \frac{\partial A}{\partial q} \frac{\partial \phi}{\partial q} \right) \hbar^1 \\ &\quad - \frac{1}{2m} e^{\frac{i}{\hbar}\phi} \left(\frac{\partial^2 A}{\partial q^2} \right) \hbar^2. \end{aligned}$$

We can now collect all the \hbar^0 terms into one equation, and all the higher order \hbar terms into another equation

$$(1) \quad -A \frac{\partial \phi}{\partial t} e^{\frac{i}{\hbar}\phi} = e^{\frac{i}{\hbar}\phi} \left(\frac{1}{2m} A \left(\frac{\partial \phi}{\partial q} \right)^2 + V A \right)$$

$$(2) \quad i \frac{\partial A}{\partial t} e^{\frac{i}{\hbar}\phi} = -\frac{i}{2m} e^{\frac{i}{\hbar}\phi} \left(A \frac{\partial^2 \phi}{\partial q^2} + 2 \frac{\partial A}{\partial q} \frac{\partial \phi}{\partial q} \right) - \frac{1}{2m} e^{\frac{i}{\hbar}\phi} \left(\frac{\partial^2 A}{\partial q^2} \right) \hbar,$$

which implies

$$(1) \quad \frac{1}{2m} \left(\frac{\partial \phi}{\partial q} \right)^2 + V + \frac{\partial \phi}{\partial t} = 0 \tag{115}$$

$$(2) \quad \frac{\partial A}{\partial t} + \frac{1}{2m} A \frac{\partial^2 \phi}{\partial q^2} + \frac{1}{m} \frac{\partial A}{\partial q} \frac{\partial \phi}{\partial q} = \frac{i}{2m} \left(\frac{\partial^2 A}{\partial q^2} \right) \hbar. \tag{116}$$

Note that if we associate ϕ with the action S as we did in the time independent WKB section, then (115) becomes the Hamilton-Jacobi equation as in (7) since $\frac{\partial \phi}{\partial q} = p$ and then

$$\begin{aligned} \frac{1}{2m} \left(\frac{\partial \phi}{\partial q} \right)^2 + V + \frac{\partial \phi}{\partial t} &= 0 \\ \Rightarrow \frac{p^2}{2m} + V + \frac{\partial S}{\partial t} &= 0 \\ \Rightarrow T + V + \frac{\partial S}{\partial t} &= 0 \\ \Rightarrow H + \frac{\partial S}{\partial t} &= 0, \end{aligned}$$

where we have used that $T = \frac{p^2}{2m}$ where T is kinetic energy, and $H = T + V$, where H is the Hamiltonian.

Now in standard WKB approximation we assume we take the semi-classical limit, $\hbar \rightarrow 0$. Thus we set the right hand side of (116) to be 0. Then (116) becomes

$$\frac{\partial A}{\partial t} + \frac{1}{2m} A \frac{\partial^2 \phi}{\partial q^2} + \frac{1}{m} \frac{\partial A}{\partial q} \frac{\partial \phi}{\partial q} = 0, \quad (117)$$

which is the transport equation [23]. Solving (115) and (117) will give us a solution for A and ϕ , however these solutions do not usually have explicit expression that we can show here.

Advanced Approach

A more advanced WKB approach is to semi-classically expand A into a power series of \hbar :

$$A = A_0 + A_1 \hbar + A_2 \hbar^2 + \dots + A_k \hbar^k.$$

Then we can plug this into equation (116) and solve for each A_i :

$$\begin{aligned} \frac{\partial A_0}{\partial t} + \frac{1}{2m} \left(A_0 \frac{\partial^2 \phi}{\partial q^2} + 2 \frac{\partial A_0}{\partial q} \frac{\partial \phi}{\partial q} \right) &= \frac{i}{2m} \frac{\partial^2 A_0}{\partial q^2} \hbar \\ \frac{\partial A_1}{\partial t} \hbar + \frac{1}{2m} \left(A_1 \frac{\partial^2 \phi}{\partial q^2} + 2 \frac{\partial A_1}{\partial q} \frac{\partial \phi}{\partial q} \right) \hbar &= \frac{i}{2m} \frac{\partial^2 A_1}{\partial q^2} \hbar^2 \\ &\vdots && \vdots \\ \frac{\partial A_k}{\partial t} \hbar^k + \frac{1}{2m} \left(A_k \frac{\partial^2 \phi}{\partial q^2} + 2 \frac{\partial A_k}{\partial q} \frac{\partial \phi}{\partial q} \right) \hbar^k &= \frac{i}{2m} \frac{\partial^2 A_k}{\partial q^2} \hbar^{k+1}, \end{aligned}$$

and then once again we can equate \hbar terms

$$\begin{aligned} \frac{\partial A_0}{\partial t} + \frac{1}{2m} \left(A_0 \frac{\partial^2 \phi}{\partial q^2} + 2 \frac{\partial A_0}{\partial q} \frac{\partial \phi}{\partial q} \right) &= 0 \\ \frac{\partial A_1}{\partial t} + \frac{1}{2m} \left(A_1 \frac{\partial^2 \phi}{\partial q^2} + 2 \frac{\partial A_1}{\partial q} \frac{\partial \phi}{\partial q} \right) &= \frac{i}{2m} \frac{\partial^2 A_0}{\partial q^2} \\ &\vdots && \vdots \\ \frac{\partial A_k}{\partial t} + \frac{1}{2m} \left(A_k \frac{\partial^2 \phi}{\partial q^2} + 2 \frac{\partial A_k}{\partial q} \frac{\partial \phi}{\partial q} \right) &= \frac{i}{2m} \frac{\partial^2 A_{k-1}}{\partial q^2}. \end{aligned}$$

Note that we can stop at A_k as the remainder term will be $\mathcal{O}(\hbar^k)$, which will be very small if \hbar is small. These equations give us our solutions, and as above, we cannot write explicit equations for A and ϕ .

It's important to note that this method only works if $\frac{\partial^2 A}{\partial q^2}$ is not large, an assumption we can make in the time independent WKB section as well. The situation where $\frac{\partial^2 A}{\partial q^2}$ is large can be read about in an adapted approach in [23]. The ideas in this paper are beyond the scope of this project, since more geometrical theory is required. Some of the ideas however are relevant to the interaction picture mentioned in §2.2.2. The methods we have covered so far in this section are a basis for further development, seen in [23].

