Utrecht University

Bachelor thesis

The path integral

Double bachelor physics and mathematics

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Abstract

In this thesis we look at Feynman's path integral. We first work on getting a useful and correct definition for this path integral, by using background from the Lagrangian mechanics, proving the equivalence to the Schrödinger Equation, showing what happens in the classical limit and by rigorously looking at the last problems which remain in the definition and searching for a way to fix them. We then look at examples, where we start with the explicit calculation for the free particle and where we then find that the use of only the classical path gives us the same result. From this we go on to the double slit experiment. There we find that the usage of the path integral gives us a particularly elegant result, for both the experiment with infinitesimal, as well as with finite slits. After that we look at a specific class of potentials, for which we can prove that using the classical path is enough to get the correct result. We then apply this to calculate the result for the harmonic oscillator.

We then define the concept of imaginary time and use this concept to get a more stable path integral, which leads us towards many applications. We then compare some of the examples which we already looked at to their imaginary time equivalent. Then the imaginary time operator leads us to spectral theory, to allow us to define this operator correctly, even when it does not have a true orthonormal basis.

Contents

1 Introduction

One of the most interesting experiments in physics is the double slit experiment, since this showed us that both light and matter can behave like waves. But when we want to calculate the results for this example, it does not clearly show us the behavior which made the experiment so famous. The way we usually look at a quantum mechanical example like this, is by using Hamiltonian mechanics and the Schrödinger Equation.

The way we will tackle the example in this thesis is by using a different starting point. We will start with Lagrangian mechanics, which will give us the action and principle of least action. We can use this as the starting point to get to Feynman's path integral. Along the road to the double slit experiment, we will find multiple definitions, as we are searching for the one which makes our calculations easiest. We will visit the equivalence to the Schrödinger Equation while we check the validity of the formula and we will look at the classical limit, to check whether that also gives us the correct result. We will then go into some of the mathematical difficulties of the formula and use two theorems to define the path integral rigorously.

Then we will look at some examples, where the free particle shows us that using its classical path gives us the same result as doing the explicit calculations. Using this result we can finally look at the double slit experiment, which is described beautifully by the path integral. After this we will look at a specific class of potentials, where we find that for these potentials using the classical path also gives the correct result. We can use this to look at another well known example, the harmonic oscillator.

After this we will look at the imaginary time operator, where analytic continuation and a more stable path integral definition will lead us to many possible applications. This will also lead us towards spectral theory, as we want everything we have seen above to be applicable to as many situations, or operators as possible.

It is like Shankar said: "We discuss Feynman's alternative, not only because of its aesthetic value, but also because it can, in a class of problems, give the full propagator with tremendous ease and also give valuable insight into the relation between classical and quantum mechanics."

But we could also add that we want to look at it for its connection to many different areas and for its many possibilities.

2 Path integral definition

In this section we will define the path integral and look at its validity in the classical limit, equivalence to the Schrödinger equation and in a more rigorous definition.

2.1 Approximation definition

We will first look at the definition of the path integral, since this is needed before we work with it. For this we will follow parts of Shankar [1].

In quantum mechanics, we usually use the Schrödinger equation, which is based on the Hamiltonian formalism of classical mechanics. In Appendix A.1 we have looked at the Lagrangian formalism of classical mechanics. We have seen that in this formalism, the principle of least action is what distinguishes the classical path from the other paths. Now we want to see if we can find a way to treat quantum mechanics, based on this principle of least action and the Lagrangian formalism.

For this we will look for the time operator, or propagator, U, for a particle which travels between x' at time t' and x at time t. The reason we want to look at this time operator, is that it is a really useful function, since it tells us the state of a particle at the final time t, when we insert the initial state into the operator, so it will tell us how the state will evolve over time. The way we do this consists of three steps.

The first step is to draw all the paths between the two points we are looking at. In Figure 1 we have drawn some paths connecting two points, but there are clearly many, many more paths which also connect these two points.

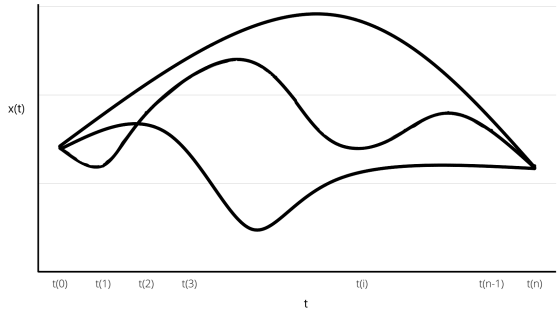


Figure 1: An example of possible paths connecting two points.

Our next step will be to calculate the action $S[x(t)]$ of each of these paths, for which we can use Equation (A.1.1). Here we use the notation $S[x(t)]$ to show that the action depends on the whole path $x(t)$, not just at some point x at time t.

Our last step is to calculate the time propagator, by calculation the path sum

$$U(x,t;x',t') = A \sum_{\text{all paths}} \exp\left(\frac{i}{\hbar} S[x(t)]\right). \tag{2.1.1}$$

Here A is some normalizing constant, at which we will look later on.

As there exist many paths between the two points and as these paths can be very close to each other, we do not know how to sum over all of these paths. Since there are so many paths to sum over we can also imagine that the sum over all the paths will tend to infinity. We will therefore look at the integral over all of the paths, in the hope that this will give us an answer we can work with. This gives us the path integral definition

$$U(x,t;x',t') = A\int \exp\left(\frac{i}{\hbar}S[x(t)]\right)\mathscr{D}[x(t)], \tag{2.1.2}$$

where $\mathscr{D}[x(t)]$ symbolizes the integration over all paths. If we now let the time operator U act on a wave function, which describes the initial state, we get the wave function which describes the final state. This wave function is then given by

$$\psi(x,t;x',t') = A\int \exp\left(\frac{i}{\hbar}S[x(t)]\right)\psi(x',t')\mathscr{D}[x(t)]. \tag{2.1.3}$$

For now it is unclear whether this is a valid definition which will give us the correct result, but in Section 2.3 we will find that this definition is equivalent to the Schrödinger equation. From that it follows that this definition will give us the correct results.

The problem we now face with Equations (2.1.2) and (2.1.3) is that we do not know how to integrate over all the paths. To fix this problem, we will discretize the paths. An example of the discretization of a single path can be found in Figures 2 and 3.

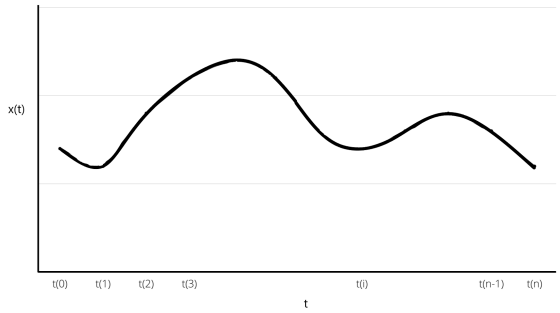


Figure 2: A single path, to which we will apply the discretization.

Now by varying all the points between $-\infty$ and ∞, except the starting point and the end point as these are fixed, we get the discrete approximation of every single path. When we now take the limit of $n \to \infty$, we will get increasingly well approximations of all the paths.

As we are looking at the particle between times t' and t and as we discretize the path into n equal pieces, the length ε of each time interval will be given by

$$\varepsilon = \frac{t-t'}{n}. \tag{2.1.4}$$

As n goes to infinity, our time intervals will become infinitesimal, as we divide by n to get the length of the time intervals. When we now look at one of these infinitesimal intervals,

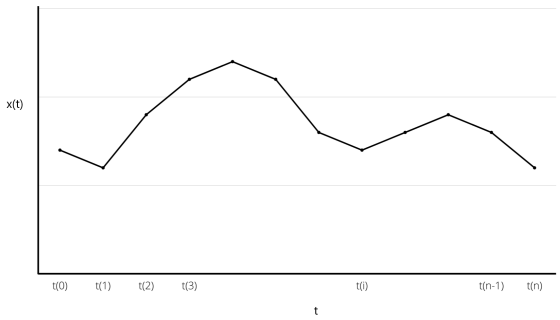


Figure 3: The discretized version of the path in Figure 2.

using Equation (2.1.3), we can get the following formula for the wave function after the time interval ε

$$\psi(t'+\varepsilon, x_{j+1}) = B\int_{\mathbb{R}} \exp\left(\frac{i}{\hbar}S(x_{j+1}, x_j)\right)\psi(t', x_j)dx_j. \tag{2.1.5}$$

Here B is again a normalizing constant, but now B will depend on the length of our interval ε. We also see in Equation (2.1.5) that $S(x_{j+1}, x_j)$ is the action of the linear path, which was given by the interpolation between these points. We can now repeat Equation (2.1.5) to get

$$\begin{aligned}\psi(t'+2\varepsilon, x_{j+2}) &= B\int_{\mathbb{R}} \exp\left(\frac{i}{\hbar}S(x_{j+2}, x_{j+1})\right)\psi(t'+\varepsilon, x_{j+1})dx_{j+1} \\ &= B\int_{\mathbb{R}} \exp\left(\frac{i}{\hbar}S(x_{j+2}, x_{j+1})\right)\left[B\int_{\mathbb{R}} \exp\left(\frac{i}{\hbar}S(x_{j+1}, x_j)\right)\psi(t', x_j)dx_j\right]dx_{j+1} \\ &= B^2\int_{\mathbb{R}\times\mathbb{R}} \exp\left(\frac{i}{\hbar}[S(x_{j+2}, x_{j+1}) + S(x_{j+1}, x_j)]\right)\psi(t', x_j)dx_j dx_{j+1}.\end{aligned} \tag{2.1.6}$$

Now that we have seen how the repetition of Equation (2.1.5) works, we can apply this repetition n times. By using Equation (2.1.4) we find that $t = t' + n\varepsilon$. Also, when we look at the discretization in Figure 3, we can see that x_0 is our starting point, so $x_0 = x'$ and that x_n is our end point, so $x_n = x$. We can now use all of this and Equation (2.1.6) to get

$$\psi(x, t; x', t') = \lim_{\substack{n\to\infty \\ \varepsilon\to 0}} B^n \int_{\mathbb{R}^{n-1}} \exp\left(\frac{i}{\hbar}\sum_{j=0}^{n-1} S(x_{j+1}, x_j)\right)\psi(t', x')dx_1\cdots dx_{n-1}. \tag{2.1.7}$$

We can now apply the same discretization and steps to Equation (2.1.2) as we have done to Equation (2.1.3). From Equation (2.1.3) followed Equation (2.1.7) and by applying the same steps, we find that from Equation (2.1.2) follows

$$U(x, t; x', t') = \lim_{\substack{n\to\infty \\ \varepsilon\to 0}} B^n \int_{\mathbb{R}^{n-1}} \exp\left(\frac{i}{\hbar}\sum_{j=0}^{n-1} S(x_{j+1}, x_j)\right)dx_1\cdots dx_{n-1}. \tag{2.1.8}$$

Now that we have found a path integral definition we can work with, Equation (2.1.8), there are some things we want to look at, before we will use this definition. We will look

at the classical limit, Section 2.2, the equivalence to the Schrödinger equation, Section 2.3, and a more rigorous definition, Section 2.4, before looking at examples, Section 3, and at the imaginary time operator, Section 4.

2.2 Classical limit

To check if the definition we found in Section 2.1 is valid, one of the things we want to check is whether we get the correct result in the classical limit. That is what we will be looking at in this section. For this we will follow some parts of Shankar [1].

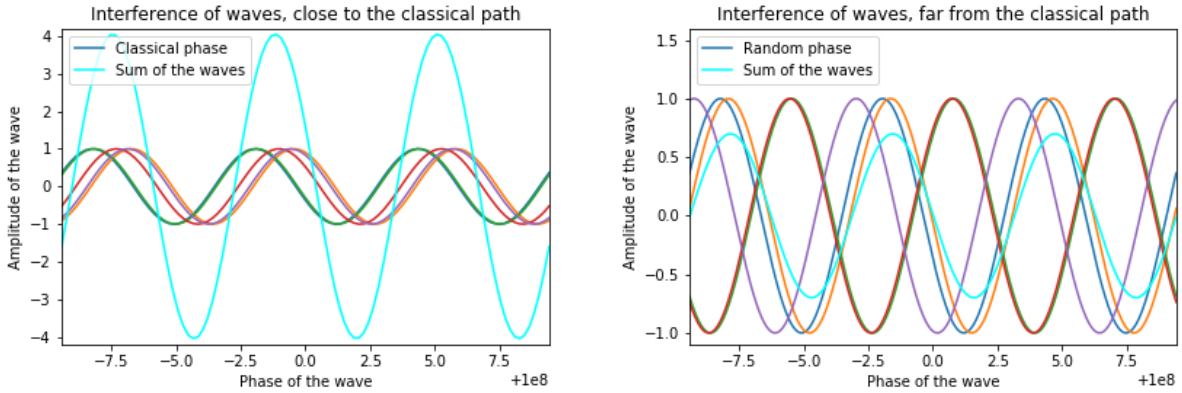
In the previous section we have seen multiple definitions for the path integral, the summation definition, the integral definition and the definition for an infinitesimal time interval. In each of these definitions, all of the paths weighed equally. Now we expect that this might become a problem in the classical limit. We know that in the classical limit, we should expect a particle to go along the classical path, but this result does not seem to follow from the path integral. But even in this path integral definition, the classical path still plays an important role. This follows from the fact that the classical path is the path of least action, as we have seen in section Appendix A.1. This must mean that the classical path resides at a minimum of the action, or at least it has to hold that $\delta S = 0$. From this it follows that for a path very near the classical one, the action must be very close to the action of the classical path. One other thing we can note by looking at Equations (2.1.1) and (2.1.2) is that the action divided by the constant $\hbar$ is actually equal to the phase of this exponential. We know that waves can interfere constructively or destructively with each other. For waves to have constructive interference, their phases have to be very close to each other. As we know that the action barely changes when we are very close to the classical path, from this it follows that there will be constructive interference close to the classical path. This tells us that this classical path will be of influence in the big picture as it will not disappear.

Now we will look at what happens to paths far from the classical one. In general we can assume that for a random path $y(t)$ we find that $\delta S[y(t)] \neq 0$. This means that the action for this path differs from the action from the paths near it. When we divide these actions by the very small constant $\hbar$ these differences in the phases become large. This tells us that the phases oscillate rapidly and thus will give destructive interference (as it is just as likely for the exponential to be positive as negative, these neighboring paths thus start to cancel each other out).

In Figure 4a we can see what happens close to the classical path. There will be constructive interference, so the sum of the waves, this is the cyan wave, has a way bigger amplitude than the other waves.

In Figure 4b we can see what happens away from the classical path. Here we started with a random path and let all the action for the other paths deviate less than 0.1 percent from this path. We still see, that even with such a small deviation and only 4 paths close to the random path, there is already destructive interference, since the sum of the path has a smaller amplitude than the other paths. So we can imagine that with even larger deviations or more paths the destructive interference will take over for a random path.

We thus find that paths close to the classical path will interfere constructively with each other, while paths far from the classical one will interfere destructively. This indeed tells us that the classical path has a special outcome in the classical limit, as this path and the ones



(a) Constructive interference, close to x_{cl}.

(b) Destructive interference, away from x_{cl}.

Figure 4: Interference close to and far from the classical path. Note that the figures have different wave amplitudes, since the constructive interference in figure (a) was so big, it did not fit in the picture when we used the same values.

close to it will be the only ones with constructive interference. As we will be working in the classical limit, the action will be huge compared to the constant $\hbar$. From this it follows that the difference in phases, the action divided by $\hbar$, will be enormous. For paths to interfere constructively with the classical path, they will have to be extremely close to the classical path. From this it follows that it will generally suffice to look at the classical path, when we look at the classical limit. We thus indeed get the result we hoped for, which is the classical path in the classical limit.

2.3 Equivalence to the Schrödinger equation

We have now shown that the path integral gives us the correct result in the classical limit. But we also have to check whether the definition of the path integral will even give us a valid result. Therefore we will now look at the equivalence between the Schrödinger equation and the path integral. For if this holds, we can conclude that we are allowed to use the path integral. For this we we largely follow Shankar [1].

We know that the Schrödinger equation is given by

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle, \tag{2.3.1}$$

where H is the Hamiltonian, which is given by

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x), \tag{2.3.2}$$

for a single particle in one dimension on which acts the potential $V(x)$. For the wave functions, we will use the following notation $|\psi(t)\rangle = \psi(t,x)$. We are now looking for a definition for the time derivative of the wave function, which we saw in Equation (2.3.1). For this we will use the wave function at time $t+\varepsilon$, where ε is an infinitesimal time interval. As the wave

functions are usually given by nice functions, we can use the Taylor expansion of this wave function around $\varepsilon = 0$ to get

$$\psi(t+\varepsilon, x) = \psi(t,x) + \frac{d}{dt}\big(\psi(t,x)\big)\varepsilon + \mathscr{O}(\varepsilon^2). \tag{2.3.3}$$

We can rewrite this to get

$$\frac{d}{dt}\psi(t,x) \approx \frac{\psi(t+\varepsilon,x) - \psi(t,x)}{\varepsilon}, \tag{2.3.4}$$

where we neglect terms which contain ε^2, or any higher orders of ε, as ε already was infinitesimal and these terms will be even smaller. We can now insert the definition for the Hamiltoninan, Equation (2.3.2), and the result we found in Equation (2.3.4) into Equation (2.3.1), to get

$$i\hbar\frac{\psi(t+\varepsilon,x) - \psi(t,x)}{\varepsilon} = \bigg(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\bigg)\psi(t,x). \tag{2.3.5}$$

We can rewrite this once more to

$$\psi(t+\varepsilon,x) - \psi(t,x) = -\frac{i\varepsilon}{\hbar}\bigg(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\bigg)\psi(t,x), \tag{2.3.6}$$

which is the equation we will be using.

Our starting point for this calculation will be the definition of the path integral from Equation (2.1.5). We will first look at the definition of the action and how we can write this. From the classical mechanics, of which a recapitulation can be found in Appendix A.1, we already know the definition of the action, which is given by

$$S(x) = \int_{t'}^{t'+\varepsilon} \left(\frac{m}{2}\left[\frac{dx}{dt}\right]^2 - V(x(t))\right)dt \tag{2.3.7}$$

for the path between x_j and x_{j+1}. When we looked at Equation (2.1.5) we used the points x_i and interpolated between the points, this means that between the points we have a straight line. This is an approximation of the path along which the particle will move. The place of this particle between two such points will be given by

$$x(t) = x_j + \frac{x_{j+1} - x_j}{(t'+\varepsilon) - t'}(t - t') = x_j + \frac{x_{j+1} - x_j}{\varepsilon}(t - t'). \tag{2.3.8}$$

Along this path, we can take the derivative of the place to the time, to get

$$\frac{dx}{dt} = \frac{x_{j+1} - x_j}{\varepsilon}. \tag{2.3.9}$$

We can already insert this into Equation (2.3.7) to get

$$S(x) \approx \int_{t'}^{t'+\varepsilon} \left(\frac{m}{2}\left[\frac{x_{j+1} - x_j}{\varepsilon}\right]^2 - V(x(t))\right)dt. \tag{2.3.10}$$

We find that the first term is no longer dependent on the time, which means we can get the following

$$\begin{aligned} S(x) &= \frac{m}{2}\left[\frac{x_{j+1}-x_j}{\varepsilon}\right]^2(t'+\varepsilon-t') - \int_{t'}^{t'+\varepsilon} V(x(t))dt \\ &= \frac{m\varepsilon}{2}\left[\frac{x_{j+1}-x_j}{\varepsilon}\right]^2 - \int_{t'}^{t'+\varepsilon} V(x(t))dt \\ &= \frac{m}{2}\frac{(x_{j+1}-x_j)^2}{\varepsilon} - \int_{t'}^{t'+\varepsilon} V(x(t))dt. \end{aligned} \tag{2.3.11}$$

We now want to find an approximation for the second term, the integral of the potential. We know that the integral is used to calculate the area under a function. As we take this integral over a very small time interval ε and as we can generally assume the potential to be a nice, bounded function, it can be approximated by treating it as a rectangle. One side has length $t'+\varepsilon-t'=\varepsilon$ and for the length of its other side, we can use $V(x_{j+1})$. This tells us that the area of the rectangle is given by $\varepsilon V(x_{j+1})$. Inserting this into Equation (2.3.11) gives us

$$S(x) = \frac{m}{2}\frac{(x_{j+1}-x_j)^2}{\varepsilon} - \varepsilon V(x_{j+1}). \tag{2.3.12}$$

Inserting this into Equation (2.1.5) gives us

$$\psi(t'+\varepsilon, x_{j+1}) = B\int_{\mathbb{R}} \exp\left(\frac{im}{2\hbar}\frac{(x_{j+1}-x_j)^2}{\varepsilon} - \frac{i\varepsilon}{\hbar}V(x_{j+1})\right)\psi(t', x_j)dx_j. \tag{2.3.13}$$

We will now simplify the expression, by using t instead of t', x instead of x_{j+1} and y instead of $x_j - x_{j+1}$. This way we can write x_j as $x+y$ and $x_j - x_{j+1}$ as $x-(x+y)=-y$. We also find that $\frac{dy}{dx_j}=1$, so $dy=dx_j$. By inserting all of this into Equation (2.3.13) we get the following equation

$$\psi(t+\varepsilon, x) = B\int_{\mathbb{R}} \exp\left(\frac{im}{2\hbar}\frac{y^2}{\varepsilon} - \frac{i\varepsilon}{\hbar}V(x)\right)\psi(t, x+y)dy, \tag{2.3.14}$$

which is equal to

$$\psi(t+\varepsilon, x) = B\int_{\mathbb{R}} \exp\left(\frac{imy^2}{2\hbar\varepsilon}\right)\exp\left(-\frac{i\varepsilon}{\hbar}V(x)\right)\psi(t, x+y)dy \tag{2.3.15}$$

or

$$\psi(t+\varepsilon, x) = B\exp\left(-\frac{i\varepsilon}{\hbar}V(x)\right)\int_{\mathbb{R}} \exp\left(\frac{imy^2}{2\hbar\varepsilon}\right)\psi(t, x+y)dy \tag{2.3.16}$$

as $V(x)$ nor one of its prefactors is dependent on y.

In Section 2.2 we have seen that paths will cancel each other out when they are far from the classical path. We have also already seen that a practical interval around the classical path, for which we do take the paths into account, is the interval for which the phases differ

less than π. In Equation (2.3.15) we can see that the phase is given by $\frac{my^2}{2\hbar\varepsilon}$. We thus want to look at the paths for which

$$\begin{aligned} \frac{my^2}{2\hbar\varepsilon} &\leq \pi \\ y^2 &\leq \frac{2\pi\hbar\varepsilon}{m} \\ |y| &\leq \sqrt{\frac{2\pi\hbar\varepsilon}{m}}. \end{aligned} \tag{2.3.17}$$

As $\hbar$ is miniscule and as we are working on a very small time interval ε, we can see that y must be very small to. Because of this, we know we can approximate $\psi(t, x+y)$ by using its Taylor expansion. We will discard terms which have ε^2, which is equivalent to y^4, as $y \sim \varepsilon^{1/2}$, or y to a higher order in it, as the contributions of these terms will be so small, we can ignore them. This gives us the following expansion

$$\psi(t, x+y) = \psi(t, x) + \frac{\partial\psi}{\partial u}y + \frac{1}{2}\frac{\partial^2\psi}{\partial^2 u}y^2 + \frac{1}{6}\frac{\partial^3\psi}{\partial^3 u}y^3 + \mathscr{O}(y^4), \tag{2.3.18}$$

where we have used du to express the differentiation to the particles coordinate. We have not used dx for this, to prevent the confusion with x, the notation we are using for x_{j+1}. We can insert this expansion into Equation (2.3.16), to get

$$\psi(t+\varepsilon, x) = B\exp\left(-\frac{i\varepsilon}{\hbar}V(x)\right)\int_{\mathbb{R}}\exp\left(\frac{imy^2}{2\hbar\varepsilon}\right)\left[\psi(t,x) + \frac{\partial\psi}{\partial u}y + \frac{1}{2}\frac{\partial^2\psi}{\partial^2 u}y^2 + \frac{1}{6}\frac{\partial^3\psi}{\partial^3 u}y^3\right]dy. \tag{2.3.19}$$

By expanding this expression, we get

$$\begin{aligned} \psi(t+\varepsilon, x) = B\exp\left(-\frac{i\varepsilon}{\hbar}V(x)\right)\int_{\mathbb{R}}\Bigg[&\psi(t,x)\exp\left(\frac{imy^2}{2\hbar\varepsilon}\right) + \frac{\partial\psi}{\partial u}y\exp\left(\frac{imy^2}{2\hbar\varepsilon}\right) \\ &+ \frac{1}{2}\frac{\partial^2\psi}{\partial^2 u}y^2\exp\left(\frac{imy^2}{2\hbar\varepsilon}\right) + \frac{1}{6}\frac{\partial^3\psi}{\partial^3 u}y^3\exp\left(\frac{imy^2}{2\hbar\varepsilon}\right)\Bigg]dy. \end{aligned} \tag{2.3.20}$$

We now find that we need to solve four Gaussian integrals, which are given by

$$\int_{\mathbb{R}}\exp\left(\frac{imy^2}{2\hbar\varepsilon}\right)dy = \int_{\mathbb{R}}\exp\left(-\frac{my^2}{2i\hbar\varepsilon}\right)dy, \tag{2.3.21}$$

$$\int_{\mathbb{R}} y\exp\left(\frac{imy^2}{2\hbar\varepsilon}\right)dy = \int_{\mathbb{R}} y\exp\left(-\frac{my^2}{2i\hbar\varepsilon}\right)dy, \tag{2.3.22}$$

$$\int_{\mathbb{R}} y^2\exp\left(\frac{imy^2}{2\hbar\varepsilon}\right)dy = \int_{\mathbb{R}} y^2\exp\left(-\frac{my^2}{2i\hbar\varepsilon}\right)dy, \tag{2.3.23}$$

$$\int_{\mathbb{R}} y^3\exp\left(\frac{imy^2}{2\hbar\varepsilon}\right)dy = \int_{\mathbb{R}} y^3\exp\left(-\frac{my^2}{2i\hbar\varepsilon}\right)dy. \tag{2.3.24}$$

As y^2 is an even function, we can easily see that $\exp\left(-\frac{my^2}{2i\hbar\varepsilon}\right)$ is also an even function. By multiplying this by y or y^3, which are odd functions, the product is an odd function as well.

As we are integrating over $\mathbb{R}$, so from $-\infty$ to ∞, we find that the integrals of these products, which are Equations (2.3.22) and (2.3.24), will be zero. To solve the remaining two integrals, we will first define $a := \frac{m}{2i\hbar\varepsilon}$. By inserting this into Equations (2.3.21) and (2.3.23) we get the following integrals

$$\int_{\mathbb{R}} \exp\big(-ay^2\big)dy, \tag{2.3.25}$$

$$\int_{\mathbb{R}} y^2 \exp\big(-ay^2\big)dy. \tag{2.3.26}$$

The first integral is the familiar Gaussian integral, which we know to be equal to $\sqrt{\pi/a}$ (more information about Gaussian integrals can be found in Blundell and Blundell [2]). We can derive the result for the second integral, Equation (2.3.26), by differentiating the first to a, which gives us

$$\begin{aligned}\int_{\mathbb{R}} y^2 \exp\big(-ay^2\big)dy &= -\int_{\mathbb{R}} \frac{\partial}{\partial a}\exp\big(-ay^2\big)dy = -\frac{\partial}{\partial a}\int_{\mathbb{R}}\exp\big(-ay^2\big)dy \\ &= -\frac{\partial}{\partial a}\sqrt{\frac{\pi}{a}} = +\frac{1}{2}\frac{\sqrt{\pi}}{a^{3/2}} = \frac{1}{2a}\sqrt{\frac{\pi}{a}}.\end{aligned} \tag{2.3.27}$$

We were allowed to move the partial derivative outside of the integral, as we know that the exponential of a quadratic function is a smooth function and as we take the partial derivative to a, while we integrate over y. We can now use $a := \frac{m}{2i\hbar\varepsilon}$ and Equation (2.3.27), to get the results for Equations (2.3.21) to (2.3.24).

$$\int_{\mathbb{R}} \exp\left(-\frac{my^2}{2i\hbar\varepsilon}\right)dy = \int_{\mathbb{R}} e^{-ay^2}dy = \sqrt{\frac{\pi}{a}} = \sqrt{\frac{2\pi\hbar\varepsilon i}{m}} \tag{2.3.28}$$

$$\int_{\mathbb{R}} y\exp\left(-\frac{my^2}{2i\hbar\varepsilon}\right)dy = 0 \tag{2.3.29}$$

$$\int_{\mathbb{R}} y^2 \exp\left(-\frac{my^2}{2i\hbar\varepsilon}\right)dy = \int_{\mathbb{R}} y^2 e^{-ay^2}dy = \frac{1}{2a}\sqrt{\frac{\pi}{a}} = \frac{2\hbar\varepsilon i}{2m}\sqrt{\frac{2\pi\hbar\varepsilon i}{m}} = \frac{\hbar\varepsilon i}{m}\sqrt{\frac{2\pi\hbar\varepsilon i}{m}} \tag{2.3.30}$$

$$\int_{\mathbb{R}} y^3 \exp\left(-\frac{my^2}{2i\hbar\varepsilon}\right)dy = 0 \tag{2.3.31}$$

We can now insert these results into Equation (2.3.20) to get

$$\begin{aligned}\psi(t+\varepsilon,x) &= B\exp\left(-\frac{i\varepsilon}{\hbar}V(x)\right)\left[\psi(t,x)\sqrt{\frac{2\pi\hbar\varepsilon i}{m}} + 0 + \frac{1}{2}\frac{\partial^2\psi}{\partial^2 u}\frac{\hbar\varepsilon i}{m}\sqrt{\frac{2\pi\hbar\varepsilon i}{m}} + 0\right] \\ &= B\sqrt{\frac{2\pi\hbar\varepsilon i}{m}}\exp\left(-\frac{i\varepsilon}{\hbar}V(x)\right)\left[\psi(t,x) + \frac{\hbar\varepsilon i}{2m}\frac{\partial^2\psi}{\partial^2 u}\right].\end{aligned} \tag{2.3.32}$$

As we have no longer any y in the equation, from now on, we will write du as dx, as we do not have to watch out for the confusion any longer. We will use this to rewrite Equation (2.3.32) to

$$\psi(t+\varepsilon,x) = B\sqrt{\frac{2\pi\hbar\varepsilon i}{m}}\exp\left(-\frac{i\varepsilon}{\hbar}V(x)\right)\left[\psi(t,x) + \frac{\hbar\varepsilon i}{2m}\frac{\partial^2\psi}{\partial^2 x}\right]. \tag{2.3.33}$$

As we have already said, we want to discard any terms with ε^2 or a higher power of ε. We still have a term of ε in the exponential with the potential, which makes it difficult for us to know which terms we can ignore. Therefore, we will use the Taylor expansion of this exponential around $\varepsilon = 0$, to simplify Equation (2.3.33). The Taylor expansion of the exponential term is given by

$$\exp\left(-\frac{i\varepsilon}{\hbar}V(x)\right) = 1 - \frac{i\varepsilon}{\hbar}V(x) + \mathscr{O}(\varepsilon^2). \tag{2.3.34}$$

We can insert this into Equation (2.3.33) and discard high order terms, to get

$$\begin{aligned}\psi(t+\varepsilon,x) &= B\sqrt{\frac{2\pi\hbar\varepsilon i}{m}}\left(1-\frac{i\varepsilon}{\hbar}V(x)\right)\left[\psi(t,x)+\frac{\hbar\varepsilon i}{2m}\frac{\partial^2\psi}{\partial^2 x}\right]\\ &= B\sqrt{\frac{2\pi\hbar\varepsilon i}{m}}\left[\psi(t,x)+\frac{\hbar\varepsilon i}{2m}\frac{\partial^2\psi}{\partial^2 x}-\frac{i\varepsilon}{\hbar}V(x)\psi(t,x)+\mathscr{O}(\varepsilon^2)\right]\\ &= B\sqrt{\frac{2\pi\hbar\varepsilon i}{m}}\left[\psi(t,x)+\frac{\hbar\varepsilon i}{2m}\frac{\partial^2\psi}{\partial^2 x}-\frac{i\varepsilon}{\hbar}V(x)\psi(t,x)\right].\end{aligned} \tag{2.3.35}$$

We can now rewrite this equation to get the following

$$\psi(t+\varepsilon,x) - B\sqrt{\frac{2\pi\hbar\varepsilon i}{m}}\psi(t,x) = -B\sqrt{\frac{2\pi\hbar\varepsilon i}{m}}\frac{i\varepsilon}{\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial^2 x}+V(x)\right]\psi(t,x). \tag{2.3.36}$$

As we can see, this equation already starts to look like the Schrödinger equation, which we have seen in Equation (2.3.6), the only main problem we have left, is the unknown constant B. We want to find a value for this constant, by looking at the Taylor expansion of $\psi(t+\varepsilon,x)$ around $\varepsilon = 0$, as both sides of the equation have to be equal at $\varepsilon = 0$. The Taylor expansion for this wave function is given by

$$\psi(t+\varepsilon,x) = \psi(t,x) + \frac{\partial\psi}{\partial t}\varepsilon + \mathscr{O}(\varepsilon^2). \tag{2.3.37}$$

We will now insert this into Equation (2.3.36) to get

$$\psi(t,x) + \frac{\partial\psi}{\partial t}\varepsilon - B\sqrt{\frac{2\pi\hbar\varepsilon i}{m}}\psi(t,x) = -B\sqrt{\frac{2\pi\hbar\varepsilon i}{m}}\frac{i\varepsilon}{\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial^2 x}+V(x)\right]\psi(t,x). \tag{2.3.38}$$

We can see that the right hand side of the equation goes to zero as long as we do not have that $B \sim \varepsilon^{-3/2}$, or any lower order of ε. When we look at the left hand side, we find that the second term goes to zero as ε does. Now we have two terms left, which gives us the following equation

$$\begin{aligned}\psi(t,x) - B\sqrt{\frac{2\pi\hbar\varepsilon i}{m}}\psi(t,x) &= 0\\ B\sqrt{\frac{2\pi\hbar\varepsilon i}{m}}\psi(t,x) &= \psi(t,x)\\ B\sqrt{\frac{2\pi\hbar\varepsilon i}{m}} &= 1\\ B &= \left(\frac{2\pi\hbar\varepsilon i}{m}\right)^{-1/2}.\end{aligned} \tag{2.3.39}$$

Of course this only holds when $\psi(t,x) \neq 0$, but it is clear that we can assume that the wave function is not 0 everywhere.

We now have found a value for the constant B, which we can plug into Equation (2.3.36) to get

$$\begin{aligned}\psi(t+\varepsilon,x) - \left(\frac{2\pi\hbar\varepsilon i}{m}\right)^{-1/2}\sqrt{\frac{2\pi\hbar\varepsilon i}{m}}\psi(t,x) = \\ -\left(\frac{2\pi\hbar\varepsilon i}{m}\right)^{-1/2}\sqrt{\frac{2\pi\hbar\varepsilon i}{m}}\frac{i\varepsilon}{\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial^2 x} + V(x)\right]\psi(t,x),\end{aligned} \tag{2.3.40}$$

which gives us

$$\psi(t+\varepsilon,x) - \psi(t,x) = -\frac{i\varepsilon}{\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial^2 x} + V(x)\right]\psi(t,x). \tag{2.3.41}$$

We can compare this result to Equation (2.3.6), to find that these are exactly the same. This means that the path integral is equivalent to the Schrödinger equation, which justifies it usage.

2.4 Rigorous definition.

Now we will go into the more rigorous definition of the path integral, to complete checking the validity of the path integral definition and to fix the remainung problems. Some background for this section is given in Appendix A.2. Those of us who are willing to take on faith that the path integral definition, which we have found in Section 2.1, works can skip this section. For this section we will largely follow Johnson and Lapidus [3].

There are some problems with the path integral formula, which we have seen in Equation (2.1.2). First of all, there exists no countable additive measure $\mathscr{D}$, which weighs all paths equally. This was a problem which we already saw coming, as we had no clue how to calculate the integral, when we used this measure $\mathscr{D}$. In Section 2.1 we discretized the path integral and looked at it for an infinitesimal time interval which we saw in Equation (2.1.7). By doing this, we could get all possible discretized paths by keeping x_0 and x_n fixed and varying all x_j for $0 < j < n$ between $-\infty$ and ∞. This way we get a true translation invariant measure, which consists of $(n-1)$ Lebesgue measures. Also, since we take the limit of $n \to \infty$ we keep taking finer and finer intervals. As the collection of such paths is dense in the space of continuous paths, they converge uniformly to the paths, which is an extra reason of why we could use this definition, given in Equation (2.1.7).

Another problem is that the space of continuous functions, which we are working on, is not compact. So even if we could have found a measure $\mathscr{D}$ which we could use, since the space is not compact, its measure would be infinite and the integrand (given by $\exp(iS[x(t)]/\hbar)$) would not be absolutely integrable.

Another problem is that, since we are allowing all continuous paths, the action will not always be well defined. This follows from the definition for the action, given in Equation (2.3.7). As we can see there, we use the derivative of the path to calculate the action, but since the paths only need to be continuous there is no guarantee that this derivative will exist. Here we find another advantage of the discretization of the paths. At each interval between points

x_j and x_{j+1} we will be interpolating, so we will have a straight line between these points. Of this line we can easily take the derivative, so even though we might not be able to take the derivative of the path, the discretized path will be piecewise differentiable. This piecewise differentiable path will be enough for us to be able to use the derivative of the path in Equation (2.1.7).

We can also note that the constant A in equations Equations (2.1.1) to (2.1.3), which we replaced in the discretization by the limit of $n \to \infty$ of the constant B^n, which was dependent on ε, was not yet known. In Section 2.3 we have found a definition for the constant B, but in general there is no guarantee that B^n will converge for $n \to \infty$. As this constant is only added for the normalization of the wave functions, the constant should not diverge, though this is not clear from its definition.

One problem which remains in Equation (2.1.7) is that when the potential V is real valued, as it usually will be, the integrand has a constant absolute value of 1 and the integral will not exist as an absolutely convergent Lebesgue integral. Even when this problem can be solved, it is still not clear in what sense the limit in Equation (2.1.7) exists. For this we use the same arguments as we have done in Section 2.2, where we argued that from the highly oscillating nature of the phase, cancellation would follow. As we have cancellation everywhere, except close to the classical path, this would essentially be the only area we would integrate over. From this it might be reasonable to assume that the limit in Equation (2.1.7) would exist, as we now take the limit over finite integrals.

One last difficulty we are facing, is that we have no clear definition for the exponential for an operator in multiple dimensions, when it has no orthonormal basis. We will look at this, using the spectral theory, in Section 4.2.

We will now look at a way of redefining the path integral, in a way which will be less problematic. For this we will follow parts of chapter 7 of Johnson and Lapidus [3]. For this we will look at the Trotter product formula for unitary groups. There exist different versions of this formula, which do not only suffice for unitary groups, but they are not needed for what we want to do. Besides the Trotter product formula, we will also use the essential self-adjointness of the Hamiltonian, which we know from Kato [4]. More information about (essential) self-adjointness can be found in Appendix A.2.

We will now use the Hamiltonian, which is given by

$$H := \frac{-\hbar^2}{2m}\Delta + V \tag{2.4.1}$$

where Δ is the Laplacian acting on functions on $\mathbb{R}^d$ and H itself is the extension to d dimensions of the operator we have already seen in equation 2.3.2.

Before we will go into the redefining of the path integral, we will first look at the integrals in the mean concept. We can then use this concept to take care of some of the difficulties which remained in Equation (2.1.7).

Definition 2.1 (Integral in the mean)**.** Let g be a $\mathbb{C}$-valued function in $L^2(\mathbb{R}^d)$. Let $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}$ be such that, for every $M > 0$,

1. $k(., \xi)$ is in $L^1([-M, M]^d)$ for almost every ξ,
2. $\int_{[-M,M]^d} k(\omega, \xi) d\omega$ is in $L^2(\mathbb{R}^d)$ as a function of ξ.

We say that g is the integral of the mean of k and abusing notation simply write

$$\int_{\mathbb{R}^d} k(\omega,\xi)d\omega = g(\xi), \tag{2.4.2}$$

provided that, as $M \to \infty$,

$$||g(.) - \int_{[-M,M]^d} k(\omega,\cdot)d\omega||_2 \to 0. \tag{2.4.3}$$

Where we use that a measurable function $f : \mathbb{R}^d \to \mathbb{R}$ (or $\mathbb{C}$) is said to be in $L^2_{loc}(\mathbb{R}^d)$ provided that it is square-integrable over every ball in $\mathbb{R}^d$ of finite radius.

Now we will split up our potential into a positive and negative part. This way we get $V = V_+ - V_-$, where $V_+(x) = \max(V(x), 0)$, so the positive term is either zero, or the value of the potential, when the potential has a positive value. In the same way we have $V_-(x) = \max(-V(x), 0)$, so the negative term will be zero, or the value of the potential, wherever it has a negative value. Finally, $L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ will denote the vector space of all $\mathbb{C}$-valued functions on $\mathbb{R}^d$ which can be written as the sum of an L^p-function and an essentially bounded function.

We can now use this to state the following theorem.