9 Conclusion

In conclusion, this project has covered some fundamental theories in quantum mechanics, and used these to build a detailed overview of different methods which explain quantum propagation techniques. We have shown this both numerically and analytically, and further, how these different approaches match up to support the same theories. Moreover, we have utilised these methods to build pictures of different scenarios, to further support theoretical claims and to gain additional insight into the behaviours of sub atomic particles. Covered within these methods are some fascinating quantum phenomena, such as superposition and scattering, which includes reflection and tunneling effects.

One key takeaway from this report is that wave packet propagation is an essential tool for understanding how quantum particles behave under different conditions. Whether we are studying atoms in a laboratory or trying to develop new technologies based on quantum computing or cryptography, our ability to simulate wave packet propagation accurately will be critical in the future.

10 Appendix

In this section we detail the code written for this project. The following code was used to create all the wave animation snapshots and the Wigner function animation snapshots in §7. The code for the different variables for each example can be found on my GitHub [26] in the ‘Quantum_Wave_Propagation’ repository in the ‘Final_Results’ notebook. We can also see all the animations in video format in the same repository under ‘README.md’. After this in 10.3, we show code used to create some of the other figures throughout the project.

10.1 Evolving and Animating Wave Packets

Here is the code create the Schrödinger class where all the wave evolution takes place.

```
#code modified from Jake Vanderplas
#email: vanderplas@astro.washington.edu
#github: http://jakevdp.github.com
#modifications made by Jess Winerborne
#github: https://github.com/JessWinterborne
#license: BSD
#free use and modification is allowed if the above information is
#retained

import numpy as np
import os
from matplotlib import pyplot as plt
from matplotlib import animation
from scipy.fftpack import fft,ifft
from matplotlib import rc
rc('animation', html='jshtml')

class Schrodinger:
    def __init__(self, x, psi_x0, V_x, k0 = None, hbar = 1, m=1, t0=0.0):
        #x = xaxis array of length N giving position
        #V_x = yaxis array of length N giving potential
        #psi_x0 = array of length N giving intial wave function at t0
        #k0 gives the minimumum value of the momentum over hbar
        #there are some constraints on this due to the FFT: k0<k<2pi/dx
        #where dx = x[1]-x[0]
        #default hbar = 1 and mass = 1 and initial time = 0
        self.x, psi_x0, self.V_x = map(np.asarray, (x, psi_x0, V_x))
        N = self.x.size
        assert self.x.shape == (N,)
        assert psi_x0.shape == (N,)
        assert self.V_x.shape == (N,)
        self.hbar = hbar
        self.m = m
        self.t = t0
        self.dt_ = None
        self.N = len(x)
```

```

        self.dx = self.x[1] - self.x[0]
        #setting the pos steps (similar to doing dx = b-a/N as
        #coordinates are evenly spaced)
        self.dk = 2 * np.pi / (self.N * self.dx)
        #dk = 2pi/Ndx (do this so FFT looks like continuous fourier
        #transform)
        #dk = 2pi/b-a

        if k0 == None:
            self.k0 = -0.5 * self.N * self.dk
        else:
            self.k0 = k0
        self.k = self.k0 + self.dk * np.arange(self.N)
        # k = k0 + dk
        self.psi_x = psi_x0
        self.psi_x = psi_x0

        #variables which hold steps in evolution
        self.x_evolve_half = None
        self.x_evolve = None
        self.k_evolve = None

        #attributes used for dynamic plotting
        self.psi_x_line = None
        self.psi_k_line = None
        self.V_x_line = None

    def _set_psi_x(self, psi_x):
        #brings it back to the original continuous version of psi(x)
        self.psi_discrete_x = (psi_x * np.exp(-1j * self.k[0] * self.x) *
                               self.dx / np.sqrt(2 * np.pi))
                               ))

    def _get_psi_x(self):
        #gives the discrete version of psi needed for the FFT
        return(self.psi_discrete_x * np.exp(1j * self.k[0] * self.x) * np.
               .sqrt(2 * np.pi) / self.dx)

#     def _set_psi_k(self, psi_k):
#         self.psi_mod_k = psi_k * np.exp(1j * self.x[0] * self.dk * np.
#                                         arange(self.N))

#     def _get_psi_k(self):
#         return self.psi_mod_k * np.exp(-1j * self.x[0] * self.dk * np.
#                                         arange(self.N))
# #can uncomment this stuff if we want to animate in momentum space too

    def _get_dt(self):
        return self.dt_

```

```

def _set_dt(self, dt):
    #how we evolve psi - half steps in position space and full steps
    #in momentum space
    #as we will see in the strang splitting method below
    if dt != self.dt_:
        self.dt_ = dt
        self.x_evolve_half = np.exp(-0.5 * 1j * self.V_x / self.hbar
                                     * dt)
        self.k_evolve = np.exp(-0.5 * 1j * self.hbar / self.m * (self
          .k * self.k) * dt)

psi_x = property(_get_psi_x, _set_psi_x)
# psi_k = property(_get_psi_k, _set_psi_k)
dt = property(_get_dt, _set_dt)
#dont really understand property functions well
#from what I understand, property assigns getter and setter functions
#to a variable

def time_step(self, dt, Nsteps = 1):
    self.dt = dt

    #strang splitting:
    for i in range(Nsteps):
        #half step in position:
        self.psi_discrete_x *= self.x_evolve_half
        #FFT
        self.psi_discrete_k = fft(self.psi_discrete_x)
        #full step in momentum
        self.psi_discrete_k *= self.k_evolve
        #iFFT
        self.psi_discrete_x = ifft(self.psi_discrete_k)
        #half step in position
        self.psi_discrete_x *= self.x_evolve_half

    self.t += dt * Nsteps
    #t = t + Nsteps*dt

def gauss_x(x, a, x0, k0):
    #wave with width a, centred at x0 with momentum k0
    return((a * np.sqrt(np.pi)) ** (-0.5) * np.exp(-0.5 * ((x - x0) * 1.
      / a) ** 2 + 1j * x * k0))
    #this is just a standard gaussian function

def gauss_k(k, a, x0, k0):
    #analytical (?) fourier transform of the gaussian in x above
    return ((a / np.sqrt(np.pi))** 0.5 * np.exp(-0.5 * (a * (k - k0)) **
      2 - 1j * (k - k0) * x0))