Theorem 2.2. *Let $V : \mathbb{R}^d \to \mathbb{R}$ and suppose that V_+ is in $L^2_{loc}(\mathbb{R}^d)$ and V_- is in $L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ Now there are restrictions on the p in $L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$. These restrictions are dependent on the dimension and are given by $p = 2$ if $d \leq 3$, $p > 2$ if $d = 4$, and $p \geq d/2$ if $d \geq 5$.*

Let $\phi \in L^2(\mathbb{R}^d)$. Then, for every $t > 0$, the integrals on the right-hand side of the following formula exist for almost every $x \in \mathbb{R}^d$ when interpreted in the mean and define a function which is in $L^2(\mathbb{R}^d)$ as a function of x:

$$\begin{aligned}
\psi_n(t,x) = &\left(\frac{-im}{2\pi\hbar\frac{t-t'}{n}}\right)^{d/2} \int_{\mathbb{R}^d} \exp\left\{\frac{i}{\hbar}\frac{m}{2\frac{t-t'}{n}}||x_n - x_{n-1}||^2\right\} \exp\left\{\frac{-i}{\hbar}\left(\frac{t-t'}{n}\right)V(x_{n-1})\right\} \\
&\times \left(\frac{-im}{2\pi\hbar\frac{t-t'}{n}}\right)^{d/2} \int_{\mathbb{R}^d} \exp\left\{\frac{i}{\hbar}\frac{m}{2\frac{t-t'}{n}}||x_{n-1} - x_{n-2}||^2\right\} \exp\left\{\frac{-i}{\hbar}\left(\frac{t-t'}{n}\right)V(x_{n-2})\right\} \\
&\times \cdots \times \left(\frac{-im}{2\pi\hbar\frac{t-t'}{n}}\right)^{d/2} \int_{\mathbb{R}^d} \exp\left\{\frac{i}{\hbar}\frac{m}{2\frac{t-t'}{n}}||x_2 - x_1||^2\right\} \exp\left\{\frac{-i}{\hbar}\left(\frac{t-t'}{n}\right)V(x_1)\right\} \\
&\times \cdots \times \left(\frac{-im}{2\pi\hbar\frac{t-t'}{n}}\right)^{d/2} \int_{\mathbb{R}^d} \exp\left\{\frac{i}{\hbar}\frac{m}{2\frac{t-t'}{n}}||x_1 - x_0||^2\right\} \exp\left\{\frac{-i}{\hbar}\left(\frac{t-t'}{n}\right)V(x_0)\right\} \\
&\times \phi(x_0)dx_0dx_1\cdots dx_{n-2}dx_{n-1},
\end{aligned} \tag{2.4.4}$$

where $x_n := x$. Also, there is a function $\psi : (0,+\infty) \times \mathbb{R}^d \to \mathbb{C}$ such that $\psi(t,\cdot) \in L^2(\mathbb{R}^d)$ for every $t > 0$ and, as $n \to \infty$,

$$||\psi(t,\cdot) - \psi_n(t,\cdot)||_2 \to 0. \tag{2.4.5}$$

Equation (2.4.4) differs from Equation (2.1.7) only in that Equation (2.1.7) was, for convenience, restricted to the case $d = 1$, and Equation (2.4.4) is written as an n-fold iterated integral instead of as a multiple integral. In Theorem 2.2 we also clearly see in which sense ψ_n converges to ψ, whereas this convergence between both sides of Equation (2.1.7) is way less clear. Also, the mode of convergence seems more natural, since the probabilities are computed using the probability densities $|\psi(t,\cdot)|^2$.

One interesting thing to note is that the hypotheses of Theorem 2.2 are already sufficient for the potentials we will be working with in this thesis. They are already so general that the positive part of the potential V_+ can have an arbitrary singularity at ∞ as well as finite range singularities as long as they are square-integrable. The assumptions on V_- are more restrictive, as $V_-(x) \to \infty$ as $||x|| \to \infty$ is not permitted and finite range singularities must be pth power integrable, where p must be the same p as we found in Theorem 2.2.

We will now look at the Trotter product formula, which we were working towards. The Trotter product formula has been extended in many different directions. We will state Trotter's original result, as this is sufficient for our discussion. Different versions of the formula and the operator theory background can be found in Johnson and Lapidus [3].

Theorem 2.3 (Trotter product formula)**.** *Let A and B be not necessarily bounded and not necessarily commuting self-adjoint operators on a Hilbert space $\mathscr{H}$. If $A + B$ is essentially self-adjoint on the intersection of the domain of A with the domain of B, then for all $\psi \in \mathscr{H}$*

$$\exp\big(-it(\overline{A+B})\big)\psi = \lim_{n\to\infty}\left(\exp\left\{-i\frac{t}{n}A\right\}\exp\left\{-i\frac{t}{n}B\right\}\right)^n\psi, \tag{2.4.6}$$

uniformly in t on all bounded subsets of $\mathbb{R}$.

Here $(\overline{A+B})$ is the unique self-adjoint extension of $A + B$, since it is its closure. This follows from the definition of essential self-adjointness in Appendix A.2.

Now we might think that Equation (2.4.6) is useless, since it expresses the left hand side, which looks quite simple, as the limit of more complicated looking expressions. The reason why it is a useful formula is that the left hand side appears easier than it actually is, since the operators are usually noncommuting. In practice, we can usually find explicit expressions for

$$\exp\left\{-i\frac{t}{n}A\right\}\exp\left\{-i\frac{t}{n}B\right\} \tag{2.4.7}$$

as is the case for the example we started with.

We can now make the connection between Theorems 2.2 and 2.3, by taking $\mathscr{H} = L^2(\mathbb{R}^d)$, $A = -\frac{\hbar}{2m}\Delta$, and $B = \frac{1}{\hbar}V$. This gives us

$$A + B = \frac{1}{\hbar}\left[-\frac{\hbar^2}{2m}\Delta + V\right] = \frac{1}{\hbar}H, \tag{2.4.8}$$

where H is the energy operator or Hamiltonian, as was given by Equation (2.4.1). This way we can get explicit formulas for both the exponential terms, which we saw in Equation (2.4.4). We can now write the first operator to act on the initial state ϕ, or the second exponential in the formula, to be

$$\exp\left\{-\frac{i}{\hbar}\frac{t}{n}V\right\}, \tag{2.4.9}$$

which is the exponential of the operator of multiplication by $-\frac{i}{\hbar}\frac{t}{n}V$. The next operator to act in Equation (2.4.4) is the only exponential which has the term x_0 in it. That is why this term is associated with integration over x_0. We know that the operator

$$\exp\left\{i\frac{t}{n}\frac{\hbar}{2m}\Delta\right\} \tag{2.4.10}$$

is the operator which has to do with the evolution of a system over a time interval of length t/n, since this is the formula we get when the potential is zero. This thus represents the free particle, at which we will look closer in Section 3.1. Now when we combine these two terms which we found at the right-hand side of Equation (2.4.4), we find that the whole right-hand side is the n-fold iteration of

$$\exp\left\{i\frac{t}{n}\frac{\hbar}{2m}\Delta\right\}\exp\left\{-\frac{i}{\hbar}\frac{t}{n}V\right\}, \tag{2.4.11}$$

just as the right-hand side of Equation (2.4.6) predicted. We thus see that this example unifies these two theorems to give the same result.

Remark. **(a)** Equation (2.4.6) expresses $\exp\{-it(A+B)\}$ in terms of $\exp\{-i\frac{t}{n}A\}$ and $\exp\{-i\frac{t}{n}B\}$. When A and B commute, the relationship is much simpler, it is just given by the familiar exponential law.

$$\exp\big\{-it(A+B)\big\} = \exp\big\{-itA\big\}\exp\big\{-itB\big\} \tag{2.4.12}$$

(For simplicity, we ignore the distinction between $A+B$ and its closure $\overline{A+B}$ in this comment.)

(b) There are alternatives to the right hand side of Equation (2.4.6). One of them is connected to the product formula for imaginary time. We will look at the path integral with imaginary time in Section 4, where we will find that this formula will have nicer stability properties, than the formulas we are working with at the moment.

(c) One can show, under the hypotheses of Theorem 2.2, that the function $\psi(t,x)$ whose existence is established by use of Theorem 2.3 satisfies the Schrödinger equation.

3 Examples

Since we have seen the definition in depth, it will now be nice to see some more of what we can actually use this definition for. Therefore we will now look at some examples.

3.1 Free particle

For now the free particle is the easiest example to start with, as we do not have to take into account the potential, as the free particle has a potential of zero. This will also be a nice example to show us how we can do an explicit calculation when using the path integral. For this section we go along the lines of Shankar [1]. As this potential is zero, we can actually calculate the time evolution operator for this example, by using the discretization for the operator and the action. So by using Equations (2.1.8) and (2.3.11) we can get the following equation for this situation

$$U(x,t;x',t') = \lim_{\substack{N\to\infty\\ \varepsilon\to 0}} B^N \int_{\mathbb{R}^{N-1}} \exp\left(\frac{i}{\hbar}\sum_{j=0}^{N-1}\left[\frac{m}{2}\frac{(x_{j+1}-x_j)^2}{\varepsilon} - \int_{t'+j\varepsilon}^{t'+(j+1)\varepsilon} V(x(t))dt\right]\right) \times dx_1\cdots dx_{N-1}. \tag{3.1.1}$$

As we know the potential to be zero, we can simplify this equation even further. We then get

$$\begin{aligned} U(x,t;x',t') &= \lim_{\substack{N\to\infty\\ \varepsilon\to 0}} B^N \int_{\mathbb{R}^{N-1}} \exp\left(\frac{i}{\hbar}\sum_{j=0}^{N-1}\frac{m}{2}\frac{(x_{j+1}-x_j)^2}{\varepsilon}\right)dx_1\cdots dx_{N-1} \\ &= \lim_{\substack{N\to\infty\\ \varepsilon\to 0}} B^N \int_{\mathbb{R}^{N-1}} \exp\left(\frac{im}{2\hbar}\sum_{j=0}^{N-1}\frac{(x_{j+1}-x_j)^2}{\varepsilon}\right)dx_1\cdots dx_{N-1}. \end{aligned} \tag{3.1.2}$$

We can also use the value we found for the constant B, in equation Equation (2.3.39), to get

$$U(x,t;x',t') = \lim_{\substack{N\to\infty\\ \varepsilon\to 0}} \left(\frac{2\pi\hbar\varepsilon i}{m}\right)^{-N/2} \int_{\mathbb{R}^{N-1}} \exp\left(\frac{im}{2\hbar}\sum_{j=0}^{N-1}\frac{(x_{j+1}-x_j)^2}{\varepsilon}\right)dx_1\cdots dx_{N-1}. \tag{3.1.3}$$

We can rewrite this to

$$\begin{aligned} U(x,t;x',t') &= \lim_{\substack{N\to\infty\\ \varepsilon\to 0}} \left(\frac{2\pi\hbar\varepsilon i}{m}\right)^{-N/2} \int_{\mathbb{R}^{N-1}} \exp\left(\frac{i^2}{i}\sum_{j=0}^{N-1}\frac{m(x_{j+1}-x_j)^2}{2\hbar\varepsilon}\right)dx_1\cdots dx_{N-1} \\ &= \lim_{\substack{N\to\infty\\ \varepsilon\to 0}} \left(\frac{m}{2\pi\hbar\varepsilon i}\right)^{N/2} \int_{\mathbb{R}^{N-1}} \exp\left(-\sum_{j=0}^{N-1}\left[\sqrt{\frac{m}{2\hbar\varepsilon i}}x_{j+1} - \sqrt{\frac{m}{2\hbar\varepsilon i}}x_j\right]^2\right) \\ &\qquad \times dx_1\cdots dx_{N-1}. \end{aligned} \tag{3.1.4}$$

We will now use the substitution $y_j = \sqrt{\frac{m}{2\hbar\varepsilon i}}x_j$. By using $\frac{dy_j}{dx_j} = \sqrt{\frac{m}{2\hbar\varepsilon i}}$ we find that $dx_j = \sqrt{\frac{2\hbar\varepsilon i}{m}}dy_j$. As the integration borders clearly stay the same under this substitution, we get

the following equation

$$\begin{aligned} U(x,t;x',t') &= \lim_{\substack{N\to\infty\\ \varepsilon\to 0}} \left(\frac{m}{2\pi\hbar\varepsilon i}\right)^{N/2} \int_{\mathbb{R}^{N-1}} \exp\Big(-\sum_{j=0}^{N-1}(y_{j+1}-y_j)^2\Big)\left[\sqrt{\frac{2\hbar\varepsilon i}{m}}\right]^{N-1} dy_1\cdots dy_{N-1} \\ &= \lim_{\substack{N\to\infty\\ \varepsilon\to 0}} \left(\frac{m}{2\pi\hbar\varepsilon i}\right)^{N/2} \left(\frac{2\hbar\varepsilon i}{m}\right)^{\frac{N-1}{2}} \int_{\mathbb{R}^{N-1}} \exp\Big(-\sum_{j=0}^{N-1}(y_{j+1}-y_j)^2\Big) dy_1\cdots dy_{N-1} \\ &= \lim_{\substack{N\to\infty\\ \varepsilon\to 0}} \pi^{-\frac{N-1}{2}} \sqrt{\frac{m}{2\pi\hbar\varepsilon i}} \int_{\mathbb{R}^{N-1}} \exp\Big(-\sum_{j=0}^{N-1}(y_{j+1}-y_j)^2\Big) dy_1\cdots dy_{N-1}. \end{aligned} \tag{3.1.5}$$

We now want to start with the integration over y_1. For this we will separate the terms containing y_1. To do this we will first rewrite Equation (3.1.5).

$$\begin{aligned} U(x,t;x',t') = \lim_{\substack{N\to\infty\\ \varepsilon\to 0}} \pi^{-\frac{N-1}{2}} \sqrt{\frac{m}{2\pi\hbar\varepsilon i}} \int_{\mathbb{R}^{N-2}} \exp\Big(-\sum_{j=2}^{N-1}(y_{j+1}-y_j)^2\Big) \\ \left[\int_{\mathbb{R}} \exp\Big(-\big((y_1-y_0)^2+(y_2-y_1)^2\big)\Big) dy_1\right] dy_2\cdots dy_{N-1} \end{aligned} \tag{3.1.6}$$

We will now first calculate the term inside the square brackets, which we will call SB_1 to simplify the notation, in Equation (3.1.6). We will start by rewriting this equation to get

$$\begin{aligned} SB_1 &= \int_{\mathbb{R}} \exp\Big\{-\big((y_1-y_0)^2+(y_2-y_1)^2\big)\Big\} dy_1 \\ &= \int_{\mathbb{R}} \exp\Big\{-\big(y_1^2-2y_0y_1+y_0^2+y_2^2-2y_1y_2+y_1^2\big)\Big\} dy_1 \\ &= \int_{\mathbb{R}} \exp\Big\{-\big(2y_1^2-2y_1(y_0+y_2)+y_0^2+y_2^2\big)\Big\} dy_1 \\ &= \int_{\mathbb{R}} \exp\Big\{-\big(2[y_1^2-2y_1\cdot\frac{1}{2}(y_0+y_2)+\frac{1}{4}(y_0+y_2)^2-\frac{1}{4}(y_0+y_2)^2]+y_0^2+y_2^2\big)\Big\} dy_1 \\ &= \int_{\mathbb{R}} \exp\left\{-\left(2\left[y_1-\frac{1}{2}(y_0+y_2)\right]^2-\frac{1}{2}(y_0+y_2)^2+y_0^2+y_2^2\right)\right\} dy_1 \\ &= \int_{\mathbb{R}} \exp\left\{-\left(2\left[y_1-\frac{(y_0+y_2)}{2}\right]^2-\frac{1}{2}(y_0^2+2y_0y_2+y_2^2)+y_0^2+y_2^2\right)\right\} dy_1 \\ &= \int_{\mathbb{R}} \exp\left\{-\left(2\left[y_1-\frac{(y_0+y_2)}{2}\right]^2+\frac{1}{2}y_0^2-y_0y_2+\frac{1}{2}y_2^2\right)\right\} dy_1 \\ &= \int_{\mathbb{R}} \exp\left\{-\left(2\left[y_1-\frac{(y_0+y_2)}{2}\right]^2+\frac{1}{2}[y_2-y_0]^2\right)\right\} dy_1 \\ &= \exp\Big\{-\frac{1}{2}[y_2-y_0]^2\Big\} \int_{\mathbb{R}} \exp\left\{-2\left[y_1-\frac{(y_0+y_2)}{2}\right]^2\right\} dy_1. \end{aligned} \tag{3.1.7}$$

We can now calculate the integral we got in the final line of Equation (3.1.7) by using the following substitution $z_1 = y_1 - \frac{(y_0+y_2)}{2}$. We can easily see that $dz_1 = dy_1$ and since we are varying y_1 in this integration, but not y_0 or y_2, we can see that the integration boundaries remain the same. This gives us a Gaussian integral to solve, but as we have already done this in Equation (2.3.28) we find that

$$SB_1 = \exp\Big\{ -\frac{1}{2}[y_2 - y_0]^2 \Big\} \int_{\mathbb{R}} \exp\Big\{ -2z_1^2 \Big\} dz_1 = \sqrt{\frac{\pi}{2}} \exp\Big\{ -\frac{1}{2}[y_2 - y_0]^2 \Big\}. \tag{3.1.8}$$

We can now insert this result for the square brackets, Equation (3.1.8), into Equation (3.1.6) to get

$$\begin{aligned} U(x,t;x',t') = \lim_{\substack{N\to\infty \\ \varepsilon\to 0}} \pi^{-\frac{N-1}{2}} \sqrt{\frac{\pi}{2}} \sqrt{\frac{m}{2\pi\hbar\varepsilon i}} \\ \int_{\mathbb{R}^{N-2}} \exp\Big(-\frac{1}{2}(y_2 - y_0)^2 - \sum_{j=2}^{N-1} (y_{j+1} - y_j)^2 \Big) dy_2 \cdots dy_{N-1}. \end{aligned} \tag{3.1.9}$$

We now want to use these same steps as we have done in Equations (3.1.6) to (3.1.8), to integrate over y_2. For this we will again separate the terms containing y_2.

$$\begin{aligned} U(x,t;x',t') = \lim_{\substack{N\to\infty \\ \varepsilon\to 0}} \pi^{-\frac{N-1}{2}} \sqrt{\frac{\pi}{2}} \sqrt{\frac{m}{2\pi\hbar\varepsilon i}} \int_{\mathbb{R}^{N-3}} \exp\Big(-\sum_{j=3}^{N-1} (y_{j+1} - y_j)^2 \Big) \\ \Big[\int_{\mathbb{R}} \exp\Big(-\big(\frac{1}{2}(y_2 - y_0)^2 + (y_3 - y_2)^2\big) \Big) dy_2 \Big] dy_3 \cdots dy_{N-1} \end{aligned} \tag{3.1.10}$$

We will now, once again look at the term in the square brackets, which we will call SB_2.

$$\begin{aligned} SB_2 &= \int_{\mathbb{R}} \exp\Big\{ -\Big(\frac{1}{2}(y_2 - y_0)^2 + (y_3 - y_2)^2\Big) \Big\} dy_2 \\ &= \int_{\mathbb{R}} \exp\Big\{ -\Big(\frac{1}{2}y_2^2 - y_0 y_2 + \frac{1}{2}y_0^2 + y_3^2 - 2y_2 y_3 + y_2^2\Big) \Big\} dy_2 \\ &= \int_{\mathbb{R}} \exp\Big\{ -\Big(\frac{3}{2}y_2^2 - y_2(y_0 + 2y_3) + \frac{1}{2}y_0^2 + y_3^2\Big) \Big\} dy_2 \\ &= \int_{\mathbb{R}} \exp\Big\{ -\Big(\frac{3}{2}\Big[y_2^2 - 2y_2 \cdot \frac{1}{2}\frac{2}{3}(y_0 + 2y_3)\Big] + \frac{1}{2}y_0^2 + y_3^2\Big) \Big\} dy_2 \\ &= \int_{\mathbb{R}} \exp\Big\{ -\Big(\frac{3}{2}\Big[y_2^2 - 2y_2 \cdot \frac{1}{3}(y_0 + 2y_3) + \frac{1}{9}(y_0 + 2y_3)^2 - \frac{1}{9}(y_0 + 2y_3)^2\Big] \\ &\qquad + \frac{1}{2}y_0^2 + y_3^2\Big) \Big\} dy_2 \\ &= \int_{\mathbb{R}} \exp\Big\{ -\Big(\frac{3}{2}\Big[y_2 - \frac{y_0 + 2y_3}{3}\Big]^2 - \frac{1}{6}(y_0 + 2y_3)^2 + \frac{1}{2}y_0^2 + y_3^2\Big) \Big\} dy_2 \\ &= \int_{\mathbb{R}} \exp\Big\{ -\Big(\frac{3}{2}\Big[y_2 - \frac{y_0 + 2y_3}{3}\Big]^2 - \frac{1}{6}y_0^2 - \frac{2}{3}y_0 y_3 - \frac{2}{3}y_3^2 + \frac{1}{2}y_0^2 + y_3^2\Big) \Big\} dy_2 \\ &= \int_{\mathbb{R}} \exp\Big\{ -\Big(\frac{3}{2}\Big[y_2 - \frac{y_0 + 2y_3}{3}\Big]^2 + \frac{1}{3}y_0^2 - \frac{2}{3}y_0 y_3 + \frac{1}{3}y_3^2\Big) \Big\} dy_2. \end{aligned} \tag{3.1.11}$$

We can continue with this calculation to get

$$\begin{aligned} SB_2 &= \int_{\mathbb{R}} \exp\left\{ -\left(\frac{3}{2}\left[y_2 - \frac{y_0+2y_3}{3}\right]^2 + \frac{1}{3}(y_3-y_0)^2\right)\right\} dy_2 \\ &= \exp\left\{ -\frac{1}{3}(y_3-y_0)^2\right\} \int_{\mathbb{R}} \exp\left\{ -\frac{3}{2}\left[y_2 - \frac{y_0+2y_3}{3}\right]^2\right\} dy_2. \end{aligned} \tag{3.1.12}$$

By now using the substitution $z_2 = y_2 - \frac{y_0+2y_3}{3}$, which gives us $dz_2 = dy_2$ and by using the same argument as before we find that the integration boundaries remain the same. This again gives us a Gaussian integral, which is given by

$$SB_2 = \exp\left\{ -\frac{1}{3}(y_3-y_0)^2\right\} \int_{\mathbb{R}} \exp\left\{ -\frac{3}{2}z_2^2\right\} dz_2 = \sqrt{\frac{2\pi}{3}} \exp\left\{ -\frac{1}{3}(y_3-y_0)^2\right\}. \tag{3.1.13}$$

We can now insert this result for the square brackets, Equation (3.1.13), into Equation (3.1.10) to get

$$\begin{aligned} U(x,t;x',t') = &\lim_{\substack{N\to\infty \\ \varepsilon\to 0}} \pi^{-\frac{N-1}{2}} \sqrt{\frac{\pi}{2}}\sqrt{\frac{2\pi}{3}}\sqrt{\frac{m}{2\pi\hbar\varepsilon i}} \\ &\int_{\mathbb{R}^{N-3}} \exp\left(-\frac{1}{3}(y_3-y_0)^2 - \sum_{j=3}^{N-1}(y_{j+1}-y_j)^2\right) dy_3\cdots dy_{N-1} \\ = &\lim_{\substack{N\to\infty \\ \varepsilon\to 0}} \pi^{-\frac{N-1}{2}} \sqrt{\frac{\pi^2}{3}}\sqrt{\frac{m}{2\pi\hbar\varepsilon i}} \\ &\int_{\mathbb{R}^{N-3}} \exp\left(-\frac{1}{3}(y_3-y_0)^2 - \sum_{j=3}^{N-1}(y_{j+1}-y_j)^2\right) dy_3\cdots dy_{N-1}. \end{aligned} \tag{3.1.14}$$

We can repeat these step for y_3 to get

$$\begin{aligned} U(x,t;x',t') = &\lim_{\substack{N\to\infty \\ \varepsilon\to 0}} \pi^{-\frac{N-1}{2}} \sqrt{\frac{\pi^3}{4}}\sqrt{\frac{m}{2\pi\hbar\varepsilon i}} \\ &\int_{\mathbb{R}^{N-4}} \exp\left(-\frac{1}{4}(y_4-y_0)^2 - \sum_{j=4}^{N-1}(y_{j+1}-y_j)^2\right) dy_4\cdots dy_{N-1}. \end{aligned} \tag{3.1.15}$$

By repeating these steps we find that

$$\begin{aligned} U(x,t;x',t') = &\lim_{\substack{N\to\infty \\ \varepsilon\to 0}} \pi^{-\frac{N-1}{2}} \sqrt{\frac{\pi^{N-2}}{N-1}}\sqrt{\frac{m}{2\pi\hbar\varepsilon i}} \\ &\int_{\mathbb{R}} \exp\left(-\frac{1}{N-1}(y_{N-1}-y_0)^2 - (y_N-y_{N-1})^2\right) dy_{N-1}. \end{aligned} \tag{3.1.16}$$

We can use the same steps as before to calculate this integral, which gives us

$$\begin{aligned} U(x,t;x',t') &= \lim_{\substack{N\to\infty \\ \varepsilon\to 0}} \pi^{-\frac{N-1}{2}} \sqrt{\frac{\pi^{N-2}}{N-1}} \sqrt{\frac{(N-1)\pi}{N}} \sqrt{\frac{m}{2\pi\hbar\varepsilon i}} \exp\Big(-\frac{1}{N}(y_N - y_0)^2 \Big) \\ &= \lim_{\substack{N\to\infty \\ \varepsilon\to 0}} \pi^{-\frac{N-1}{2}} \sqrt{\frac{\pi^{N-1}}{N}} \sqrt{\frac{m}{2\pi\hbar\varepsilon i}} \exp\Big(-\frac{1}{N}(y_N - y_0)^2 \Big) \\ &= \lim_{\substack{N\to\infty \\ \varepsilon\to 0}} \pi^{-\frac{N-1}{2}} \pi^{\frac{N-1}{2}} \sqrt{\frac{m}{2\pi\hbar N\varepsilon i}} \exp\Big(-\frac{1}{N}(y_N - y_0)^2 \Big) \\ &= \lim_{\substack{N\to\infty \\ \varepsilon\to 0}} \sqrt{\frac{m}{2\pi\hbar N\varepsilon i}} \exp\Big(-\frac{1}{N}(y_N - y_0)^2 \Big). \end{aligned} \tag{3.1.17}$$

We can now insert the substitution $y_j = \sqrt{\frac{m}{2\hbar\varepsilon i}} x_j$ into Equation (3.1.18) to get

$$\begin{aligned} U(x,t;x',t') &= \lim_{\substack{N\to\infty \\ \varepsilon\to 0}} \sqrt{\frac{m}{2\pi\hbar N\varepsilon i}} \exp\Big(-\frac{1}{N}\Big[\sqrt{\frac{m}{2\hbar\varepsilon i}} x_N - \sqrt{\frac{m}{2\hbar\varepsilon i}} x_0\Big]^2 \Big) \\ &= \lim_{\substack{N\to\infty \\ \varepsilon\to 0}} \sqrt{\frac{m}{2\pi\hbar N\varepsilon i}} \exp\Big(-\frac{1}{N}\frac{m}{2\hbar\varepsilon i}\big[x_N - x_0\big]^2 \Big) \\ &= \lim_{\substack{N\to\infty \\ \varepsilon\to 0}} \sqrt{\frac{m}{2\pi\hbar N\varepsilon i}} \exp\Big(-\frac{m}{2\hbar N\varepsilon i}\big[x_N - x_0\big]^2 \Big). \end{aligned} \tag{3.1.18}$$

As we know that $x_N = x$, $x_0 = x'$ and as we defined $t = t' + N\varepsilon$, we find that $N\varepsilon = t - t'$. We can insert all of this into Equation (3.1.18) to get

$$\begin{aligned} U(x,t;x',t') &= \lim_{\substack{N\to\infty \\ \varepsilon\to 0}} \sqrt{\frac{m}{2\pi\hbar(t-t')i}} \exp\Big(-\frac{m}{2\hbar(t-t')i}\big[x - x'\big]^2 \Big) \\ &= \sqrt{\frac{m}{2\pi\hbar(t-t')i}} \exp\Big(-\frac{m}{2\hbar(t-t')i}\big[x - x'\big]^2 \Big). \end{aligned} \tag{3.1.19}$$

Now by using the discretization we were actually able to calculate the time operator for a free particle, which gave us the result we saw in Equation (3.1.19).

3.1.1 Free particle in classical limit

We are now wondering what happens when we look at the path integral formula and insert the classical path into this. If we look at the classical path of a free particle that travels between x' and x in time t' and t, we know that the equation of the path is given by

$$x_{cl}(s) = x' + \frac{x - x'}{t - t'}(s - t'). \tag{3.1.20}$$

As we know that for the action we take the time derivative of the path, we will also calculate this. This gives us

$$\dot{x}_{cl}(s) = \frac{x - x'}{t - t'}. \tag{3.1.21}$$

We can now use the definition for the action, given in Equation (2.3.7), to calculate the action for the classical path. As we are working with the free particle, we know the potential to be zero, which gives us

$$S_{cl} = \int_{t'}^{t} \frac{1}{2} m \left(\frac{x - x'}{t - t'} \right)^2 ds = \frac{m}{2} \left(\frac{x - x'}{t - t'} \right)^2 (t - t') = \frac{m}{2} \frac{(x - x')^2}{t - t'}. \tag{3.1.22}$$

As the classical path for a free particle is given by a straight line through these points, there is no need for us to use the discretization and interpolation of the path. This shows us that we can use the formula given in Equation (2.1.8), where we set $N = 1$, as this will already give us the exact formula for our path. As we have $N = 1$, there will be no x_j left, to integrate over. Also, as we have $\varepsilon = \frac{t-t'}{N}$, we now find that $\varepsilon = t - t'$. This gives us, by using Equation (2.3.39) that

$$B = \sqrt{\frac{m}{2\pi\hbar(t - t')i}} \tag{3.1.23}$$

in our case. We can insert all of this into Equation (2.1.8) to get

$$\begin{aligned} U(x, t; x', t') &= \sqrt{\frac{m}{2\pi\hbar(t - t')i}} \exp\left(\frac{i}{\hbar} \frac{m}{2} \frac{(x - x')^2}{t - t'} \right) \\ &= \sqrt{\frac{m}{2\pi\hbar(t - t')i}} \exp\left(- \frac{m}{2\hbar(t - t')i} (x - x')^2 \right). \end{aligned} \tag{3.1.24}$$

The interesting result is that we find that this result, Equation (3.1.24), is exactly equal to Equation (3.1.19). This is a very interesting result as using the classical path thus gives us the exact same result as the explicit calculation. This not only tells us that for this example the classical limit will indeed give us the classical answer, it also makes our calculations way easier. We did not expect this result, but we find that an approximation, where we only use the classical path suffices to calculate the time evolution operator of the free particle.

We can also rewrite Equation (3.1.19) or Equation (3.1.24) to be

$$U(x, t; x', t') = \sqrt{\frac{m}{2\pi\hbar(t - t')i}} \exp\left(i \frac{m}{2\hbar(t - t')} (x - x')^2 \right). \tag{3.1.25}$$

Here we can see that Equation (3.1.25) starts to look like a wave, where the term in the exponential, without the factor i, plays the role of the phase. We will use this wave like property of the solution later on.

3.2 Double slit experiment

Now we want to look at the double slit experiment, as this is a very important quantum mechanical example. We will first assume that the slits are infinitesimally small and then look at the example with slits with finite width. We know that the only constraint for a particle in the double slit experiment is given by the slits, since it has to go through either one of them. Therefore we know that everywhere else the particle can just act like a free particle. Since we have seen in Equation (3.1.25) that the free particle has a wave-like property, we will use this in our calculations.

3.2.1 Double slit experiment with infinitesimal width

In Figure 5 we find the set-up of the double slit experiment. The interesting result of the

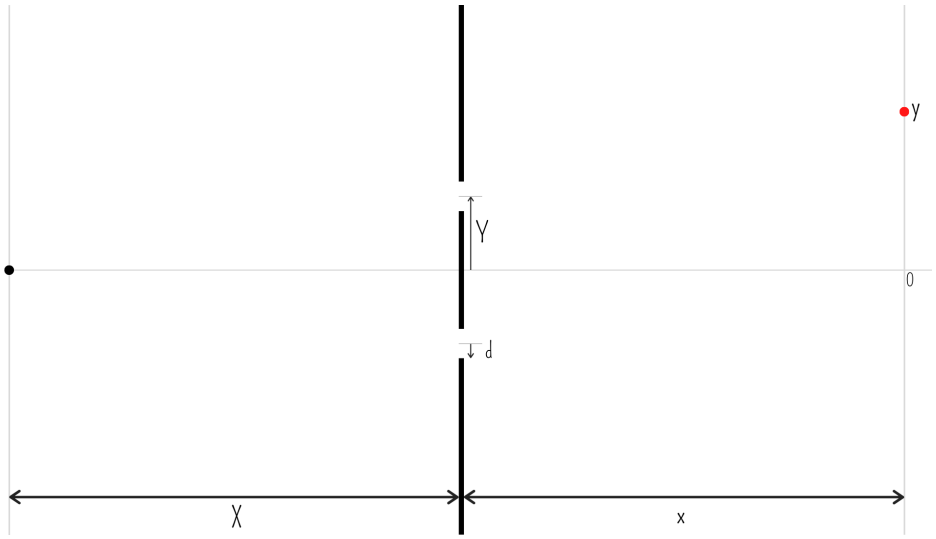


Figure 5: The set-up of the double slit experiment.

double slit experiment is that it is an example that both light and particles can behave as waves. The way we will look at this example is through these waves. We will now look at the case where the slits have infinitesimal width and reside at a distance $2Y$ from one another.

If we have waves coming through both slits, these waves will start interfering with each other. As these waves both come from the same source, this is the black dot in Figure 5, they will have the same wavelength λ and amplitude a. To look at the interference between two waves after they have gone through the slits, we will look at two waves, which go through the slits with the same angle θ. In Figure 6 we can see that the two waves with the same wavelength, will have a path difference. We will now calculate the path difference between these two paths. In Figure 6 we can see half the path difference is given by s, which is the side of the triangle, opposite to the blue angle θ. Now we already know that the side between the yellow and the blue angle has length Y. Since we can see in Figure 6 that we are working with a right triangle, we can now calculate the length of the side s, which is given by $s = Y\sin(\theta)$.

Using the length of this side s and the symmetry of the angles, we can see that the lower wave will have traveled a distance $2s$ more than the upper wave. We will write that the lower wave traveled a relative distance of $-s$ and the upper wave traveled a distance of $+s$, to mirror the symmetry of the situation. Now we can calculate the phase difference between the two waves, by using the formula for the phase difference, which can be found in Chapter 10 of Hecht [5]. The formula for the phase difference is given by $\Delta\phi = \frac{2\pi}{\lambda}\Delta y$, where Δy is the difference in traveled distance, so for us this is given by $\Delta y = \pm s = \pm Y\sin(\theta)$. Now the phase difference for the upper wave is given by $\Delta\phi_u = -\frac{2\pi}{\lambda}Y\sin(\theta)$ and for the lower wave this is given by $\Delta\phi_l = \frac{2\pi}{\lambda}Y\sin(\theta)$. Using this, we can calculate the relative wave functions, one for the wave from the upper slit, the other for the wave of the lower slit. For the upper

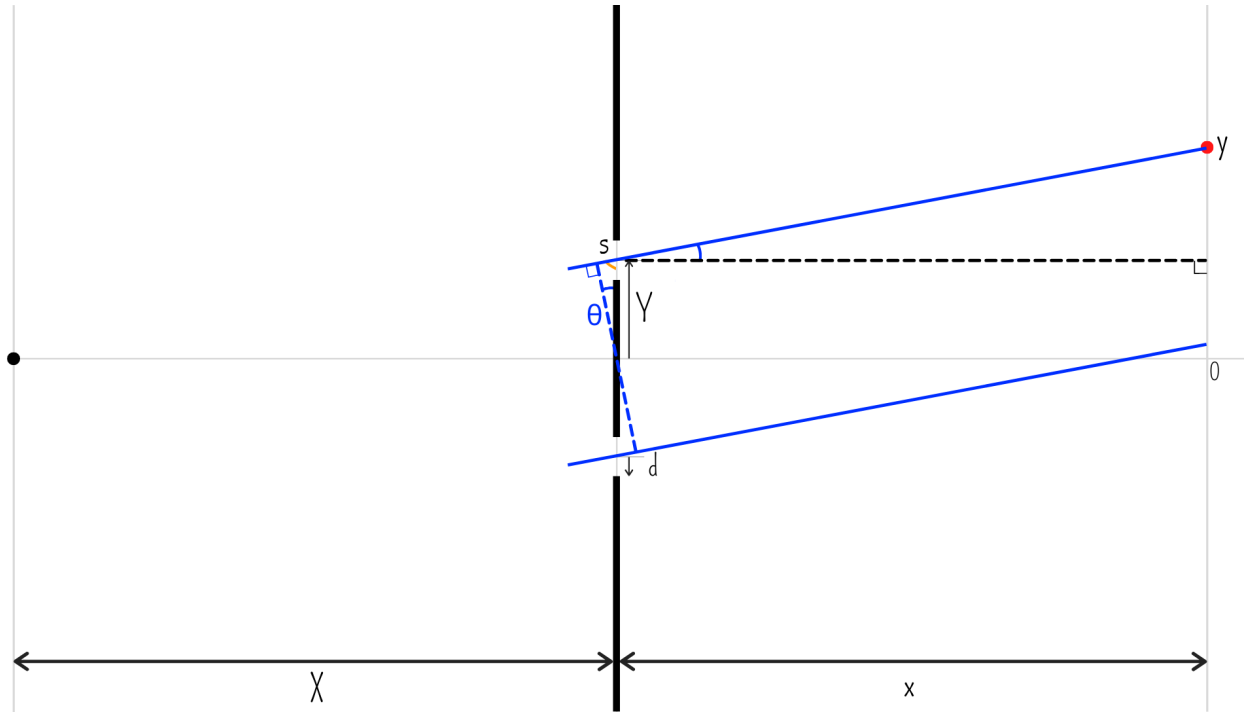


Figure 6: The path difference between two waves traveling through the slits with the same angle θ.

slit this relative wave function will be given by

$$\psi_u = a \exp\left(- i\frac{2\pi}{\lambda} Y \sin(\theta)\right) \tag{3.2.1}$$

and for the lower slit this will be given by

$$\psi_l = a \exp\left(i\frac{2\pi}{\lambda} Y \sin(\theta)\right). \tag{3.2.2}$$

We know from Hecht [5] about superposition of waves, which means that we are allowed to add the waves. We want to calculate the total wave after the slits and can now do this by adding the wave functions, or probability amplitudes, which we already know from Equations (3.2.1) and (3.2.2). So the probability amplitude for the total wave is given by

$$\begin{aligned} U(\theta) =& a \exp\left(i\frac{2\pi}{\lambda} Y \sin(\theta)\right) + a \exp\left(- i\frac{2\pi}{\lambda} Y \sin(\theta)\right) \\ =& a\left[\exp\left(i\frac{2\pi}{\lambda} Y \sin(\theta)\right) + \exp\left(- i\frac{2\pi}{\lambda} Y \sin(\theta)\right)\right] \\ =& 2a \cos\left(\frac{2\pi}{\lambda} Y \sin(\theta)\right). \end{aligned} \tag{3.2.3}$$

We can use this to get the intensity of the interference pattern, which is given by the square of the probability amplitude, so we get

$$I(\theta) = 4a^2 \cos^2\left(\frac{2\pi}{\lambda} Y \sin(\theta)\right). \tag{3.2.4}$$

Now we want to find a definition for the angle θ, so we can rewrite the formula for the intensity to something we can work with. Now if we look at Figure 6 we see that there is one other angle blue, this is also the angle θ. We know this, because in the triangle with the blue and the yellow angle, which we will call α, we know that the third angle is a right angle. As all the angles of a triangle combined have to be 180°, we know that the angle θ is given by $\theta = 180° - 90° - \alpha$. As the blue line is a straight line, the blue angle between this line and the striped black line will be given by $180° - 90° - \alpha$. So we find that this angle must be equal to θ.

Now we want to find a definition for the angle θ, which we will do by using the blue angle, which we just found to be equal to θ. Of the three sides of the triangle which contains this blue angle, we can easily deduce the length of two of the sides. By using Figure 6 we find the length of the side opposite to the blue angle, this length is given by $y - Y$. Using Figure 6 we can also see that the side adjacent to the blue angle has length x. Now we can calculate the blue angle, which is equal to θ, by using

$$\tan(\theta) = \frac{y - Y}{x}, \tag{3.2.5}$$

so we get

$$\theta = \tan^{-1}\left(\frac{y - Y}{x}\right). \tag{3.2.6}$$

We can now insert Equation (3.2.6) into Equations (3.2.3) and (3.2.4) to get

$$U(\theta) = 2a\cos\left[\frac{2\pi}{\lambda}Y\sin\left(\tan^{-1}\left(\frac{y - Y}{x}\right)\right)\right] \tag{3.2.7}$$

and

$$I(\theta) = 4a^2\cos^2\left[\frac{2\pi}{\lambda}Y\sin\left(\tan^{-1}\left(\frac{y - Y}{x}\right)\right)\right]. \tag{3.2.8}$$

We can now use Equation (3.2.8)to plot the intensity of the double slit experiment with infinitesimal width. This result is given in Figure 7.

3.2.2 Double slit experiment with finite width

We will now look at the double slit experiment, where the slits have finite width. We will find that several aspects of the calculations will stay the same, but since we have to take into account the width of the slits, we will have to take a few extra steps. In Equations (3.2.1) and (3.2.2) we have seen the relative waves for the upper and lower slit.

Now we will first look at waves that have gone through the lower slit. In Equation (3.2.2) we saw that the wave depended on Y, which is the distance between the middle of the wall and to the middle of the slit, as we can see in Figure 6. As the slits were infinitesimal in the previous section, this was not a problem. However, as this is no longer the case, we will substitute Y by $Y + \delta$. Here $-d \leq \delta \leq d$, where $2d$ is the width of the slit.