```

This is an example of some of the variables that we can change

```

#specify x grid
N = 2 ** 11 #2048
dx = 0.1
x = dx * (np.arange(N) - 0.5 * N)
dy = dx
y = x

#potential barrier
def gauss_barrier(x, a, x0):
    x = np.asarray(x)
    return (a * np.sqrt(np.pi))** (-0.5) * np.exp(-0.5 * ((x - x0)*1./a)
                                                   ** 2)

V_x = gauss_barrier(x, 3, 0)
V0 = np.max(V_x)

#potential 'walls' at either end
V_x[x < -98] = 1E6
V_x[x > 98] = 1E6

#variables
dt = 0.01
N_steps = 50
t_max = 200
frames = 151

#specifying constants
hbar = 1.0
m = 1.0 #mass
p0 = np.sqrt(2 * m * V0) #initial momentum
k0 = p0 / hbar #initial wave number
v0 = p0 / m #initial velocity
d = 4.0 #initial width of wavepacket
x0 = -20 #initial centre of wavepacket
k0_ft_y = -np.pi / dy

#wavefunction
def gauss_x(x, a, x0, k0):
    #wave with width a, centred at x0 with momentum k0
    return((a * np.sqrt(np.pi)) ** (-0.5) * np.exp(-0.5 * ((x - x0) * 1.
                                                               / a) ** 2 + 1j * x * k0))

psi_x0 = gauss_x(x, d, x0, k0)

#creating the schrodinger object
S = Schrodinger(x=x, psi_x0=psi_x0, V_x=V_x, hbar=hbar, m=m, k0=-28)

```

Here is a function to automate saving the individual frames and the whole animation.

```
def save_wave(xlim, ylim, S, frames, dt, N_steps, name, scaling, save =
```

```

        True):
fig = plt.figure(dpi=300)
ax = fig.add_subplot(111, xlim=xlim, ylim=ylim)
#have subplot so we can add in a plot for the momentum if we wanted (
#see below)
psi_x_line, = ax.plot([], [], c='r', label=r'$|\psi(q)|^2$')
# psi_k_line, = ax2.plot([], [], c='r', label=r'$|\psi(k)|$')
V_x_line, = ax.plot([], [], c='k', label=r'$V(q)$')
title = ax.set_title('')
ax.legend(prop = dict(size=12))
ax.set_xlabel('$q$')
ax.set_ylabel(r'$|\psi(q)|^2$')
V_x_line.set_data(S.x, S.V_x)
def init():
    psi_x_line.set_data([], [])
    V_x_line.set_data([], [])
    return (psi_x_line, V_x_line)
if save == True:
    try:
        os.mkdir(os.path.join(os.getcwd(), 'wave_frames'))
    except FileExistsError:
        print("Frames folder found, overwritting")
def animate(i):
    psi_x_line.set_data(S.x, scaling*abs(S.psi_x)**2)
    #factor in front just scales the wave function up
    V_x_line.set_data(S.x, S.V_x)
    title.set_text('t=% .2f' % S.t)
    if save == True:
        plt.savefig('wave_frames/wave_frame=%2f.png'%i)
S.time_step(dt, N_steps)
return (psi_x_line, V_x_line)

anim = animation.FuncAnimation(fig, animate, init_func=init, frames=
                               frames, interval=40, blit=True)
if save == True:
    anim.save(name+'.mp4')
else:
    return(anim)

```

To use this all you would have to do is run something along the lines of this.

```

#saving the wave animation
xlim = (-75, 85)
ylim = (0,0.6)
save_wave(xlim=xlim, ylim=ylim, S=S, frames=frames, dt=dt, N_steps=
          N_steps, name='single_barrier_equal',
          scaling = 1.5, save=True)

```

10.2 Plotting, Evolving and Animating the Wigner Function

Here we have a function which plots the Wigner function.

```
import numpy as np
import os
from matplotlib import pyplot as plt, cm, colors
from scipy.fftpack import fft, ifft
from scipy.ndimage import shift

def wigner_plot(psi_x0, x, y, dx, dy, k0_ft_y, t_max, view, limit, xmin,
                xmax, save_fig = False, frame_num = None, density = True, surface =
                False):
    if save_fig == True:
        assert frame_num is not None, "Please provide framenumber if
                                        saving"

    x, y = map(np.asarray, (x, y))

    #getting rid of for loops could be one way of speeding it up

    #setting the values of psi(x+y)
    psi_x0_plus = np.zeros((len(y), len(x)), dtype=complex)
    for i in range(len(y)):
        psi_x0_plus[i][:] = shift(psi_x0, int(-1/dy)*y[i], cval=0.0)

    #setting the values of psi*(x-y)
    psi_x0_minus = np.zeros((len(y), len(x)), dtype=complex)
    for i in range(len(y)):
        psi_x0_minus[i][:] = np.conjugate(shift(psi_x0, int(1/dy)*y[i],
                                                cval=0.0))

    #multiplying the two wavefunction together so our function is of the
    #form psi(x+y)psi*(x-y)
    wigner_to_transform = np.multiply(psi_x0_plus, psi_x0_minus)

    #discretising the function so we can fourier transform correctly
    discrete_wigner_to_tranform = np.zeros((len(y), len(x)), dtype =
                                            complex)
    for i in range(len(y)):
        discrete_wigner_to_tranform[i][:] = wigner_to_transform[i] * np.
            exp(-1j * k0_ft_y * y[i]) *
            dy / np.sqrt(2 * np.pi)

    #fast fourier transforming
    discrete_fourier_wigner = fft(discrete_wigner_to_tranform, axis = 0)

    #un-discretising the function
    wigner = np.zeros((len(y), len(x)), dtype = complex)
    for i in range(len(y)):
        wigner[i][:] = (discrete_fourier_wigner[i] * np.exp(1j * k0_ft_y
```

```

* y[i]) * np.sqrt(2 * np.pi)
/ dy)

#checking all the values of the wigner function are real:
assert np.allclose(wigner.imag, 0, rtol=0, atol=1e-9), 'wigner has
non-zero imaginary components'

wigner = np.real(wigner)

#creating a folder for the frames
#we will use these frames to animate
if save_fig == True and frame_num == 0:
    try:
        os.mkdir(os.path.join(os.getcwd(), 'wigner_frames'))
    except FileExistsError:
        print("Frames folder found, overwritting")

#plotting:

#3D surface plot
if surface:
    fig = plt.figure(figsize=(8,6))
    ax = fig.add_subplot(111, projection='3d')
    y_smaller = y[int(79*(1/dy)):int(-80*(1/dy))]
    x_smaller = x[int((99+xmin)*(1/dx)):int(-(100-xmax)*(1/dx))]
    X, Y = np.meshgrid(x_smaller,y_smaller)
    Z = wigner[int(79*(1/dy)):int(-80*(1/dy)),int((99+xmin)*(1/dx)) :
               int(-(100-xmax)*(1/dx))]
    ax.set_zlim3d(-limit, limit)
    ax.set_zticks(np.arange(-limit, limit+1, 5.0))
    ax.set_xlabel('q')
    ax.set_ylabel('p')
    ax.set_zlabel('W(q,p)')
    if frame_num is not None:
        if frame_num == 0:
            ax.set_title('t=%.2f' %(0))
        else:
            ax.set_title('t=%.2f' %(100*(int(frame_num)/int(t_max))))
    surf = ax.plot_surface(X,Y,Z)
    # fig.colorbar(surf, shrink = 0.25)
    ax.view_init(azim = view)

    #saving the frame
    if save_fig == True:
        plt.savefig(f'wigner_frames/3d_{frame_num}', dpi=300)
        plt.close(fig)

#density plot
if density:
    fig = plt.figure(figsize=(6,5))
    y_smaller = y[int(79*(1/dy)):int(-80*(1/dy))]