In the previous section, we have also seen that if we want to know the wave after the slits, we can sum over them. Now to calculate the wave after a single slit, we will use the same

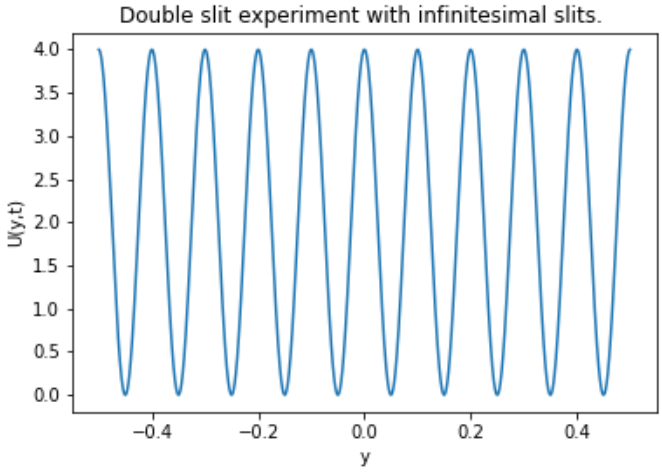


Figure 7: The intensity of the interference pattern of double slits with infinitesimal width.

method. But since the slit has a length of $2d$ and we cannot sum over a continuous interval, to find the wave after a single slit, we will have to do the following

$$\begin{aligned}
\psi_{l,d}(y) &= \int_{-d}^{d} a \exp\left(i\frac{2\pi}{\lambda}(Y+\delta)\sin(\theta)\right)d\delta \\
&= a\exp\left(i\frac{2\pi}{\lambda}Y\sin(\theta)\right)\int_{-d}^{d}\exp\left(i\frac{2\pi}{\lambda}\delta\sin(\theta)\right)d\delta \\
&= a\exp\left(i\frac{2\pi}{\lambda}Y\sin(\theta)\right)\left[\frac{\lambda}{2\pi i\sin(\theta)}\exp\left(i\frac{2\pi}{\lambda}\delta\sin(\theta)\right)\right]_{-d}^{d} \\
&= a\exp\left(i\frac{2\pi}{\lambda}Y\sin(\theta)\right)\frac{\lambda}{2\pi i\sin(\theta)}\left[\exp\left(i\frac{2\pi}{\lambda}d\sin(\theta)\right)-\exp\left(-i\frac{2\pi}{\lambda}d\sin(\theta)\right)\right] \\
&= 2ad\exp\left(i\frac{2\pi}{\lambda}Y\sin(\theta)\right)\frac{\lambda}{2\pi d\sin(\theta)}\sin\left(\frac{2\pi}{\lambda}d\sin(\theta)\right) \\
&= 2ad\exp\left(i\frac{2\pi}{\lambda}Y\sin(\theta)\right)\mathrm{sinc}\left(\frac{2\pi}{\lambda}d\sin(\theta)\right),
\end{aligned} \tag{3.2.9}$$

where $\mathrm{sinc}(x) = \sin(x)/x$. If we now use the value we found for θ in Equation (3.2.6), we can plot the squared wave function, which can be found in Figure 9, to find the diffraction pattern we get from a single slit with finite width.

We will now use the same steps as we did in Equation (3.2.9) to get the relative wave

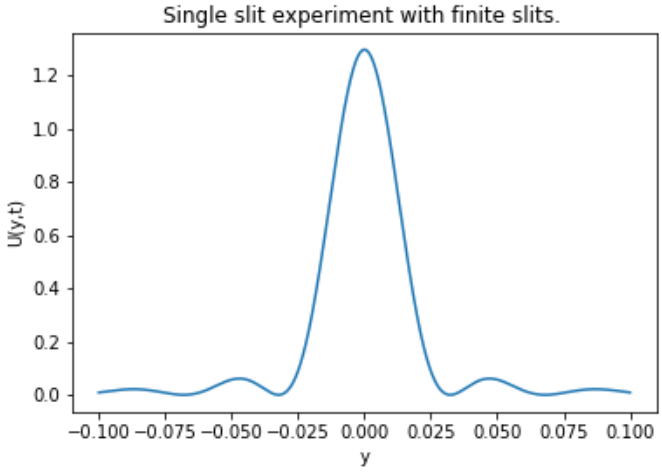


Figure 8: The diffraction pattern of a single slit with finite width.

after the upper slit with finite width.

$$
\begin{aligned}
\psi_{u,d}(y) &= \int_{-d}^{d} a \exp\left(-i\frac{2\pi}{\lambda}(Y+\delta)\sin(\theta)\right) d\delta \\
&= a\exp\left(-i\frac{2\pi}{\lambda}Y\sin(\theta)\right)\int_{-d}^{d}\exp\left(-i\frac{2\pi}{\lambda}\delta\sin(\theta)\right)d\delta \\
&= a\exp\left(-i\frac{2\pi}{\lambda}Y\sin(\theta)\right)\left[-\frac{\lambda}{2\pi i\sin(\theta)}\exp\left(-i\frac{2\pi}{\lambda}\delta\sin(\theta)\right)\right]_{-d}^{d} \\
&= -a\exp\left(-i\frac{2\pi}{\lambda}Y\sin(\theta)\right)\frac{\lambda}{2\pi i\sin(\theta)}\left[\exp\left(-i\frac{2\pi}{\lambda}d\sin(\theta)\right) - \exp\left(i\frac{2\pi}{\lambda}d\sin(\theta)\right)\right] \\
&= -2ad\exp\left(i\frac{2\pi}{\lambda}Y\sin(\theta)\right)\frac{\lambda}{2\pi d\sin(\theta)}\sin\left(-\frac{2\pi}{\lambda}d\sin(\theta)\right) \\
&= -2ad\exp\left(i\frac{2\pi}{\lambda}Y\sin(\theta)\right)\frac{\lambda}{2\pi d\sin(\theta)}\cdot -\sin\left(\frac{2\pi}{\lambda}d\sin(\theta)\right) \\
&= 2ad\exp\left(-i\frac{2\pi}{\lambda}Y\sin(\theta)\right)\frac{\lambda}{2\pi d\sin(\theta)}\sin\left(\frac{2\pi}{\lambda}d\sin(\theta)\right) \\
&= 2ad\exp\left(-i\frac{2\pi}{\lambda}Y\sin(\theta)\right)\mathrm{sinc}\left(\frac{2\pi}{\lambda}d\sin(\theta)\right)
\end{aligned}
\tag{3.2.10}
$$

We can now use the superposition of waves once again, to calculate the total relative wave

after the two slits.

$$\begin{aligned}
U(\theta) =& \psi_{l,d}(y) + \psi_{u,d}(y) = 2ad\exp\left(i\frac{2\pi}{\lambda}Y\sin(\theta)\right)\mathrm{sinc}\left(\frac{2\pi}{\lambda}d\sin(\theta)\right) \\
&+ 2ad\exp\left(-i\frac{2\pi}{\lambda}Y\sin(\theta)\right)\mathrm{sinc}\left(\frac{2\pi}{\lambda}d\sin(\theta)\right) \\
=& 2ad\left[\exp\left(i\frac{2\pi}{\lambda}Y\sin(\theta)\right) + \exp\left(-i\frac{2\pi}{\lambda}Y\sin(\theta)\right)\right]\mathrm{sinc}\left(\frac{2\pi}{\lambda}d\sin(\theta)\right) \qquad (3.2.11) \\
=& 2ad2\cos\left(\frac{2\pi}{\lambda}Y\sin(\theta)\right)\mathrm{sinc}\left(\frac{2\pi}{\lambda}d\sin(\theta)\right) \\
=& 4ad\cos\left(\frac{2\pi}{\lambda}Y\sin(\theta)\right)\mathrm{sinc}\left(\frac{2\pi}{\lambda}d\sin(\theta)\right)
\end{aligned}$$

We can now use the fact that the intensity is the probability amplitude squared to get

$$I(\theta) = 16a^2d^2\cos^2\left(\frac{2\pi}{\lambda}Y\sin(\theta)\right)\mathrm{sinc}^2\left(\frac{2\pi}{\lambda}d\sin(\theta)\right). \qquad (3.2.12)$$

We can now use Equation (3.2.6) to get

$$U(\theta) = 4ad\cos\left(\frac{2\pi}{\lambda}Y\sin\left(\tan^{-1}\left(\frac{y-Y}{x}\right)\right)\right)\mathrm{sinc}\left(\frac{2\pi}{\lambda}d\sin\left(\tan^{-1}\left(\frac{y-Y}{x}\right)\right)\right) \qquad (3.2.13)$$

and

$$I(\theta) = 16a^2d^2\cos^2\left(\frac{2\pi}{\lambda}Y\sin\left(\tan^{-1}\left(\frac{y-Y}{x}\right)\right)\right)\mathrm{sinc}^2\left(\frac{2\pi}{\lambda}d\sin\left(\tan^{-1}\left(\frac{y-Y}{x}\right)\right)\right). \qquad (3.2.14)$$

In Figure 9 we find the plot of the intensity of the double slit experiment with the finite width. In this figure we can see the diffraction pattern, which we already saw in Figure 8, and the interference pattern, which we saw in Figure 7, combined. In Figure 10 we find the plot of the intensity of the double slit, Equation (3.2.14), and the intensity of the single slit. In this figure we can also clearly see that the diffraction pattern is the reason for the missing orders in the double slit result.

More information about interference and diffraction can for example be found in Chapters 35 and 36 of Young and Freedman [6].

3.3 Harmonic oscillator (and similar potentials)

To further understand the calculations and possibilities which follow from the path integral, we will look at another example. The first example that comes to mind is the harmonic oscillator. We will look at this example by first looking at a class of potentials to which the harmonic oscillator belongs. To be exact, we will be looking at potentials which are given by $V = a + bx + cx^2 + d\dot{x} + ex\dot{x}$. Our goal is to solve the path integral for this class of potentials and to derive the solution of the harmonic oscillator from this. We will do this by largely following Shankar [1].

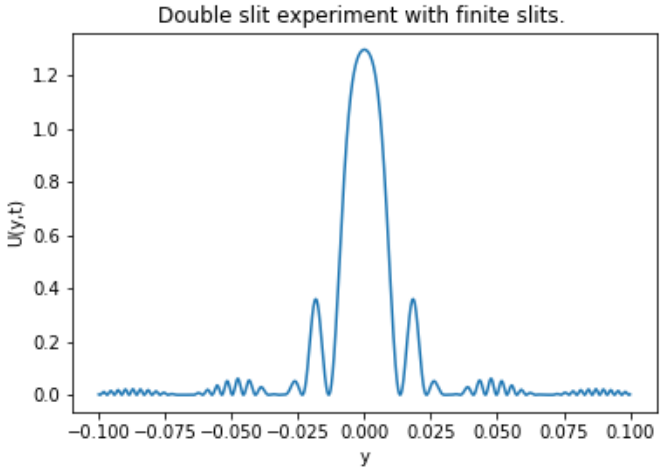


Figure 9: The interference pattern of two slits with finite width.

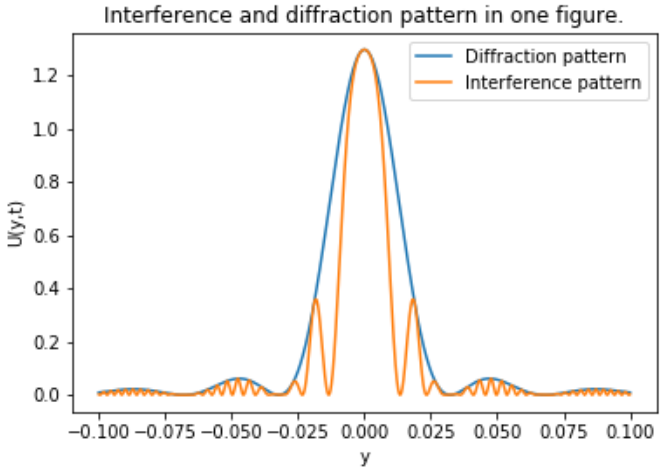


Figure 10: The interference and diffraction pattern for a double and single slit.

Before we will try to calculate the path integral for these potentials, we will rewrite the formula for the path. We will separate the path x into the classical path x_{cl} and its deviation from the classical path y. We can now write every path as

$$x(s) = x_{cl}(s) + y(s). \tag{3.3.1}$$

From this it follows that

$$\dot{x}(s) = \dot{x}_{cl}(s) + \dot{y}(s). \tag{3.3.2}$$

We know that all paths start at x' and end at x. We can take the time at the start to be 0 and at the end to be t. We then get that for each path, including the classical path, it holds that $x(0) = x'$ and $x(t) = x$. This thus tells us that $y(0) = 0$ and $y(t) = 0$ as none of the paths deviates from the classical path at these points.

As we have done before, we can now discretize these paths, which gives us

$$x_i = x(s_i) = x_{cl}(s_i) + y(s_i) = x_{cl}(s_i) + y_i. \tag{3.3.3}$$

For every path $x_{cl}(s_i)$ is the same, since it is just some constant at time s_i. Therefore we find that $dx_i = dy_i$. As the path $x(t)$ goes from x' to x and the path $y(t)$ goes from 0 to 0, we find that

$$\int_{x'}^{x} \mathscr{D}[x(s)] = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} dx_1 \cdots dx_{N-1} = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} dy_1 \cdots dy_{N-1} = \int_{0}^{0} \mathscr{D}[y(s)]. \tag{3.3.4}$$

We can now use Equation (2.1.2) to get

$$U(x,t;x') = \int_{x'}^{x} e^{\frac{i}{\hbar}S[x(s)]}\mathscr{D}[x(s)] = \int_{0}^{0} e^{\frac{i}{\hbar}S[x(s)]}\mathscr{D}[y(s)] = \int_{0}^{0} e^{\frac{i}{\hbar}S[x_{cl}(s)+y(s)]}\mathscr{D}[y(s)]. \tag{3.3.5}$$

We will now look at the term $S[x_{cl}(s) + y(s)]$ as we do not know how to work with this term. To get a definition we can use, we will use a Taylor expansion around $x_{cl}(s)$, as we have already seen in Section 2.2 that the only paths we will usually need to take into account will be paths close to the classical one. We know that the formula for the action is given by Equation (A.1.1), which in our case will become

$$S[x_{cl}(s) + y(s)] = \int_0^t \mathscr{L}(x_{cl} + y, \dot{x}_{cl} + \dot{y})ds. \tag{3.3.6}$$

Since the Lagrangian is dependent on the path and its derivative, the Taylor expansion will become

$$\begin{aligned}\mathscr{L}(x_{cl} + y, \dot{x}_{cl} + \dot{y}) =& \mathscr{L}(x_{cl}, \dot{x}_{cl}) + \left(\frac{\partial \mathscr{L}}{\partial x}\bigg|_{x_{cl}} y + \frac{\partial \mathscr{L}}{\partial \dot{x}}\bigg|_{x_{cl}} \dot{y}\right) \\ &+ \frac{1}{2}\left(\frac{\partial^2 \mathscr{L}}{\partial x^2}\bigg|_{x_{cl}} y^2 + 2\frac{\partial^2 \mathscr{L}}{\partial x \partial \dot{x}}\bigg|_{x_{cl}} y\dot{y} + \frac{\partial^2 \mathscr{L}}{\partial \dot{x}^2}\bigg|_{x_{cl}} \dot{y}^2\right).\end{aligned} \tag{3.3.7}$$

We only work until the second derivative, as we know that the highest orders of the terms in the kinetic part $T = \frac{1}{2}m\dot{x}^2$ and the specific potentials we are working with will be quadratic. In other words, any third (or higher order) derivative of the Lagrangian will be zero, therefore we do not include them in the formula.

We will calculate the integral over the Lagrangian, which gives us the action, in three parts. These will be the three terms we found in Equation (3.3.7). The first term gives us, through the definition of the action,

$$\int_0^t \mathscr{L}(x_{cl}, \dot{x}_{cl})ds = S[x_{cl}(s)] = S_{cl}. \tag{3.3.8}$$

For the second term we will use the equation of motion, which we have found in Equa-

tion (A.1.9), and the fact that $y(0) = y(t) = 0$ to get

$$\begin{aligned}\int_0^t \left(\frac{\partial \mathscr{L}}{\partial x}\bigg|_{x_{cl}} y + \frac{\partial \mathscr{L}}{\partial \dot{x}}\bigg|_{x_{cl}} \dot{y}\right) ds &= \int_0^t \left(\frac{\partial \mathscr{L}}{\partial x}\bigg|_{x_{cl}} y + \frac{\partial \mathscr{L}}{\partial \dot{x}}\bigg|_{x_{cl}} \dot{y} + \left[\frac{d}{dt}\frac{\partial \mathscr{L}}{\partial \dot{x}}\bigg|_{x_{cl}}\right] y - \left[\frac{d}{dt}\frac{\partial \mathscr{L}}{\partial \dot{x}}\bigg|_{x_{cl}}\right] y\right) ds \\ &= \int_0^t \left(\left[\frac{\partial \mathscr{L}}{\partial x}\bigg|_{x_{cl}} - \frac{d}{dt}\frac{\partial \mathscr{L}}{\partial \dot{x}}\bigg|_{x_{cl}}\right] y + \frac{\partial \mathscr{L}}{\partial \dot{x}}\bigg|_{x_{cl}} \left[\frac{d}{dt} y\right] + \left[\frac{d}{dt}\frac{\partial \mathscr{L}}{\partial \dot{x}}\bigg|_{x_{cl}}\right] y\right) ds \\ &= \int_0^t \left(0 \cdot y + \frac{d}{dt}\left[\frac{\partial \mathscr{L}}{\partial \dot{x}}\bigg|_{x_{cl}} y\right]\right) ds = \left[\frac{\partial \mathscr{L}}{\partial \dot{x}}\bigg|_{x_{cl}} y\right]_0^t \\ &= \frac{\partial \mathscr{L}}{\partial \dot{x}}\bigg|_{x_{cl},t} y(t) + \frac{\partial \mathscr{L}}{\partial \dot{x}}\bigg|_{x_{cl},0} y(0) = \frac{\partial \mathscr{L}}{\partial \dot{x}}\bigg|_{x_{cl},t} \cdot 0 + \frac{\partial \mathscr{L}}{\partial \dot{x}}\bigg|_{x_{cl},0} \cdot 0 = 0.\end{aligned} \tag{3.3.9}$$

To simplify the third term we use the fact that we are looking at potentials of the form $V = a + bx + cx^2 + d\dot{x} + ex\dot{x}$. This tells us that our Lagrangian is given by $\mathscr{L} = \frac{1}{2}m\dot{x}^2 - a - bx - cx^2 - d\dot{x} - ex\dot{x}$. From this we find

$$\frac{\partial^2 \mathscr{L}}{\partial x^2} = -2c, \tag{3.3.10}$$

$$2\frac{\partial^2 \mathscr{L}}{\partial x \partial \dot{x}} = 2 \cdot -e = -2e, \tag{3.3.11}$$

$$\frac{\partial^2 \mathscr{L}}{\partial \dot{x}^2} = m. \tag{3.3.12}$$

We can use Equations (3.3.10) to (3.3.12) to calculate the third integral, which gives us

$$\begin{aligned}&\int_0^t \frac{1}{2}\left(\frac{\partial^2 \mathscr{L}}{\partial x^2}\bigg|_{x_{cl}} y^2 + 2\frac{\partial^2 \mathscr{L}}{\partial x \partial \dot{x}}\bigg|_{x_{cl}} y\dot{y} + \frac{\partial^2 \mathscr{L}}{\partial \dot{x}^2}\bigg|_{x_{cl}} \dot{y}^2\right) ds \\ &\qquad = \int_0^t \frac{1}{2}\Big(- 2cy^2 - 2ey\dot{y} + m\dot{y}^2\Big) ds = \int_0^t \big(- cy^2 - ey\dot{y} + \frac{1}{2}m\dot{y}^2\big) ds.\end{aligned} \tag{3.3.13}$$

We can insert the results from Equations (3.3.7) to (3.3.9) and (3.3.13) into Equation (3.3.6) to get

$$\begin{aligned}S[x_{cl}(s) + y(s)] &= \int_0^t \mathscr{L}(x_{cl} + y, \dot{x}_{cl} + \dot{y}) ds = S_{cl} + 0 + \int_0^t \big(- cy^2 - ey\dot{y} + \frac{1}{2}m\dot{y}^2\big) ds \\ &= S_{cl} + \int_0^t \big(- cy^2 - ey\dot{y} + \frac{1}{2}m\dot{y}^2\big) ds.\end{aligned} \tag{3.3.14}$$

We can now insert the result from Equation (3.3.14) into Equation (3.3.5) to get

$$\begin{aligned}U(x, t; x') &= \int_0^0 \exp\left\{\frac{i}{\hbar}\left(S_{cl} + \int_0^t \big(- cy^2 - ey\dot{y} + \frac{1}{2}m\dot{y}^2\big) ds\right)\right\} \mathscr{D}[y(s)] \\ &= \exp\left(\frac{i}{\hbar} S_{cl}\right) \int_0^0 \exp\left\{\frac{i}{\hbar}\int_0^t \big(- cy^2 - ey\dot{y} + \frac{1}{2}m\dot{y}^2\big) ds\right\} \mathscr{D}[y(s)].\end{aligned} \tag{3.3.15}$$

We can now see that this integral is no longer dependent on the classical path x_{cl}, it will only be dependent on the time. Using this, we can rewrite Equation (3.3.15) to be

$$U(x,t;x') = A(t)\exp\left(\frac{i}{\hbar}S_{cl}\right), \tag{3.3.16}$$

where

$$A(t) = \int_0^0 \exp\left\{\frac{i}{\hbar}\int_0^t \big(-cy^2 - ey\dot{y} + \frac{1}{2}m\dot{y}^2\big)ds\right\}\mathscr{D}[y(s)] \tag{3.3.17}$$

is some prefactor which we can calculate when we know which specific potential we are using. For example, when we look at the free particle, we know that $a = b = c = d = e = 0$ and we already know the constant, which was given by Equation (3.1.23). We can note that Equation (3.3.17) does not depend on a, b or d. This tells us that the prefactor for potentials of the form $V = a + bx + d\dot{x}$ will also be given by Equation (3.1.23).