```

```

x_smaller = x[int((99+xmin)*(1/dx)):int(-(100-xmax)*(1/dx))]
X, Y = np.meshgrid(x_smaller,y_smaller)
Z = wigner[int(79*(1/dy)):int(-80*(1/dy)),int((99+xmin)*(1/dx)):
            int(-(100-xmax)*(1/dx))]
plt.pcolormesh(X, Y, Z, shading='auto')
plt.clim(-limit, limit)
cbar = plt.colorbar()
cbar.set_label('W(q,p)')
plt.xlabel('q')
plt.ylabel('p', rotation = 0)
if frame_num is not None:
    if frame_num == 0:
        plt.title('t=%.2f' %(0))
    else:
        plt.title('t=%.2f' %(100*(int(frame_num)/int(t_max))))
#saving the frame
if save_fig == True:
    plt.savefig(f'wigner_frames/density_{frame_num}', dpi=300)
    plt.close(fig)
else:
    plt.show()

```

In order to plot the time evolution of the wave function, we use the Schrödinger class from earlier and use this loop.

```

#creating the wigner plot frames
#we can do either the desnity plot, or the surface plot, or both
xmin = -75
xmax = 85
psi_x0_input = psi_x0
for frame in range(frames):
    S = Schrodinger(x=x, psi_x0=psi_x0_input, V_x=V_x, hbar=hbar, m=m, k0
                    =-28.0)
    wigner_plot(psi_x0_input, x, y, dx, dy, k0_ft_y, t_max, view = 230,
                limit = 10, xmin = xmin, xmax =
                xmax, save_fig = True, frame_num
                = frame, density = True,
                surface = False)
    S.time_step(dt, N_steps)
    psi_x0_input = S.psi_x

```

Here we have a function that takes the Wigner frames that have been saved and animates them.

```

import cv2
import os

def anim_wigner(density = True, surface = False):
    path = os.path.join(os.getcwd(),'wigner_frames')

```

```

if density:
    # Get images in each folder
    density_files_unsorted = [os.path.join(path,f) for f in os.listdir(path) if (f.endswith('.png') and f.startswith('density'))]
    # Sort frames in correct order (0,1,2...10,11) instead of (0,1,10,11..2,20)
    density_dict = {}

    for img_file in density_files_unsorted:
        frame_number = int(os.path.basename(str(img_file)).split('_')[-1].split('.')[0])
        density_dict[frame_number] = img_file

    density_files = [value for key,value in sorted(density_dict.items())]

    # Create video writers
    fps = 25
    fourcc = cv2.VideoWriter_fourcc(*'mp4v')
    density_frame_size = cv2.imread(density_files[0]).shape[:2]

    # Reverse shape tuple order from (height,width) to (width,height)
    density_frame_size = density_frame_size[::-1]

    density_out = cv2.VideoWriter('density.mp4', fourcc, fps,
                                  density_frame_size)

    # Loop through each frame
    for i in range(len(density_files)):
        density_img = cv2.imread(density_files[i])
        density_out.write(density_img)

    density_out.release()
    cv2.destroyAllWindows()

if surface:
    surface_files_unsorted = [os.path.join(path,f) for f in os.listdir(path) if (f.endswith('.png') and f.startswith('3d'))]
    surface_dict = {}

    for img_file in surface_files_unsorted:
        frame_number = int(os.path.basename(str(img_file)).split('_')[-1].split('.')[0])
        surface_dict[frame_number] = img_file

    surface_files = [value for key,value in sorted(surface_dict.items())]

```

```
fps = 25
fourcc = cv2.VideoWriter_fourcc(*'mp4v')

surface_frame_size = cv2.imread(surface_files[0]).shape[:2]

surface_frame_size = surface_frame_size[::-1]

surface_out = cv2.VideoWriter('3d.mp4', fourcc, fps,
                             surface_frame_size)

for i in range(len(surface_files)):
    surface_img = cv2.imread(surface_files[i])
    surface_out.write(surface_img)

surface_out.release()
cv2.destroyAllWindows()
```

10.3 Figures

All figures in this project have been generated by myself in Python. The figures that required non trivial calculations are detailed below.

Reflection and Transmission Rectangular Barrier

Code to create Fig. 11.

```
import numpy as np
import matplotlib.pyplot as plt

x = np.linspace(0.1, 10, 1000)
#x plays the role of E, so x>=0

def transmission(x,a,V0):
    y = np.zeros(len(x))
    for i in range(len(x)):
        if x[i] == V0:
            y[i] = (1+((a**2)*V0)*0.5)**(-1)
        if x[i]>V0:
            y[i] = (((V0**2)*(np.sin((np.sqrt(2*(x[i]-V0)))*a))**2)*(4*x[i]*(x[i]-V0))**(-1)+1)**(-1)
        if x[i]<V0:
            y[i] = (((V0**2)*(np.sinh((np.sqrt(2*(V0-x[i])))*a))**2)*(4*x[i]*(V0-x[i]))**(-1)+1)**(-1)
    return y

def reflection(t):
    y = np.ones(len(t))
    return y - t

#graph number 1
T = transmission(x,1,1.5)
R = reflection(T)

plt.plot(x,T, label='T(E)')
plt.plot(x,R, label='R(E)')
plt.title('T(E) and R(E) for $a=1$ and $V_{0} = 1.5$')
plt.xlabel('E')
plt.legend()
plt.savefig('RandT1', dpi=500)

#graph number 2
T = transmission(x,2,1.5)
R = reflection(T)

plt.plot(x,T, label='T(E)')
plt.plot(x,R, label='R(E)')
plt.title('T(E) and R(E) for $a=2$ and $V_{0} = 1.5$')
```

```

plt.xlabel('E')
plt.legend()
plt.savefig('RandT2', dpi=500)

#graph number 3
T = transmission(x,3,1.5)
R = reflection(T)

plt.plot(x,T, label='T(E)')
plt.plot(x,R, label='R(E)')
plt.title('T(E) and R(E) for $a=3$ and $V_{0} = 1.5$')
plt.xlabel('E')
plt.legend()
plt.savefig('RandT3', dpi=500)

```

Airy Functions

Code to create Fig. 13.

```

import numpy as np
from scipy import special
import matplotlib.pyplot as plt

x = np.linspace(-10, 5, 201)
ai, aip, bi, bip = special.airy(x)

plt.plot(x, ai, 'r', label='Ai(q)')
plt.plot(x, bi, 'b--', label='Bi(q)')
plt.ylim(-0.5, 1.0)
plt.grid()
plt.title('Airy Functions of the First and Second Kind')
plt.axhline(0,color='black')
plt.axvline(0,color='black')
plt.xlabel('q')
# plt.ylabel('y', rotation=0)
plt.legend(loc='upper left')
# plt.show()
plt.savefig('airy.png', dpi = 500)

```

Asymptotic Airy Functions

Code to create Fig. 15.

```

import numpy as np
from scipy import special
import matplotlib.pyplot as plt

#airy function of the first kind

x = np.linspace(-10, 5, 201)
ai, aip, bi, bip = special.airy(x)

```

```

def airyexp(x):
    y = np.zeros(len(x))
    for i in range(len(x)):
        if x[i] == 0:
            y[i] = float('inf')
        if x[i] > 0 :
            y[i] = np.exp(-(x[i])**1.5 / 1.5) / (2 * np.sqrt(np.pi) * (x[i])**0.25)
        if x[i]<0:
            y[i] = np.sin((-x[i])**1.5 / 1.5 + np.pi/4) / (np.sqrt(np.pi) * (-x[i])**0.25)
    return y

y1 = airyexp(x)

plt.plot(x, ai, c='r', label = 'Ai(q)')
plt.plot(x, y1, c='m', linestyle = 'dashed', label = 'Asymptotic Expansion')
plt.ylim(-0.75, 1.6)
plt.grid()
plt.title('Ai(q) Plotted Against its Asymptotic Expansion')
plt.axhline(0,color='black')
plt.axvline(0,color='black')
plt.xlabel('q')
# plt.ylabel('y', rotation=0)
plt.legend()
# plt.show()
plt.savefig('ai_asymptotic.png', dpi = 500)

#airy function of the second kind

x = np.linspace(-10, 3, 201)
ai, aip, bi, bip = special.airy(x)

def bairyexp(x):
    y = np.zeros(len(x))
    for i in range(len(x)):
        if x[i] == 0:
            y[i] = float('inf')
        if x[i] > 0 :
            y[i] = np.exp(x[i]**1.5 / 1.5) / (np.sqrt(np.pi) * x[i]**0.25)
        if x[i]<0:
            y[i] = np.cos((-x[i])**1.5 / 1.5 + np.pi/4) / (np.sqrt(np.pi) * (-x[i])**0.25)
    return y

y2 = bairyexp(x)

plt.plot(x, bi, c='b', label = 'Bi(q)')
plt.ylim(-0.75, 1.9)

```

```

plt.plot(x, y2, c='m', linestyle = 'dashed', label = 'Asymptotic Expansion')
plt.grid()
plt.title('Bi(q) Plotted Against its Asymptotic Expansion')
plt.axhline(0,color='black')
plt.axvline(0,color='black')
plt.xlabel('q')
# plt.ylabel('y', rotation=0)
plt.legend()
# plt.show()
plt.savefig('bi_asymptotic.png', dpi = 500)

```

Linear Potential for Connection Formulae

Code to create Fig. 16 and Fig. 17.

```

#turning point at a

import numpy as np
import matplotlib.pyplot as plt

# Define the logistic function
def logistic(x):
    return 1 / (1 + np.exp(-(3*x)))

# Define the x values to plot
x = np.linspace(-5, 5, 1000)

# Calculate the y values using the logistic function
y = logistic(x)

for i in range(len(x)):
    if x[i]<-1:
        y[i] = np.nan
    if x[i]>1:
        y[i]= np.nan

# print(logistic(0,L,k,x0))

def derivative(x):
    return (3*np.exp(-3*x))/((1+np.exp(-3*x))**2)

y2 = logistic(0) + derivative(0)*x

for i in range(len(x)):
    if x[i]<-1.5:
        y2[i] = np.nan
    if x[i]>1.5:
        y2[i] = np.nan

ymax = np.nanmax(y)
ymin =np.nanmin(y)

```

```

# Plot the logistic curve
plt.figure(figsize=(9,6))
plt.plot(x,y2, label='Linear Potential')
plt.plot(x, y, label='Potential')
plt.xlim(-0.75, 0.75)
plt.ylim(ymin, ymax)

# Set the axis labels and title
# plt.xlabel('q')
# plt.ylabel('y')
plt.title('Region of Gaussain Potential Around Turning Point at a')

plt.tick_params(axis='y',which='both',bottom=False, left=False,top=False,
                labelleft=False, )
plt.tick_params(axis='x',which='both',bottom=False, left=False,top=False,
                labelbottom=False,)

plt.axhline(0.5, -0.5, 0.5, color='forestgreen', linestyle='--')
plt.text(-0.8, 0.49, 'E', color='forestgreen', fontsize=12)

plt.axvline(0, 0, 0.5, color='forestgreen', linestyle='--')
plt.text(-0.01, 0, 'a', color='forestgreen', fontsize=12)

plt.axvline(-0.3, 0, 1, color='mediumpurple', linestyle='--')
plt.axvline(0.3, 0, 1, color='mediumpurple', linestyle='--')

plt.legend(loc='center right')

# Show the plot
# plt.show()
plt.savefig("wkb_airy_connection_a.png",dpi=500)

#turning point at b

import numpy as np
import matplotlib.pyplot as plt

# Define the logistic function
def logistic(x):
    return 1 / (1 + np.exp((3*x)))

# Define the x values to plot
x = np.linspace(-5, 5, 1000)

# Calculate the y values using the logistic function
y = logistic(x)

for i in range(len(x)):
    if x[i]<-1:

```

```

        y[i] = np.nan
    if x[i]>1:
        y[i]= np.nan

def derivative(x):
    return (-3*np.exp(3*x))/((1+np.exp(3*x))**2)

y2 = logistic(0) + derivative(0)*x

for i in range(len(x)):
    if x[i]<-1.5:
        y2[i] = np.nan
    if x[i]>1.5:
        y2[i] = np.nan

ymax = np.nanmax(y)
ymin =np.nanmin(y)

# Plot the logistic curve backwards

# Plot the logistic curve
plt.figure(figsize=(9,6))
plt.plot(x,y2, label='Linear Potential')
plt.plot(x, y, label='Potential')
plt.xlim(-0.75, 0.75)
plt.ylim(ymin, ymax)

plt.title('Region of Gaussain Potential Around Turning Point at b')

plt.tick_params(axis='y',which='both',bottom=False, left=False, top=False,
                labelleft=False,)
plt.tick_params(axis='x',which='both',bottom=False, left=False, top=False,
                labelbottom=False,)

plt.axhline(0.5, -0.5, 0.5, color='forestgreen', linestyle='--')
plt.text(-0.8, 0.49, 'E', color='forestgreen', fontsize=12)

plt.axvline(0, 0, 0.5, color='forestgreen', linestyle='--')
plt.text(-0.01, 0, 'b', color='forestgreen', fontsize=12)

plt.axvline(-0.3, 0, 1, color='mediumpurple', linestyle='--')
plt.axvline(0.3, 0, 1, color='mediumpurple', linestyle='--')

plt.legend(loc='center right')

# Show the plot
# plt.show()
plt.savefig("wkb_airy_connection_b.png",dpi=500)

```

Reflection and Transmission Coefficients from Animations

This code was used to create all the reflection and transmission graphs in §7. In this case, all the specific variables for the different examples can be found on my GitHub project repository [26] in the ‘R_and_T_from_Schrodinger’ notebook.

```
import numpy as np
import os
from matplotlib import pyplot as plt
from matplotlib import animation
from scipy.fftpack import fft,ifft
from matplotlib import rc
rc('animation', html='jshtml')
from animate_wave import save_wave
from schrodinger_class import Schrodinger

def gauss_x(x, a, x0, k0):
    #wave with width a, centred at x0 with momentum k0
    return((a * np.sqrt(np.pi)) ** (-0.5) * np.exp(-0.5 * ((x - x0) * 1.
        / a) ** 2 + 1j * x * k0))
    #this is just a standard gaussian function

#A single Gaussian barrier:
#specify x grid
N = 2 ** 11 #2048
dx = 0.1
# x = dx * (np.arange(N) - 0.5 * N)
x=np.arange(-600,600,0.1)
dy = dx
y = x

#potential barrier
def gauss_barrier(x, a, x0):
    x = np.asarray(x)
    return (a * np.sqrt(np.pi))** (-0.5) * np.exp(-0.5 * ((x - x0)*1./a)
        ** 2)

V_x = gauss_barrier(x, 3, 0)
V0 = np.max(V_x)

#potential 'walls' at either end
# V_x[x < -598] = 1E6
# V_x[x > 598] = 1E6

#variables
dt = 0.01
N_steps = 50s
t_max = 200
frames = 501

energies = np.linspace(0, 3*V0, 100)
```

```

reflections = []
transmissions = []

for E in energies:
    #specifying constants
    hbar = 1.0
    m = 1.0 #mass
    p0 = np.sqrt(2 * m * E) #initial momentum
    k0 = p0 / hbar #initial wave number
    v0 = p0 / m #initial velocity
    d = 4.0 #initial width of wavepacket
    x0 = -20 #initial centre of wavepacket
    k0_ft_y = -np.pi / dy

    psi_x0 = gauss_x(x, d, x0, k0)

    inputpsi = psi_x0
#    S = Schrodinger(x=x, psi_x0=inputpsi, V_x=V_x, hbar=hbar, m=m, k0=-28)

    for i in range(frames):
        S = Schrodinger(x=x, psi_x0=inputpsi, V_x=V_x, hbar=hbar, m=m, k0=-28)
        S.time_step(dt, N_steps)
        inputpsi = S.psi_x

    index = []
    for i in range(len(x)):
        if V_x[i]>0.01:
            index.append(i)

    modsquared = np.abs(inputpsi)**2

    reflection = np.sum(modsquared[0:np.min(index)-1])*0.1
    transmission = np.sum(modsquared[np.max(index):-1])*0.1

    reflections.append(reflection)
    transmissions.append(transmission)

plt.plot(energies, transmissions, label = 'T(E)')
plt.plot(energies, reflections, label = 'R(E)')
plt.axvline(V0, linestyle = '--', c = 'g', label = '$V_0$')
plt.title('T(E) and R(E) for a Single Gaussian Potential')
plt.xlabel('E')
plt.legend()
plt.savefig('RandT_Single_Gaussian', dpi=500)

#      xlim = (-600, 600)

```

```

#      ylim = (0,0.6)
#      save_wave(xlim=xlim, ylim=ylim, S=S, frames=frames, dt=dt, N_steps=
#                  N_steps, name=f'single_barrier_{E}', scaling = 1.5, save=True)

#A rectangular barrier:
#specify x grid
N = 2 ** 11 #2048
dx = 0.1
# x = dx * (np.arange(N) - 0.5 * N)
x=np.arange(-800,800,0.1)
dy = dx
y = x

#potential barrier
def rectangular_barrier(x, a, b, V0):
    potential = np.zeros(len(x))
    for i in range(len(x)):
        if x[i]<a:
            potential[i] = 0
        if x[i]>= a and x[i]<= b:
            potential[i] = V0
        if x[i]>b:
            potential[i] = 0
    return potential

V0 = 0.5
a = -2
b = 2
V_x = rectangular_barrier(x,a,b,V0)

#potential 'walls' at either end
# V_x[x < -798] = 1E6
# V_x[x > 798] = 1E6

#variables
dt = 0.01
N_steps = 50
t_max = 200
frames = 501

energies = np.linspace(0, 4*V0, 100)

reflections = []
transmissions = []

for E in energies:
    #specifying constants
    hbar = 1.0
    m = 1.0 #mass
    p0 = np.sqrt(2 * m * E) #intial momentum