Now that we have looked at this general example, we can look at the harmonic oscillator. For this we will calculate the exponential of the classical action, but we will not go into the prefactor $A(t)$ for this example, as this requires quite some technical calculations. For the readers who wish to know more about this, a calculation for the prefactor can be found in section 3.11 of Feynman, Hibbs and Styer [7].

We will calculate the exponential for the harmonic oscillator. To do this, we will first calculate the classical path. We can then use the classical path, to calculate the Lagrangian. From the Lagrangian we can get the classical action, which we can use to calculate the exponential. We know that the potential for the harmonic oscillator is given by

$$V(x) = \frac{1}{2}m\omega^2x^2. \tag{3.3.18}$$

Using Equation (3.3.18), we get that the Lagrangian is given by

$$\mathscr{L} = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2x^2. \tag{3.3.19}$$

From classical mechanics, Equation (A.1.9), we know that the equation of motion for the classical path, in one dimension, is given by

$$\frac{d}{dt}\frac{\partial\mathscr{L}}{\partial\dot{x}} - \frac{\partial\mathscr{L}}{\partial x} = 0. \tag{3.3.20}$$

As we find that $\frac{\partial\mathscr{L}}{\partial x} = -m\omega^2x$ and $\frac{d}{dt}\frac{\partial\mathscr{L}}{\partial\dot{x}} = \frac{d}{dt}m\dot{x} = m\ddot{x}$ our equation of motion is given by

$$\ddot{x} = -\omega^2x^2. \tag{3.3.21}$$

We can use this to find that the classical path needs to have the form $x_{cl}(s) = A\cos(\omega s) + B\sin(\omega s)$, where we use s to denote the time variable. We will use $(x',0)$ as the starting point for the path and (x,t) as the end point. This gives us the following equations:

$$x' = x_{cl}(0) = A\cos(0) + B\sin(0) = A \tag{3.3.22}$$

and

$$x = x_{cl}(t) = x'\cos(\omega t) + B\sin(\omega t), \tag{3.3.23}$$

which we can rewrite to be

$$B = \frac{x - x'\cos(\omega t)}{\sin(\omega t)}. \tag{3.3.24}$$

Using Equations (3.3.22) and (3.3.24), we find that the classical path is given by

$$x_{cl}(s) = x'\cos(\omega s) + \frac{x - x'\cos(\omega t)}{\sin(\omega t)}\sin(\omega s) \tag{3.3.25}$$

We can now easily find the time derivative of the path, which is given by

$$\dot{x}_{cl}(s) = -\omega x'\sin(\omega s) + \omega\frac{x - x'\cos(\omega t)}{\sin(\omega t)}\cos(\omega s). \tag{3.3.26}$$

We can insert the results we found in Equations (3.3.25) and (3.3.26) into the Lagrangian, which we found in Equation (3.3.19), to get

$$\begin{aligned}
\mathscr{L} &= \frac{1}{2}m\bigg(-\omega x'\sin(\omega s) + \omega\frac{x - x'\cos(\omega t)}{\sin(\omega t)}\cos(\omega s)\bigg)^2 \\
&\quad -\frac{1}{2}m\omega^2\bigg(x'\cos(\omega s) + \frac{x - x'\cos(\omega t)}{\sin(\omega t)}\sin(\omega s)\bigg)^2 \\
&= \frac{1}{2}m\bigg(\omega^2 x'^2\sin^2(\omega s) - 2\omega^2\frac{x - x'\cos(\omega t)}{\sin(\omega t)}x'\cos(\omega s)\sin(\omega s) \\
&\qquad + \omega^2\bigg[\frac{x - x'\cos(\omega t)}{\sin(\omega t)}\bigg]^2\cos^2(\omega s)\bigg) - \frac{1}{2}m\omega^2\bigg(x'^2\cos^2(\omega s) \\
&\qquad + 2\frac{x - x'\cos(\omega t)}{\sin(\omega t)}x'\cos(\omega s)\sin(\omega s) + \bigg[\frac{x - x'\cos(\omega t)}{\sin(\omega t)}\bigg]^2\sin^2(\omega s)\bigg) \\
&= \frac{1}{2}m\omega^2\bigg(-x'^2\Big[\cos^2(\omega s) - \sin^2(\omega s)\Big] - 4\frac{x - x'\cos(\omega t)}{\sin(\omega t)}x'\cos(\omega s)\sin(\omega s) \\
&\qquad + \bigg[\frac{x - x'\cos(\omega t)}{\sin(\omega t)}\bigg]^2\Big[\cos^2(\omega s) - \sin^2(\omega s)\Big]\bigg) \\
&= \frac{1}{2}m\omega^2\bigg(\bigg\{\bigg[\frac{x - x'\cos(\omega t)}{\sin(\omega t)}\bigg]^2 - x'^2\bigg\}\Big[\cos^2(\omega s) - \sin^2(\omega s)\Big] \\
&\qquad - 4\frac{x - x'\cos(\omega t)}{\sin(\omega t)}x'\cos(\omega s)\sin(\omega s)\bigg) \\
&= \frac{1}{2}m\omega^2\bigg(\bigg\{\bigg[\frac{x - x'\cos(\omega t)}{\sin(\omega t)}\bigg]^2 - x'^2\bigg\}\cos(2\omega s) - 2\frac{x - x'\cos(\omega t)}{\sin(\omega t)}x'\sin(2\omega s)\bigg).
\end{aligned} \tag{3.3.27}$$

Now that we have found a definition for the Lagrangian, we can use Equation (A.1.1), which in our case will become

$$S[x(t)] = \int_0^t \mathscr{L}(x, \dot{x})ds, \tag{3.3.28}$$

to calculate the action of the harmonic oscillator. We can now insert the result we found in Equation (3.3.27) into Equation (3.3.28) to get

$$\begin{aligned}
S_{cl} &= \int_0^t \frac{1}{2}m\omega^2\bigg(\bigg\{\bigg[\frac{x-x'\cos(\omega t)}{\sin(\omega t)}\bigg]^2 - x'^2\bigg\}\cos(2\omega s) - 2\frac{x-x'\cos(\omega t)}{\sin(\omega t)}x'\sin(2\omega s)\bigg)ds \\
&= \frac{1}{2}m\omega^2\bigg(\bigg\{\bigg[\frac{x-x'\cos(\omega t)}{\sin(\omega t)}\bigg]^2 - x'^2\bigg\}\int_0^t \cos(2\omega s)ds \\
&\qquad - 2\frac{x-x'\cos(\omega t)}{\sin(\omega t)}x'\int_0^t \sin(2\omega s)ds\bigg) \\
&= \frac{1}{2}m\omega^2\bigg(\bigg\{\bigg[\frac{x-x'\cos(\omega t)}{\sin(\omega t)}\bigg]^2 - x'^2\bigg\}\bigg[\frac{1}{2\omega}\sin(2\omega s)\bigg]_0^t \\
&\qquad - 2\frac{x-x'\cos(\omega t)}{\sin(\omega t)}x'\bigg[-\frac{1}{2\omega}\cos(2\omega s)\bigg]_0^t\bigg) \\
&= \frac{1}{4}m\omega\bigg(\bigg\{\bigg[\frac{x-x'\cos(\omega t)}{\sin(\omega t)}\bigg]^2 - x'^2\bigg\}\bigg[\sin(2\omega t) - \sin(0)\bigg] \\
&\qquad + 2\frac{x-x'\cos(\omega t)}{\sin(\omega t)}x'\bigg[\cos(2\omega t) - \cos(0)\bigg]\bigg) \\
&= \frac{1}{4}m\omega\bigg(\bigg\{\bigg[\frac{x-x'\cos(\omega t)}{\sin(\omega t)}\bigg]^2 - x'^2\bigg\}\sin(2\omega t) + 2\frac{x-x'\cos(\omega t)}{\sin(\omega t)}x'\bigg[\cos(2\omega t) - 1\bigg]\bigg).
\end{aligned} \tag{3.3.29}$$

We can now rewrite this formula, to get

$$\begin{aligned}
S_{cl} =& \frac{1}{4}m\omega\bigg(\bigg\{\bigg[\frac{x^2 - 2xx'\cos(\omega t) + x'^2\cos^2(\omega t)}{\sin^2(\omega t)}\bigg] - x'^2\bigg\}\sin(2\omega t) \\
&\qquad + 2\frac{x-x'\cos(\omega t)}{\sin(\omega t)}x'\bigg[\cos(2\omega t) - 1\bigg]\bigg) \\
=& \frac{1}{4}m\omega\bigg(\bigg\{\bigg[\frac{x^2 - 2xx'\cos(\omega t) + x'^2\cos^2(\omega t)}{\sin^2(\omega t)}\bigg] - \frac{x'^2\sin^2(\omega t)}{\sin(\omega t)}\bigg\}2\cos(\omega t)\sin(\omega t) \\
&\qquad + 2\frac{x-x'\cos(\omega t)}{\sin(\omega t)}x'\bigg[1 - 2\sin^2(\omega t) - 1\bigg]\bigg) \\
=& \frac{1}{2}m\omega\bigg(\bigg\{\frac{x^2 - 2xx'\cos(\omega t) + x'^2\cos^2(\omega t) - x'^2\sin^2(\omega t)}{\sin^2(\omega t)}\bigg\}\cos(\omega t)\sin(\omega t) \\
&\qquad - 2\frac{x-x'\cos(\omega t)}{\sin(\omega t)}x'\sin^2(\omega t)\bigg).
\end{aligned} \tag{3.3.30}$$

We can simplify this equation further by taking $1/\sin(\omega t)$ out of the brackets. This gives us

$$\begin{aligned}
S_{cl} =& \frac{1}{2}\frac{m\omega}{\sin(\omega t)}\big((x^2 - 2xx'\cos(\omega t) + x'^2\cos^2(\omega t) - x'^2\sin^2(\omega t))\cos(\omega t) - 2(x - x'\cos(\omega t))x'\sin^2(\omega t)\big) \\
=& \frac{m\omega}{2\sin(\omega t)}\big(x^2\cos(\omega t) - 2xx'\cos^2(\omega t) + x'^2\cos^3(\omega t) - x'^2\cos(\omega t)\sin^2(\omega t) \\
& \qquad - 2xx'\sin^2(\omega t) + 2x'^2\cos(\omega t)\sin^2(\omega t)\big) \\
=& \frac{m\omega}{\sin(\omega t)}\big(x^2\cos(\omega t) - 2xx'(\cos^2(\omega t) + \sin^2(\omega t)) + x'^2\cos^3(\omega t) + x'^2\cos(\omega t)\sin^2(\omega t)\big) \\
=& \frac{m\omega}{2\sin(\omega t)}\big(x^2\cos(\omega t) - 2xx'\cdot 1 + x'^2\cos(\omega t)\big(\cos^2(\omega t) + \sin^2(\omega t)\big)\big) \\
=& \frac{m\omega}{2\sin(\omega t)}\big(x^2\cos(\omega t) - 2xx' + x'^2\cos(\omega t)\cdot 1\big) \\
=& \frac{m\omega}{2\sin(\omega t)}\big((x^2 + x'^2)\cos(\omega t) - 2xx'\big).
\end{aligned} \tag{3.3.31}$$

We can now use equation Equations (3.3.16) and (3.3.31) to find the solution for the harmonic oscillator, which is given by

$$U(x,t;x') = A(t)\exp\left(\frac{im\omega}{2\hbar\sin(\omega t)}\big((x^2 + x'^2)\cos(\omega t) - 2xx'\big)\right). \tag{3.3.32}$$

The reason why we are so glad with this result is because we only needed to calculate the classical action, to find the time propagator. As the calculation for the classical action is way easier than the path integral would be, this is a great advantage.

4 Imaginary time operator

We will now look at the imaginary time operator, since this leads us to many applications of the path integral formula. For this section we will follow parts of Shankar [1] and Hall [8].

One of the problems, especially in mathematics is the fact that we work with a lot of complex numbers. Now in general this is not a problem, as we have a very well established way of working with them. Their difficulty however is that they make the results less intuitive and that they make it more difficult to talk about the convergence of the integral. We already saw this in Section 2.2, when we talked about the convergence in the classical limit and had to use the cancellation of the phases argument. One trick we can use to make the situation easier is the imaginary time, where we define $\tau = it$. From this we can, for example, rewrite the time operator in the Hamiltonian formalism. The normal time operator was given by $\exp(-itH/\hbar)$, which becomes imaginary time operator $\exp(-\tau H/\hbar)$. We do not have a correct definition for either $\exp(-itH/\hbar)$ or $\exp(-\tau H/\hbar)$ yet, when they do not have a true orthonormal basis of eigenvectors. We will look at a way to define them without this basis in Section 4.2.

We can now also look at the imaginary Schrödinger equation. We know that the normal Schrödinger equation is given by Equation (2.3.1), so we can use the imaginary time to get

$$-\hbar\frac{d}{d\tau}|\psi(\tau)\rangle = \mathscr{H}|\psi(\tau)\rangle. \tag{4.0.1}$$

The idea is that if we can use path integrals to understand imaginary time operators, we can go back to the real time operator by analytic continuation with respect to t. An interesting result is that we get the same eigenvalues and eigenfunctions from the Hamiltonian in both situations. Then by using $\exp(-itH/\hbar)$ or $\exp(-\tau H/\hbar)$, we can derive the solution of either one, from the solution of the other. This tells us that when we can solve a problem in imaginary time, we can also do it for the original situation.

We can, for example, use this imaginary time, to get a definition for the imaginary time path integral. For this we will use Equation (2.1.8) and the approximation for the action, which we found in Equation (2.3.12) to get

$$U(x,t;x') = \lim_{\substack{n\to\infty\\ \varepsilon\to 0}} B^n \int_{\mathbb{R}^{n-1}} \exp\left(\frac{i}{\hbar}\sum_{j=0}^{n-1}\left[\frac{m}{2}\frac{(x_{j+1}-x_j)^2}{\varepsilon} - \varepsilon V(x_{j+1})\right]\right) dx_1\cdots dx_{n-1}, \tag{4.0.2}$$

where ε was the length of an infinitesimal time interval and where we took $t' = 0$, so t' disappeared from the equation. Now we can use the imaginary time in this equation. For this we will use that $\tau' = i\varepsilon$ and $1/\tau' = 1/i\varepsilon = -i/\varepsilon$. As we had $t' = 0$, we know that $N\varepsilon = t$, in the same way we can define $\tau = N\tau'$. This gives us

$$\begin{aligned} U(x,\tau;x') &= \lim_{\substack{n\to\infty\\ \varepsilon\to 0}} B^n \int_{\mathbb{R}^{n-1}} \exp\left(-\frac{1}{\hbar}\sum_{j=0}^{n-1}\left[\frac{m}{2}\frac{(x_{j+1}-x_j)^2}{\tau'} + \tau' V(x_{j+1})\right]\right) dx_1\cdots dx_{n-1} \\ &= \lim_{\substack{n\to\infty\\ \varepsilon\to 0}} B^n \int_{\mathbb{R}^{n-1}} \exp\left(-\frac{1}{\hbar}\sum_{j=0}^{n-1}\tau'\left[\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\tau'}\right)^2 + V(x_{j+1})\right]\right) dx_1\cdots dx_{n-1}. \end{aligned} \tag{4.0.3}$$

Now in the same way that Equation (2.1.8) is related to Equation (2.1.7), by using Equation (4.0.3) we can get the following equation

$$\psi(x,\tau;x') = \lim_{\substack{n\to\infty \\ \varepsilon\to 0}} B^n \int_{\mathbb{R}^{n-1}} \exp\left(-\frac{1}{\hbar}\sum_{j=0}^{n-1} \tau' \left[\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\tau'} \right)^2 + V(x_{j+1}) \right] \right) \psi(x') dx_1 \cdots dx_{n-1}. \tag{4.0.4}$$

Now just as Equation (2.1.7) is the discretization of Equation (2.1.3), we can now take the limit of Equation (4.0.4) to get

$$\psi(x,\tau;x') = A \int \exp\left(-\frac{1}{\hbar}\int_0^\tau \left[\frac{m}{2}\left(\frac{dx}{ds} \right)^2 + V(x(s)) \right] ds \right) \psi(x') \mathscr{D}[x(\tau)]. \tag{4.0.5}$$

The reasoning as to why the discretization of the kinetic energy and potential energy in Equation (4.0.4) leads to the potential energy and kinetic energy found in Equation (4.0.5) can be found in Section 2.3 as we used the same steps to find the discretization there.

One big advantage of the imaginary time path integral over the normal path integral is that its convergence in the classical limit is way clearer. For the imaginary time operator, we can easily find that, as the classical path has the least action, the action of all other paths will be larger and as there is a minus sign in the exponential, all other paths will be suppressed by this. So the convergence of the imaginary path integral will be more intuitive in the classical limit than the convergence of the normal path integral was.

One disadvantage of Equation (4.0.3) is that the action is no longer the action as we had defined it before, as it now has a plus sign in front of the potential, which used to be a minus sign. This means that when we look at an imaginary time example, the particle will see the potential upside down, as there is no longer a minus sign in front of the potential.

As the kinetic energy is the same for every example, just the potential energy changes, we can define a measure which contains this kinetic energy term. So we will try to interpret

$$A \exp\left(-\frac{1}{\hbar}\int_0^\tau \frac{m}{2}\left(\frac{dx}{ds} \right)^2 ds \right) \psi(x') \mathscr{D}[x(\tau)] \tag{4.0.6}$$

as a measure, for which we fill follow parts of Chapter 20 of Hall [8]. For this we will once again use the discretization, as we do not know how to interpret the measure $\mathscr{D}[x(\tau)]$. That means we want to interpret

$$B^n \int_{\mathbb{R}^{n-1}} \exp\left(-\frac{1}{\hbar}\sum_{j=0}^{n-1} \frac{m}{2}\frac{(x_{j+1}-x_j)^2}{\tau'} \right) \psi(x') dx_1 \cdots dx_{n-1} \tag{4.0.7}$$

as a measure. For this we can see the discrete intervals of this imaginary time interval as the increments of a Brownian path of which more information can for example be found in [9]. For the Brownian paths, there exists the Wiener measure, and since we can interpret the discretized path as a Brownian path, we can apply the following theorem to it.

Theorem 4.1. *For each vector $x_0 \in \mathbb{R}^n$ and each pair of positive numbers σ and τ, there exists a unique measure $\mu^\sigma_{x_0}$ on the borel σ-algebra in $\mathcal{C}_{x_0}([0,\tau];\mathbb{R}^n)$ such that the following*

condition holds. For each sequence $0 = \tau_0 < \tau_1 < \cdots < \tau_N \leq \tau$ *of real numbers and each non-negative measurable function* f *on* $(\mathbb{R}^n)^N$*, we have*

$$\begin{aligned}&\int_{C_{x_0}([0,\tau];\mathbb{R}^n)} f(x(\tau_1), x(\tau_2), \ldots, x(\tau_N)) d\mu^{\sigma}_{x_0}(x) \\ &= C \int_{\mathbb{R}^N} \exp\left\{ -\frac{1}{2\sigma} \sum_{j=1}^{N} \frac{|x_j - x_{j-1}|^2}{\tau_j - \tau_{j-1}} \right\} f(x_1, x_2, \ldots, x_N) dx_1 \ldots dx_N,\end{aligned} \tag{4.0.8}$$

where

$$C = \prod_{j=1}^{N} \frac{1}{\sqrt{2\pi\sigma(\tau_j - \tau_{j-1})}}. \tag{4.0.9}$$

Using this theorem, we can define Equation (4.0.7) as a measure. The notation we use for this is that the length of the time intervals is given by τ', so we use τ' instead of $\tau_j - \tau_{j-1}$. We also use that $\tau_N = \tau$, so we will not integrate over dx_N and since we used n instead of N, we will set $n = N$. Finally, we also can see that $\sigma = \hbar/m$, to find the exact link between Equation (4.0.7) and Theorem 4.1.