```

```

k0 = p0 / hbar #initial wave number
v0 = p0 / m #initial velocity
d = 4.0 #initial width of wavepacket
x0 = -20 #initial centre of wavepacket
k0_ft_y = -np.pi / dy

psi_x0 = gauss_x(x, d, x0, k0)

inputpsi = psi_x0
# S = Schrodinger(x=x, psi_x0=inputpsi, V_x=V_x, hbar=hbar, m=m, k0=-28)

for i in range(frames):
    S = Schrodinger(x=x, psi_x0=inputpsi, V_x=V_x, hbar=hbar, m=m, k0=-28)
    S.time_step(dt, N_steps)
    inputpsi = S.psi_x

index = []
for i in range(len(x)):
    if V_x[i]>0.01:
        index.append(i)

modSquared = np.abs(inputpsi)**2

reflection = np.sum(modSquared[0:np.min(index)-1])*0.1
transmission = np.sum(modSquared[np.max(index):-1])*0.1

reflections.append(reflection)
transmissions.append(transmission)

plt.plot(energies, transmissions, label = 'T(E)')
plt.plot(energies, reflections, label = 'R(E)')
plt.axvline(V0, linestyle = '--', c = 'g', label = '$V_0$')
plt.title('T(E) and R(E) for a Rectangular Potential')
plt.xlabel('E')
plt.legend()
plt.savefig('RandT_Rectangle', dpi=500)

# xlim = (-800, 800)
# ylim = (0, 0.6)
# save_wave(xlim=xlim, ylim=ylim, S=S, frames=frames, dt=dt, N_steps=N_steps, name=f'single_barrier_{E}', scaling = 1.5, save=True)

#A double equal barrier:
#specify x grid
N = 2 ** 11 #2048

```

```

dx = 0.1
x = np.arange(-200, 200, 0.1)
dy = dx
y = x

#potential barrier
def gauss_barrier(x, a, x0):
    x = np.asarray(x)
    return (a * np.sqrt(np.pi))** (-0.5) * np.exp(-0.5 * (((x-20) - x0)*1
        ./a)** 2) + (a * np.sqrt(np.pi))** (-0.5) * np.exp(-0.5 * (((x+20) - x0)*1./a)** 2)

V_x = gauss_barrier(x, 3, 0)
V0 = np.max(V_x)

#potential 'walls' at either end
# V_x[x < -198] = 1E6
# V_x[x > 198] = 1E6

#variables
dt = 0.01
N_steps = 50
t_max = 200
frames = 251

energies = np.linspace(0, 4*V0, 100)

reflections = []
transmissions = []

for E in energies:
    #specifying constants
    hbar = 1.0
    m = 1.0 #mass
    p0 = np.sqrt(2 * m * E) #intial momentum
    k0 = p0 / hbar #intial wave number
    v0 = p0 / m #initial velocity
    d = 4.0 #initial width of wavepacket
    x0 = -40 #initial centre of wavepacket
    k0_ft_y = -np.pi / dy

    psi_x0 = gauss_x(x, d, x0, k0)

    inputpsi = psi_x0
#    S = Schrodinger(x=x, psi_x0=inputpsi, V_x=V_x, hbar=hbar, m=m, k0=-28)

    for i in range(frames):
        S = Schrodinger(x=x, psi_x0=inputpsi, V_x=V_x, hbar=hbar, m=m, k0

```

```

            == 28)

S.time_step(dt, N_steps)
inputpsi = S.psi_x

index = []
for i in range(len(x)):
    if V_x[i]>0.01:
        index.append(i)

modSquared = np.abs(inputpsi)**2

reflection = np.sum(modSquared[0:np.min(index)-1])*0.1
transmission = np.sum(modSquared[np.max(index):-1])*0.1

reflections.append(reflection)
transmissions.append(transmission)

plt.plot(energies, transmissions, label = 'T(E)')
plt.plot(energies, reflections, label = 'R(E)')
plt.title('T(E) and R(E) for Double Gaussian Barriers with Equal Heights')
plt.xlabel('E')
plt.legend()
plt.savefig('RandT_Equal_Double', dpi=500)

#creating the schrodinger object
S = Schrodinger(x=x, psi_x0=psi_x0, V_x=V_x, hbar=hbar, m=m, k0==28)

#An unequal double barrier:
#specify x grid
N = 2 ** 11 #2048
dx = 0.1
# x = dx * (np.arange(N) - 0.5 * N)
x=np.arange(-800,800,0.1)
dy = dx
y = x
#potential barrier
def gauss_barrier(x, a, x0):
    return (a * np.sqrt(np.pi))** (-0.5) * np.exp(-0.5 * (((x-20) - x0)*1./a)** 2)+ 0.5*(a * np.sqrt(np.pi))** (-0.5) * np.exp(-0.5 * (((x+20) - x0)*1./a)** 2)

V_x = gauss_barrier(x, 3, 0)
V0 = np.max(V_x)

```

```

#potential 'walls' at either end
# V_x[x < -198] = 1E6
# V_x[x > 198] = 1E6

#variables
dt = 0.01
N_steps = 50
t_max = 200
frames = 651

energies = np.linspace(0, 3*V0, 100)

reflections = []
transmissions = []

for E in energies:
    #specifying constants
    hbar = 1.0
    m = 1.0 #mass
    p0 = np.sqrt(2 * m * E) #initial momentum
    k0 = p0 / hbar #initial wave number
    v0 = p0 / m #initial velocity
    d = 4.0 #initial width of wavepacket
    x0 = -40 #initial centre of wavepacket
    k0_ft_y = -np.pi / dy

    psi_x0 = gauss_x(x, d, x0, k0)

    inputpsi = psi_x0
    # S = Schrodinger(x=x, psi_x0=inputpsi, V_x=V_x, hbar=hbar, m=m, k0=-28)

    for i in range(frames):
        S = Schrodinger(x=x, psi_x0=inputpsi, V_x=V_x, hbar=hbar, m=m, k0=-28)
        S.time_step(dt, N_steps)
        inputpsi = S.psi_x

    index = []
    for i in range(len(x)):
        if V_x[i]>0.01:
            index.append(i)

    modsquared = np.abs(inputpsi)**2

    reflection = np.sum(modsquared[0:np.min(index)-1])*0.1
    transmission = np.sum(modsquared[np.max(index):-1])*0.1

    reflections.append(reflection)
    transmissions.append(transmission)

```

```

plt.plot(energies, transmissions, label = 'T(E)')
plt.plot(energies, reflections, label = 'R(E)')
plt.title('T(E) and R(E) for Double Gaussian Barriers with Unequal
           Heights ')
plt.xlabel('E')
plt.legend()
plt.savefig('RandT_Unequal_Double', dpi=500)

#creating the schrodinger object
S = Schrodinger(x=x, psi_x0=psi_x0, V_x=V_x, hbar=hbar, m=m, k0=-28)

```

References

- [1] H. Goldstein, *Classical Mechanics, 2nd edition.* Reading, MA: Addison-Wesley Publishing Company, Inc, 1980.
- [2] D. Tannor, *Introduction to Quantum Mechanics: A Time-Dependent Perspective, 1st edition.* Sausalito, CA: University Science Books, 2008.
- [3] B. C. Hall, *Quantum Theory for Mathematicians*, vol. 1. New York: Springer, 2013.
- [4] D. J. Griffiths, *Introduction to Quantum Mechanics, 2nd edition.* Upper Saddle River, NJ: Pearson Prentice Hall, 2005.
- [5] K. Konishi and P. Giampiero, *Quantum Mechanics: A New Introduction.* Oxford, UK: Oxford University Press, 2009.
- [6] K. Hannabuss, *An Introduction to Quantum Theory.* Oxford, UK: Oxford University Press, 1997.
- [7] C. Lubich, *From Quantum to Classical Molecular Dynamics: Reduced Models and Numerical Analysis.* Zürich, Switzerland: European Mathematical Society, 2008.
- [8] D. Hughes-Hallett, A. M. Gleason, and W. G. McCallum, *Calculus: Single and Multivariable, 4th edition.* John Wiley, 2005.
- [9] C. R. Harris, K. J. Millman, S. J. van der Walt, R. Gommers, P. Virtanen, D. Cournapeau, E. Wieser, J. Taylor, S. Berg, N. J. Smith, R. Kern, M. Picus, S. Hoyer, M. H. van Kerkwijk, M. Brett, A. Haldane, J. F. del Río, M. Wiebe, P. Peterson, P. Gérard-Marchant, K. Sheppard, T. Reddy, W. Weckesser, H. Abbasi, C. Gohlke, and T. E. Oliphant, “Array programming with NumPy,” *Nature*, vol. 585, pp. 357–362, Sept. 2020.
- [10] P. Virtanen, R. Gommers, T. E. Oliphant, M. Haberland, T. Reddy, D. Cournapeau, E. Burovski, P. Peterson, W. Weckesser, J. Bright, S. J. van der Walt, M. Brett, J. Wilson, K. J. Millman, N. Mayorov, A. R. J. Nelson, E. Jones, R. Kern, E. Larson, C. J. Carey, I. Polat, Y. Feng, E. W. Moore, J. VanderPlas, D. Laxalde, J. Perktold, R. Cimrman, I. Henriksen, E. A. Quintero, C. R. Harris, A. M. Archibald, A. H. Ribeiro, F. Pedregosa, P. van Mulbregt, and SciPy 1.0 Contributors, “SciPy 1.0: Fundamental Algorithms for Scientific Computing in Python,” *Nature Methods*, vol. 17, pp. 261–272, 2020.
- [11] J. D. Hunter, “Matplotlib: A 2d graphics environment,” *Computing In Science & Engineering*, vol. 9, no. 3, pp. 90–95, 2007.
- [12] M. S. Child, *Semiclassical Mechanics with Molecular Applications, 2nd edition.* Oxford, UK: Oxford University Press, 2014.
- [13] G. Wentzel, “Eine verallgemeinerung der quantenbedingungen für die zwecke der wellenmechanik,” *Zeitschrift für Physik*, vol. 38, no. 6-7, pp. 518–529, 1926.

- [14] H. A. Kramers, “Wellenmechanik und halbzahlige quantisierung,” *Zeitschrift für Physik*, vol. 39, no. 10-11, pp. 828–840, 1926.
- [15] L. Brillouin, “La mécanique ondulatoire de schrödinger: une méthode générale de résolution par approximations successives,” *Comptes Rendus de l'Académie des Sciences*, vol. 183, pp. 24–26, 1926.
- [16] H. Jeffreys, “On certain approximate solutions of linear differential equations of the second order,” *Proceedings of the London Mathematical Society*, vol. s2-23, no. 1, pp. 428–436, 1925.
- [17] H. Waalkens, R. Schubert, and S. Wiggins, “Wigner’s dynamical transition state theory in phase space: Classical and quantum,” *Nonlinearity*, vol. 21, no. 1, p. R1, 2007.
- [18] C. M. Bender and S. A. Orszag, *Advanced Mathematical Methods for Scientists and Engineers: Asymptotic Methods and Perturbation Theory*. New York: McGraw-Hill Inc, 1978.
- [19] M. de Gosson, *Symplectic Geometry and Quantum Mechanics*, vol. 166. Basel, Switzerland: Birkhäuser Verlag, 2006.
- [20] E. Wigner, “On the quantum correction for thermodynamic equilibrium,” *Phys. Rev.*, vol. 40, pp. 749–759, 1932.
- [21] E. Joos, H. D. Zeh, C. Kiefer, D. Giulini, J. Kupsch, and I. O. Stamatescu, *Decoherence and the Appearance of a Classical World in Quantum Theory, 2nd edition*. New York: Springer, 2003.
- [22] T. Plastow, “Semiclassical methods for investigating open quantum systems and decoherence, phd thesis,” 2020.
- [23] R. Schubert, R. O. Vallejos, and F. Toscano, “How do wave packets spread? time evolution on ehrenfest time scales,” *Journal of Physics A: Mathematical and Theoretical*, vol. 45, no. 21, p. 5307, 2012.
- [24] N. Aishan, T. Yusufu, and Y. Turek, “Amplitude-squared squeezing of schrödinger cat states via postselected von neumann measurement,” *The European Physical Journal Plus*, vol. 137, no. 2, pp. 1–10, 2022.
- [25] P. Bracken, “A time dependent version of the quantum wkb approximation,” *arXiv preprint math-ph/0608011*, 2006.
- [26] J. Winterborne, “Quantum wave propagation.” GitHub.com. Accessed on: 2023-02-05. Available at: https://github.com/JessWinterborne/Quantum_Wave_Propagation.