We will now check if the constant B^n will also be equal to the constant C which we saw in Theorem 4.1. We have found the value for B in Equation (2.3.39), now we can use this to get

$$B^n = \left(\frac{2\pi\hbar\tau'}{m} \right)^{-n/2}, \tag{4.0.10}$$

where we use that $\tau' = i\varepsilon$. Now we know the constant C from Equation (4.0.9), which we can rewrite by using $\tau' = \tau_j - \tau_{j-1}$ for all j, $n = N$ and $\sigma = \hbar/m$. We then find C to be

$$C = \prod_{j=1}^{N} \frac{1}{\sqrt{2\pi\sigma(\tau_j - \tau_{j-1})}} = \prod_{j=1}^{n} \left(\frac{m}{2\pi\hbar\tau'} \right)^{1/2} = \left(\frac{m}{2\pi\hbar\tau'} \right)^{n/2} = \left(\frac{2\pi\hbar\tau'}{m} \right)^{-n/2}. \tag{4.0.11}$$

So we indeed find that $B^n = C$, so we find that we can indeed apply Theorem 4.1 to Equation (4.0.7), to define the following measure

$$d\mu^{\sigma} = B^n \exp\left(-\frac{1}{\hbar} \sum_{j=0}^{n-1} \frac{m}{2} \frac{(x_{j+1} - x_j)^2}{\tau'} \right) dx_1 \cdots dx_{n-1}. \tag{4.0.12}$$

Using the fact that we have found this measure, we can use this to define the Feynman-Kac formula, which is given in the following theorem.

Theorem 4.2. *Suppose* $V : \mathbb{R}^3 \to \mathbb{R}$ *can be expressed as the sum of a function in* $L^2(\mathbb{R}^3)$ *and a bounded function. Then for all* $x_0 \in \mathbb{R}^3$*, we have*

$$(e^{-\tau H/\hbar}\psi)(x_0) = \int_{\mathscr{C}_{x_0}([0;\tau];\mathbb{R}^3)} \exp\left\{ -\frac{1}{\hbar} \int_0^{\tau} V(x(s)) ds \right\} \psi(x(t)) d\mu^{\sigma}_{x_0}(x), \tag{4.0.13}$$

where $\mu^{\sigma}_{x_0}$ *is the Wiener measure on* $\mathscr{C}_{x_0}([0,\tau];\mathbb{R}^3)$ *and where* $\sigma = \hbar/m$*.*

We thus find that there are some restrictions on the potential, but for all potentials which fulfill these restrictions, we can use this Wiener measure.

If we now take the potential to be zero in Equation (4.0.13), then this becomes the heat equation expressed as a Wiener integral, more information about this can be found in Glimm and Jaffe [10].

4.1 Examples

We now want to look at some examples to see how we can apply the formula we found in Section 4. For this we will use parts of Shankar [1].

In the previous section we have found Equation (4.0.13) as the Feynman-Kac formula. This is a nice result, but when we want to look at examples, it is quite difficult to work with. An easier way to look at the examples is through analytic continuation. For this we use the definition $\tau = it$, or $t = -i\tau$. We can implement these formulas into results we already knew to get the correct imaginary time result.

If we now look at Equation (3.1.19), this is the solution for the free particle. We can now use analytic continuation, to get the following.

$$\begin{aligned} U(x,\tau;x',\tau') &= \sqrt{\frac{m}{2\pi\hbar((-i\tau)-(-i\tau'))i}}\exp\left(-\frac{m}{2\hbar((-i\tau)-(-i\tau'))i}\big[x-x'\big]^2\right) \\ &= \sqrt{\frac{m}{2\pi\hbar(-i)(\tau-\tau')i}}\exp\left(-\frac{m}{2\hbar(-i)(\tau-\tau')i}\big[x-x'\big]^2\right) \\ &= \sqrt{\frac{m}{2\pi\hbar(-i^2)(\tau-\tau')}}\exp\left(-\frac{m}{2\hbar(-i^2)(\tau-\tau')}\big[x-x'\big]^2\right) \\ &= \sqrt{\frac{m}{2\pi\hbar(\tau-\tau')}}\exp\left(-\frac{m}{2\hbar(\tau-\tau')}\big[x-x'\big]^2\right) \end{aligned} \tag{4.1.1}$$

We can go through the same steps for the harmonic oscillator example, which original result we can find in Equation (3.3.32). By using the analytic continuation we get

$$\begin{aligned} U(x,\tau;x') &= A(\tau)\exp\left(\frac{im\omega}{2\hbar\sin(\omega(-i\tau))}\big((x^2+x'^2)\cos(\omega(-i\tau))-2xx'\big)\right) \\ &= A(\tau)\exp\left(\frac{im\omega}{2\hbar(\exp\{i\omega(-i\tau)\}-\exp\{-i\omega(-i\tau)\})/(2i)}\right. \\ &\qquad\left.\times\big((x^2+x'^2)(\exp\{i\omega(-i\tau)\}+\exp\{-i\omega(-i\tau)\})/2-2xx'\big)\right) \\ &= A(\tau)\exp\left(\frac{im\omega\cdot 2i}{2\hbar(\exp\{\omega\tau\}-\exp\{-\omega\tau\})}\right. \\ &\qquad\left.\times\big((x^2+x'^2)(\exp\{\omega\tau\}+\exp\{-\omega\tau\})/2-2xx'\big)\right) \\ &= A(\tau)\exp\left(\frac{-2m\omega}{2\hbar 2\sinh(\omega\tau)}\big((x^2+x'^2)2\cosh(\omega\tau)/2-2xx'\big)\right) \\ &= A(\tau)\exp\left(\frac{-m\omega}{2\hbar\sinh(\omega\tau)}\big((x^2+x'^2)\cosh(\omega\tau)-2xx'\big)\right), \end{aligned} \tag{4.1.2}$$

where we have used that $(\exp\{x\} - \exp\{-x\})/2 = \sinh(x)$ and $(\exp\{x\} + \exp\{-x\})/2 = \cosh(x)$.

So by simply using analytic continuation we have found the imaginary time result for the free particle and for the harmonic oscillator. These results are the same as the ones we could calculate from the imaginary time operator, which can be found in Shankar [1].

We also know that in the calculation for the path integral, we integrate the Lagrangian over time. When we now look at this from the imaginary time formula and if we take 0 and $\beta\hbar$ as our integration borders, we can find a connection to statistical physics. More information on this connection can be found in Feynman, Hibbs and Styer [7] and in Shankar [1].

4.2 Spectral theory

We will now look at spectral theory, but first we want to answer a question: What is spectral theory and why would we need it? Spectral theory helps us to define 'functional calculus', or in essence, a way of working with operators without a true orthonormal basis of eigenvectors. This also immediately tells us why we would need it, that is, to find a way of working with such operators. We have already come across a few operators which might be problematic, but until now we have skipped over this. One example is Equation (A.1.1) where we take the integral of the Lagrangian and another one is Equation (4.0.13) where we use the exponential of some constants times the Hamiltonian, to calculate $\psi(x_n)$. Since we cannot expect the Lagrangian and Hamiltonian to always have a true orthonormal basis of eigenvectors, we want to look at spectral theory. This way we can find a way in which we will be able to work with them, even when they lack this basis. For this we will follow parts of Ch. 9 of Hall [8].

To find this way of working with the operators, we will first define the spectrum of an operator. The values in the spectrum are somewhat like the eigenvalues, but since we are looking at the case where an operator does not need to have a true basis, we can not call them eigenvalues.

Definition 4.3. Suppose A is an unbounded operator on $\mathscr{H}$. A number $\lambda \in \mathbb{C}$ belongs to the resolvent set of A if there exists a bounded operator B with the following properties:

1. For all $\psi \in \mathscr{H}$, $B\psi$ belongs to $\mathrm{Dom}(A)$ and $(A - \lambda I)B\psi = \psi$,
2. for all $\psi \in \mathrm{Dom}(A)$ we have $B(A - \lambda I)\psi = \psi$.

If no such bounded operator B exists, then λ belongs to the **spectrum** of A.

Now we have used the definition for unbounded operators, since this is more general, but we can also look at the definition for the spectrum for bounded operators, which is given by

Definition 4.4. For all $A \in \mathcal{B}(\mathscr{H})$, the resolvent set of A, denoted by $\rho(A)$, is given by the set of all $\lambda \in \mathbb{C}$ such that the operator $(A - \lambda I)$ has a bounded inverse. The **spectrum** of A, denoted by $\sigma(A)$, is the complement in $\mathbb{C}$ of the resolvent set.

Now we can see that indeed, both Definitions 4.3 and 4.4 are given in the same way, only Definition 4.3 needed a more general definition, since we assumed the operators to be unbounded.

Using these definitions, we can postulate the following theorem

Theorem 4.5. *Suppose A is a self-adjoint operator on $\mathscr{H}$. Then there is a unique projection-valued measure μ^A on $\sigma(A)$ with values in $\mathcal{B}(\mathscr{H})$ such that*

$$\int_{\sigma(A)} \lambda d\mu^A(\lambda) = A. \tag{4.2.1}$$

Now we do not really know how we can use this theorem yet, but from this, the following definition follows.

Definition 4.6. For any measurable function f on $\sigma(A)$, define a (possibly unbounded) operator, denoted $f(A)$, by

$$f(A) = \int_{\sigma(A)} f(\lambda) d\mu^A(\lambda). \tag{4.2.2}$$

This is the definition we wanted to work towards, since this offers us a way of working with possibly unbounded operators. There are two things we want to note here. The first is that in Theorem 4.5 we say that the operator A needs to be self-adjoint on $\mathscr{H}$. Now we know from Kato [4], that the Hamiltonian is essentially self-adjoint under quite general circumstances. Since we know from Appendix A.2 that we can take the closure of an essentially self-adjoint operator to get a self-adjoint extension of our original operator. So since we can get a self-adjoint extension, it is enough to assume that the operator is essentially self-adjoint.

The second is that in both Theorem 4.5 and definition 4.6 we can see that we use the spectrum $\sigma(A)$, which we defined in Definitions 4.3 and 4.4. We can now see in Definition 4.6 that we only use the values in the spectrum of the operator A and their function value $f(\lambda)$ to calculate $f(A)$. This shows use that we can calculate the functions of operators, even if they do not have a true orthonormal basis, by just using their spectrum and the function value at each point of the spectrum. Also, since we are working with unbounded operators, the spectrum of an operator can be continuous, hence the integration over the spectrum, instead of a summation.

Some examples of the application of the spectral theory to operators in the Hamiltonian formalism can be found in Chapters 6 and 9 of Hall [8].

5 Conclusions and discussion

In this thesis we looked at Feynman's path integral. We used discretrization to get a path integral we could work with. Then we used Taylor approximations to show that the path integral is equal to the Schrödinger Equation. After that we looked at the classical limit, where we saw that we would expect to get the correct result, by using the interference argument. We continued towards a more rigorous definition where we used the Trotter product formula, to find a more precise definition and a clearer sense of the limit in which ψ_n would go to ψ.

We then went on to the examples, where we looked at the free particle example and a specific class of potentials, where we saw that their exact results are exactly equal to the results we get by simply using the classical action, instead of looking at the action of all the paths. We also looked at the double slit experiment and saw a very elegant result and we clearly saw both the interference and the diffraction pattern.

Lastly we looked at the imaginary time operator. This led us towards the imaginary path integral, for which the classical limit was way more intuitive than for the original path integral. We also saw that this imaginary path integral had connections to multiple different areas, such as the heat equation and statistical mechanics. We then looked at spectral theory to find out in what sense the time evolution operator exists, when we do not have a true orthonormal basis of eigenvectors.

There are many applications of the path integral left, one could for example look further into the integral representation of the heat equation, about which more information can be found in Glimm and Jaffe [10]. Or we could go into the connection between statistical mechanics and the path integral. For this we could look towards Shankar [1]. Even more applications of the path integral can be found in quantum field theory, which can be found in Zee [11].

A Appendix

A.1 Classical Lagrangian mechanics

In this section we will look at some of the classical mechanics background for the path integral and its definition. As the path integral definition depends heavily on the Lagrangian mechanics, this is what we will be looking at in this section. For this section we follow parts of Shankar [1].

In the Lagrangian formalism, the problem of a single particle in a potential $V(x)$ is posed in a different way: given that the particle is at x_i at time t_i and at x_f at time t_f, what is it that distinguishes the actual trajectory $x_{cl}(t)$ from all other trajectories or paths that connect these points? We can give the answer to this question in three parts.

First we will define a function $\mathscr{L}$, which is called the Lagrangian, given by $\mathscr{L} = T - V$, where T is the kinetic energy and V is the potential energy of the particle. Now this Lagrangian will be dependent on the location x of the particle and its direction $\dot{x}$. The Lagrangian could also directly depend on t, but as this only happens when the particle is in an external time-dependent field, we can assume this will not be the case in the situations we will be working with.

Secondly for each path $x(t)$ connecting x_i at time t_i and x_f at time t_f, we can calculate the action $S[x(t)]$, where we use the $[x(t)]$ notation to show that the action depends on the path $x(t)$, not just at x at some time t. The formula for the action is given by

$$S[x(t)] = \int_{t_i}^{t_f} \mathscr{L}(x, \dot{x}) dt. \tag{A.1.1}$$

Last of all, we will look at what separates the classical path from all other paths in this situation. We will call this condition the principle of least action, as it states that the classical path is the path with the least action, so for which S is a minimum. In our calculations we will only assume the action to be an extremum, as we only use the first derivative of the action.

We will first check the validity of this formulation, before we look into it any further. To verify this principle, we will show that it is equivalent to Newtons second law. We know that, for a particle of mass m moving along the x axis under a potential $V(x)$, Newtons second law is given by

$$m\frac{d^2x}{dt^2} = -\frac{dV}{dx}. \tag{A.1.2}$$

This can be found in many classical mechanics books, e.g. Ch. 2 of Shankar [1].

To verify this equivalency we will start with the principle of least action. This principle states that the classical path will reside at an extremum of the action. This means that the derivative of the action of the classical path will be zero, or $\delta S_{cl} = 0$. If we now take a path $x(t)$ we from x_i at time t_i to x_f at time t_f, we can write this path as a sum of the classical path $x_{cl}(t)$ and some deviation from the classical path $y(t)$. As the path $x(t)$ and the classical path connect the same two points, we know that the deviation at these points will be zero, so $y(t_i) = y(t_f) = 0$. So we can write the path as

$$x(t) = x_{cl}(t) + y(t) \tag{A.1.3}$$

and its derivative as

$$\dot{x}(t) = \dot{x}_{cl}(t) + \dot{y}(t). \tag{A.1.4}$$

If we now take the path $x(t)$ to be close to the classical path, we can use the Taylor expansion of the action around the classical path, which gives

$$S[x_{cl}(t) + y(t)] = S_{cl} + \delta S_{cl} y(t) + \mathscr{O}(y^2(t)). \tag{A.1.5}$$

Now we know that the action depends on the Lagrangian, which depends on the path and its derivative. We can use this to calculate the Taylor expansion, which is given by

$$\begin{aligned} S[x_{cl}(t) + y(t)] &= \int_{t_i}^{t_f} \Big(\mathscr{L}(x_{cl} + y, \dot{x}_{cl} + \dot{y}) \Big) dt \\ &= \int_{t_i}^{t_f} \left(\mathscr{L}(x_{cl}, \dot{x}_{cl}) + \left[\frac{\partial \mathscr{L}}{\partial x} \bigg|_{x_{cl}} y + \frac{\partial \mathscr{L}}{\partial \dot{x}} \bigg|_{x_{cl}} \dot{y} \right] + ... \right) dt \\ &\approx S_{cl} + \int_{t_i}^{t_f} \left(\frac{\partial \mathscr{L}}{\partial x} \bigg|_{x_{cl}} y + \frac{\partial \mathscr{L}}{\partial \dot{x}} \bigg|_{x_{cl}} \dot{y} \right) dt. \end{aligned} \tag{A.1.6}$$

We thus find, using the fact that $\delta S_{cl} = 0$, that

$$\begin{aligned} 0 = \delta S_{cl} &= \int_{t_i}^{t_f} \left(\frac{\partial \mathscr{L}}{\partial x} \bigg|_{x_{cl}} y + \frac{\partial \mathscr{L}}{\partial \dot{x}} \bigg|_{x_{cl}} \dot{y} \right) dt \\ &= \int_{t_i}^{t_f} \left(\frac{\partial \mathscr{L}}{\partial x} \bigg|_{x_{cl}} y + \frac{\partial \mathscr{L}}{\partial \dot{x}} \bigg|_{x_{cl}} \dot{y} + \left[\frac{d}{dt} \frac{\partial \mathscr{L}}{\partial \dot{x}} \bigg|_{x_{cl}} \right] y - \left[\frac{d}{dt} \frac{\partial \mathscr{L}}{\partial \dot{x}} \bigg|_{x_{cl}} \right] y \right) dt \\ &= \int_{t_i}^{t_f} \left(\frac{\partial \mathscr{L}}{\partial x} \bigg|_{x_{cl}} y - \left[\frac{d}{dt} \frac{\partial \mathscr{L}}{\partial \dot{x}} \bigg|_{x_{cl}} \right] y + \frac{\partial \mathscr{L}}{\partial \dot{x}} \bigg|_{x_{cl}} \frac{d}{dt} y + \left[\frac{d}{dt} \frac{\partial \mathscr{L}}{\partial \dot{x}} \bigg|_{x_{cl}} \right] y \right) dt \\ &= \int_{t_i}^{t_f} \left(\left[\frac{\partial \mathscr{L}}{\partial x} \bigg|_{x_{cl}} - \frac{d}{dt} \frac{\partial \mathscr{L}}{\partial \dot{x}} \bigg|_{x_{cl}} \right] y + \frac{d}{dt} \left[\frac{\partial \mathscr{L}}{\partial \dot{x}} \bigg|_{x_{cl}} y \right] \right) dt \\ &= \int_{t_i}^{t_f} \left[\frac{\partial \mathscr{L}}{\partial x} \bigg|_{x_{cl}} - \frac{d}{dt} \frac{\partial \mathscr{L}}{\partial \dot{x}} \bigg|_{x_{cl}} \right] y dt + \left[\frac{\partial \mathscr{L}}{\partial \dot{x}} \bigg|_{x_{cl}} y \right]_{t_i}^{t_f} \\ &= \int_{t_i}^{t_f} \left[\frac{\partial \mathscr{L}}{\partial x} \bigg|_{x_{cl}} - \frac{d}{dt} \frac{\partial \mathscr{L}}{\partial \dot{x}} \bigg|_{x_{cl}} \right] y dt + \frac{\partial \mathscr{L}}{\partial \dot{x}} \bigg|_{x_{cl}, t_f} y(t_f) - \frac{\partial \mathscr{L}}{\partial \dot{x}} \bigg|_{x_{cl}, t_i} y(t_i). \end{aligned} \tag{A.1.7}$$

Now we know that $y(t_i) = y(t_f) = 0$, so we will get

$$0 = \delta S_{cl} = \int_{t_i}^{t_f} \left[\frac{\partial \mathscr{L}}{\partial x} \bigg|_{x_{cl}} - \frac{d}{dt} \frac{\partial \mathscr{L}}{\partial \dot{x}} \bigg|_{x_{cl}} \right] y dt. \tag{A.1.8}$$

As Equation (A.1.8) has to hold for all paths close to the classical path, we know y will not be zero. To get that $\delta S = 0$, it thus has to hold that

$$\left[\frac{\partial \mathscr{L}}{\partial x} - \frac{d}{dt} \frac{\partial \mathscr{L}}{\partial \dot{x}} \right]_{x_{cl}} = 0, \tag{A.1.9}$$

which is equal to

$$\frac{\partial \mathscr{L}}{\partial x}\bigg|_{x_{cl}} = \frac{d}{dt}\frac{\partial \mathscr{L}}{\partial \dot{x}}\bigg|_{x_{cl}}, \tag{A.1.10}$$

where Equation (A.1.9) is called the Euler-Lagrange equation, or the equation of motion.

Now we already know that $\mathscr{L} = T - V$, $T = \frac{1}{2}m\dot{x}$ and $V = V(x)$. We can insert this into Equation (A.1.10) to get

$$\frac{\partial \mathscr{L}}{\partial x} = \frac{\partial}{\partial x}\left(\frac{1}{2}m\dot{x} - V(x)\right) = -\frac{dV(x)}{dx}, \tag{A.1.11}$$

$$\frac{d}{dt}\frac{\partial \mathscr{L}}{\partial \dot{x}} = \frac{d}{dt}\frac{\partial}{\partial \dot{x}}\left(\frac{1}{2}m\dot{x} - V(x)\right) = \frac{d}{dt}m\dot{x} = m\frac{d^2x}{dt^2}, \tag{A.1.12}$$

$$m\frac{d^2x}{dt^2} = -\frac{dV(x)}{dx}. \tag{A.1.13}$$

We find that Equation (A.1.13) is equal to Equation (A.1.2) and thus that the principle of least action is equivalent to Newtons second law.

Now we have seen the validity of the Lagrangian scheme, we will quickly note two advantages of this formalism and then look at an example of the calculation of the action.

The first advantage of the Lagrangian scheme is that the Euler-Lagrange equations, or equations of motions have the same form for multiple dimensions and for any general set of independent coordinates. The equations will then just be given by

$$\frac{d}{dt}\frac{\partial \mathscr{L}}{\partial \dot{q}_i} = \frac{\partial \mathscr{L}}{\partial q_i}. \tag{A.1.14}$$

The second advantage of Lagrangian is the fact that once we know this Lagrangian, we can easily derive the equations of motion from it. We will only have to take simple derivatives to find the equations of motion in this formalism.

We will now look at an example, where we will calculate the classical action. In this example, we have a particle under a constant force f, which moves from x_i at time t_i to x_f at time t_f. We are working in one dimension, so the potential will be given by $V(x) = -fx$, which gives us the following Lagrangian

$$\mathscr{L}(x, \dot{x}) = \frac{1}{2}m\dot{x} + fx. \tag{A.1.15}$$

We will first use the equation of motion, which we saw in Equation (A.1.9), to get

$$\frac{\partial \mathscr{L}}{\partial x} = \frac{\partial}{\partial x}\left(\frac{1}{2}m\dot{x} + fx\right) = f, \tag{A.1.16}$$

$$\frac{d}{dt}\frac{\partial \mathscr{L}}{\partial \dot{x}} = \frac{d}{dt}\frac{\partial}{\partial \dot{x}}\left(\frac{1}{2}m\dot{x} + fx\right) = \frac{d}{dt}m\dot{x} = m\ddot{x}, \tag{A.1.17}$$

$$m\ddot{x} = f. \tag{A.1.18}$$

Using Equation (A.1.18) we find that the classical path, which satisfies the equation of motion, will be given by

$$x_{cl}(t') = \frac{f}{2m}t'^2 + ct' + d, \tag{A.1.19}$$

where c and d are some constants. For our convenience we will use the substitution $t' = t - t_i$, which gives us

$$x_{cl}(t) = \frac{f}{2m}(t - t_i)^2 + c(t - t_i) + d. \tag{A.1.20}$$

We already know that $x(t_i) = x_i$ and $x(t_f) = x_f$, which we will use to find values for the constants c and d.

$$x_i = x(t_i) = \frac{f}{2m}(t_i - t_i)^2 + c(t_i - t_i) + d = 0 + 0 + d = d \tag{A.1.21}$$

$$\begin{aligned} x_f = x(t_f) &= \frac{f}{2m}(t_f - t_i)^2 + c(t_f - t_i) + x_i \\ c(t_f - t_i) &= x_f - x_i - \frac{f}{2m}(t_f - t_i)^2 \\ c &= \frac{x_f - x_i}{t_f - t_i} - \frac{f}{2m}(t_f - t_i) \end{aligned} \tag{A.1.22}$$

We will insert the results from Equations (A.1.21) and (A.1.22) into Equation (A.1.20) to get

$$x_{cl}(t) = \frac{f}{2m}(t - t_i)^2 + \left(\frac{x_f - x_i}{t_f - t_i} - \frac{f}{2m}(t_f - t_i)\right)(t - t_i) + x_i. \tag{A.1.23}$$

We now want to use this formula for the path to calculate the Lagrangian, which was given by Equation (A.1.15). We will first calculate the time derivative of the path, as we need this to calculate the Lagrangian.

$$\dot{x}_{cl}(t) = \frac{f}{m}(t - t_i) + \left(\frac{x_f - x_i}{t_f - t_i} - \frac{f}{2m}(t_f - t_i)\right) \tag{A.1.24}$$

We can now use Equations (A.1.23) and (A.1.24) to calculate the Lagrangian. For now we will still use the constant c instead of the value we found in Equation (A.1.21), to keep our calculations easier.

$$\begin{aligned} \mathscr{L}(x, \dot{x}) =& \frac{1}{2}m\dot{x}_{cl} + fx_{cl} = \frac{1}{2}m\left[\frac{f}{m}(t - t_i) + c\right]^2 + f\left[\frac{f}{2m}(t - t_i)^2 + c(t - t_i) + x_i\right] \\ =& \frac{1}{2}m\left[\frac{f^2}{m^2}(t - t_i)^2 + 2c\frac{f}{m}(t - t_i) + c^2\right] + \frac{f^2}{2m}(t - t_i)^2 + cf(t - t_i) + fx_i \\ =& \frac{f^2}{2m}(t - t_i)^2 + cf(t - t_i) + \frac{1}{2}mc^2 + \frac{f^2}{2m}(t - t_i)^2 + cf(t - t_i) + fx_i \\ =& \frac{f^2}{m}(t - t_i)^2 + 2cf(t - t_i) + \frac{1}{2}mc^2 + fx_i \end{aligned} \tag{A.1.25}$$

We can now use the Lagrangian to calculate the action, for which we will use Equation (A.1.1).

$$\begin{aligned} S[x_{cl}(t)] =& \int_{t_i}^{t_f} \mathscr{L}(x,\dot{x})dt = \int_{t_i}^{t_f} \left(\frac{f^2}{m}(t-t_i)^2 + 2cf(t-t_i) + \frac{1}{2}mc^2 + fx_i\right)dt \\ =& \left(\frac{f^2}{3m}(t-t_i)^3 + cf(t-t_i)^2 + \frac{1}{2}mc^2(t-t_i) + fx_i(t-t_i)\right)_{t_i}^{t_f} \\ =& \frac{f^2}{3m}(t_f-t_i)^3 + cf(t_f-t_i)^2 + \frac{1}{2}mc^2(t_f-t_i) + fx_i(t_f-t_i) \end{aligned} \tag{A.1.26}$$

We will now insert the value we found for the constant c, in Equation (A.1.21), into the equation. This way we get

$$\begin{aligned} S_{cl} =& \frac{f^2}{3m}(t_f-t_i)^3 + cf(t_f-t_i)^2 + \frac{1}{2}mc^2(t_f-t_i) + fx_i(t_f-t_i) \\ =& \frac{f^2}{3m}(t_f-t_i)^3 + \left(\frac{x_f-x_i}{t_f-t_i} - \frac{f}{2m}(t_f-t_i)\right)f(t_f-t_i)^2 \\ &+ \frac{1}{2}m\left(\frac{x_f-x_i}{t_f-t_i} - \frac{f}{2m}(t_f-t_i)\right)^2(t_f-t_i) + fx_i(t_f-t_i) \\ =& \frac{f^2}{3m}(t_f-t_i)^3 + f(x_f-x_i)(t_f-t_i) - \frac{f^2}{2m}(t_f-t_i)^3 \\ &+ \frac{1}{2}m\left(\frac{(x_f-x_i)^2}{(t_f-t_i)^2} - 2\frac{f}{2m}(x_f-x_i) + \frac{f^2}{4m^2}(t_f-t_i)^2\right)(t_f-t_i) + fx_i(t_f-t_i) \\ =& \frac{f^2}{3m}(t_f-t_i)^3 + fx_f(t_f-t_i) - \frac{f^2}{2m}(t_f-t_i)^3 \\ &+ \frac{1}{2}m\frac{(x_f-x_i)^2}{t_f-t_i} - \frac{f}{2}(x_f-x_i)(t_f-t_i) + \frac{f^2}{8m}(t_f-t_i)^3 \\ =& \frac{f^2}{3m}(t_f-t_i)^3 - \frac{f^2}{2m}(t_f-t_i)^3 + \frac{f^2}{8m}(t_f-t_i)^3 \\ &+ \frac{1}{2}m\frac{(x_f-x_i)^2}{t_f-t_i} + fx_f(t_f-t_i) - \frac{f}{2}x_f(t_f-t_i) + \frac{f}{2}x_i(t_f-t_i) \\ =& -\frac{f^2}{24m}(t_f-t_i)^3 + \frac{1}{2}m\frac{(x_f-x_i)^2}{t_f-t_i} + \frac{f}{2}(x_f+x_i)(t_f-t_i). \end{aligned} \tag{A.1.27}$$

By using the formulas we had defined before and by doing explicit calculations, we were able to determine the action of the classical path for a particle under a force f. We found that the action for the classical path was given by

$$S_{cl} = -\frac{f^2}{24m}(t_f-t_i)^3 + \frac{1}{2}m\frac{(x_f-x_i)^2}{t_f-t_i} + \frac{f}{2}(x_f+x_i)(t_f-t_i). \tag{A.1.28}$$

A.2 Self-adjoint operators

In this section we will look at self-adjoint and essentially self-adjoint operators, since this is background we need for Sections 2.4 and 4.2. We will mainly look at the definitions and

theorems and only go into some proofs. Some more background information and proofs can be found in Chapter 9 of Hall [8], along which lines we will mainly go.

We will look mainly at unbounded self-adjoint operators. In physics a lot of operators will not be defined on the whole Hilbert space, only on a dense subspace. For these operators there is no constant $C > 0$ such that $||A\psi|| \leq C||\psi||$ for all ψ for which A is defined, so the operator A is unbounded.

As we work with unbounded operators, it will be a bit more difficult to give a definition of self-adjointness as this definition will not be given by the probable candidate $\langle \phi, A\psi \rangle = \langle A\phi, \psi \rangle$, which follows from the definition for bounded operators. Instead we will define A^*, the adjoint of A, with its own domain. Now A is self-adjoint and thus $A^* = A$ when they have the same domain.

In the following, we will use $\mathscr{H}$ to denote a separable Hilbert space over $\mathbb{C}$.

Definition A.1. An unbounded operator A on $\mathscr{H}$ is a linear map of some dense subspace $\mathrm{Dom}(A) \subset \mathscr{H}$ into $\mathscr{H}$.

Unbounded means not necessarily bounded, so we permit the case that $\mathrm{Dom}(A) = \mathscr{H}$ and A is bounded.

If A is bounded then for any ϕ we get that $\langle \phi, A \cdot \rangle$ is bounded so there exists (by using the Riesz theorem) a unique χ such that $\langle \phi, A \cdot \rangle = \langle \chi, \cdot \rangle$, we then define A^*, the adjoint of A, by setting $A^*\phi = \chi$. For the bounded case, we have thus found a definition for the adjoint of A.

If A is unbounded, then $\langle \phi, A \cdot \rangle$ is not necessarily bounded, although it may be bounded for certain ϕ. If it is bounded for certain $\phi \in \mathscr{H}$, there has to exist a unique bounded extension from $\mathrm{Dom}(A)$ to $\mathscr{H}$, according to the BLT theorem, which can be found in Hall [8]. We can then use Riesz' theorem once more to find that there exists a unique χ such that the linear function is equal to the inner product with χ.

Definition A.2. Suppose A is an operator defined on a dense subspace $\mathrm{Dom}(A) \subset \mathscr{H}$. Let $\mathrm{Dom}(A^*)$ be the space of all $\phi \in \mathscr{H}$ for which the linear functional

$$\psi \mapsto \langle \phi, A\psi \rangle, \quad \psi \in \mathrm{Dom}(A),$$

is bounded. For $\phi \in \mathrm{Dom}(A^*)$, define $A^*\phi$ to be the unique vector such that $\langle \phi, A\psi \rangle = \langle A^*\phi, \psi \rangle$ for all $\psi \in \mathrm{Dom}(A)$.

Saying that $\langle \phi, A\cdot \rangle$ is bounded means that there exists a constant C such that $|\langle \phi, A\psi \rangle| \leq C||\psi||$ for all $\psi \in \mathrm{Dom}(A)$. We now once again find that the operator A^* is linear on its domain and is called the *adjoint* of A. We will quickly show that A^* is linear, that is we want to show that $A^*(\alpha\phi + \beta\chi) = \alpha A^*\phi + \beta A^*\chi$, where α, β are some constants and $\phi, \chi \in \mathrm{Dom}(A^*)$. For this we will use the linearity of the inner product and Definition A.2. This gives us that there exists a $\psi \in \mathrm{Dom}(A)$ such that

$$\begin{aligned} \langle A^*(\alpha\phi + \beta\chi), \psi \rangle &= \langle \alpha\phi + \beta\chi, A\psi \rangle = \alpha\langle \phi, A\psi \rangle + \beta\langle \chi, A\psi \rangle = \alpha\langle A^*\phi, \psi \rangle + \beta\langle A^*\chi, \psi \rangle \\ &= \langle \alpha A^*\phi, \psi \rangle + \langle \beta A^*\chi, \psi \rangle = \langle \alpha A^*\phi + \beta A^*\chi, \psi \rangle. \end{aligned} \tag{A.2.1}$$

Since we found in Definition A.2 that the adjoint vector would be unique, this tells us that $A^*(\alpha\phi + \beta\chi) = \alpha A^*\phi + \beta A^*\chi$, so we indeed find that A^* is linear.

Another way of thinking about the definition of A^* is as follows. Given a vector ϕ, if there exists a vector χ such that $\langle \phi, A\psi\rangle = \langle \chi, \psi\rangle$ for all $\psi \in \mathrm{Dom}(A)$, then ϕ belongs to $\mathrm{Dom}(A^*)$ and $A^*\phi = \chi$. By using Riesz' theorem once more, we find that such a χ will exist if and only if $\langle \phi, A\,\cdot\,\rangle$ is bounded, which means this way of thinking about the adjoint A^* is equivalent to Definition A.2.

One problem we might face, is that given a densely defined operator A, the adjoint A^* of A does not necessarily have to be densely defined itself. As this situation does not usually occur for operators of interest in applications, which we are looking at in this thesis, we will only go into the operators with a densely defined adjoint now.

Definition A.3. An unbounded operator A on $\mathscr{H}$ is **symmetric** if

$$\langle \phi, A\psi\rangle = \langle A\phi, \psi\rangle \tag{A.2.2}$$

for al $\phi, \psi \in \mathrm{Dom}(A)$.

If A is symmetric, then A^* is an extension of A, where the definition of an extension is given by Definition A.4.

Definition A.4. An unbounded operator A is an **extension** of an unbounded operator B if $\mathrm{Dom}(B) \subset \mathrm{Dom}(A)$ and $A = B$ on $\mathrm{Dom}(B)$.

If A is an extension of B, then very likely A will be given by the same formula as B. For example, if $\mathscr{H} = L^2(\mathbb{R})$ two operators might be given by the formula $-i\hbar\frac{d}{dx}$ on their respective domains, but if $\mathrm{Dom}(A) \neq \mathrm{Dom}(B)$, these two operators still differ from one another.

We can now give a definition of a self-adjoint unbounded operator, which is what we have been working towards.

Definition A.5. An unbounded operator A on $\mathscr{H}$ is **self-adjoint** if $\mathrm{Dom}(A^*) = \mathrm{Dom}(A)$ and $A^*\phi = A\phi$ for all $\phi \in \mathrm{Dom}(A)$.

It may now seem easier to give the definition of self-adjointness by saying that A is self-adjoint if $A^* = A$. But one of the important things which easily gets neglected in that case, is the requirement of equality of domains. By using Proposition A.6 we know that every self-adjoint operator is symmetric, but not every symmetric operator is self-adjoint as the domains do not have to be equal. We can expand this to say that a symmetric operator is self-adjoint if and only if $\mathrm{Dom}(A) = \mathrm{Dom}(A^*)$, but the difficulty with this is having to show that $\mathrm{Dom}(A^*)$ does not contain more elements than $\mathrm{Dom}(A)$.

The following proposition will be a stepping stone towards the definition of essential self-adjointness for unbounded operators.

Proposition A.6. *An unbounded operator A is symmetric if and only if A^* is an extension of A.*

We will now prove this proposition.

Proof. We will first start with the symmetric operator A and show that A^* is an extension of A and we will then proof the implication the other way around. If A is symmetric, we can use Definition A.3 to find that $|\langle\phi, A\psi\rangle| = |\langle A\phi, \psi\rangle|$ for all $\phi, \psi \in \text{Dom}(A)$. We can now use the Chauchy-Schwarz inequality on the left-hand side of the equation to show that $|\langle A\phi, \psi\rangle| \leq ||A\phi||\ ||\psi||$ and thus $|\langle\phi, A\psi\rangle| \leq ||A\phi||\ ||\psi||$. From this inequality and Definition A.2 it follows that $\phi \in \text{Dom}(A^*)$. Now Definition A.2 also tells us that $A^*\phi$ is the unique vector for which $\langle\phi, A\psi\rangle = \langle A^*\phi, \psi\rangle$. But when we now also use Equation (A.2.2), we find that this unique vector $A^*\phi$ must be equal to $A\phi$. So for all $\phi \in \text{Dom}(A)$, we find that $A^*\phi = A\phi$, so A^* and A are equal on $\text{Dom}(A)$. It could still be the case that $\text{Dom}(A^*) \supset \text{Dom}(A)$, but since they are equal on $\text{Dom}(A)$ we can use Definition A.4 to find that A^* is an extension of A.

Now if we start with A^* being an extension of A, we know that $A = A^*$ on $\text{Dom}(A)$. So for all $\phi \in \text{Dom}(A)$, we know that $\phi \in \text{Dom}(A^*)$. If we now take $\psi \in \text{Dom}(A)$, Definition A.2 tells us that $\langle\phi, A\psi\rangle = \langle A^*\phi, \psi\rangle$. Since $A = A^*$ on $\text{Dom}(A)$ this also tells us that $\langle A^*\phi, \psi\rangle = \langle A\phi, \psi\rangle$, so $\langle\phi, A\psi\rangle = \langle A\phi, \psi\rangle$. So we can see that A is symmetric for all $\phi, \psi \in \text{Dom}(A)$. ■

By using this proposition we can get the following definition.

Definition A.7. An unbounded operator A on $\mathscr{H}$ is said to be **closed** if the graph of A is a closed subset of $\mathscr{H} \times \mathscr{H}$. An unbounded operator A on $\mathscr{H}$ is said to be **closable** if the closure in $\mathscr{H} \times \mathscr{H}$ of the graph A is the graph of a function. If A is closable then the closure A^{cl} of A is the operator with graph equal to the closure of the graph of A.

An operator A is closed if and only if the following condition holds: suppose a sequence ψ_n belongs to $\text{Dom}(A)$ and suppose that there exist vectors ψ and ϕ in $\mathscr{H}$ with $\psi_n \to \psi$ and $A\psi_n \to \phi$. Then ψ belongs to $\text{Dom}(A)$ and $A\psi = \phi$. We can compare this to the following situation. If A is closed and there is a sequence ψ_n which belongs to $\text{Dom}(A)$ and suppose that there exist vectors ψ and ϕ in $\mathscr{H}$ with $\psi_n \to \psi$ and $A\psi_n \to \phi$, then it has to hold that $\psi \in \text{Dom}(A)$ as we know that A is closed. As we also saw that $A\psi_n \to \phi$, this also tells us that $A\psi = \phi$ as $A\psi_n \to A\psi = \phi$.

Regarding closability, an operator A is not closable if there exist two elements in the closure of the graph of A of the form (ϕ, ψ) and (ϕ, χ) with $\psi \neq \chi$. Another way of putting it is that A is closable if there exists some closed extension of it. Then the closure of A as defined in Definition A.7 is the smallest closed extension of A. To compare this to an example in one dimension, the interval $(0, 1)$ is not closed, but there are multiple closures possible, for example $[-100, 500]$, $[-10, 6]$ or $[0, 1]$. In this case it is clear that the smallest closed extension would be $[0, 1]$, which we would thus call the closure of $(0, 1)$.

The notion of the closure of a closable operator is useful because it sweeps away some of the arbitrariness in the choice of a domain of an operator. If we consider, for example, the operator $A = -i\hbar\frac{d}{dx}$ as an unbounded operator on $L^2(\mathbb{R})$, there are many different reasonable choices for $\text{Dom}(A)$. As it turns out, in this case, many choices for $\text{Dom}(A)$ lead to the same operator A^{cl}. For example the space of C^∞ functions of compact support and the space of C^1 functions ψ, where both ψ and ψ' belong to $L^2(\mathbb{R})$ both give the same closure for the operator A. Not every choice for this domain gives us the same closure, but often many reasonable choices do lead to the same closure. It is clear that this is a huge advantage as

in general our choice for the domain will matter less, as many choices will lead to the same closure.

We can now give the following definition:

Definition A.8. An unbounded operator A on $\mathscr{H}$ is said to be **essentially self-adjoint** if A is symmetric and closable and if A^{cl} is self-adjoint.

As it turns out, a symmetric operator is always closable. But as many closures A^{cl} will not be self-adjoint, many symmetric operators will not be essentially self-adjoint, let alone self-adjoint.

Proposition A.9. *If A is a closable operator on $\mathscr{H}$, then the adjoint of A^{cl} coincides with the adjoint of A.*

We will now look at some criteria for determining whether a symmetric operator is (essentially) self-adjoint.

Theorem A.10. *If A is a symmetric operator on $\mathscr{H}$, then A is essentially self-adjoint if and only if Range$(A - iI)$ and Range$(A + iI)$ are dense subspaces of $\mathscr{H}$.*

Which is equivalent to the following corollary:

Corollary A.11. *If A is a symmetric operator on $\mathscr{H}$, then A is essentially self-adjoint if and only if the operators $A^* + iI$ and $A^* - iI$ are injective on Dom(A^*).*

It is essential that we require both operators to be injective, as it is possible to have one of them be injective, while the other one fails to be injective. From this we can also get the following proposition, which can also be used as criterium to check the self-adjointness of an operator.

Proposition A.12. *If A is a symmetric operator on $\mathscr{H}$, then A is self-adjoint if and only if Range$(A - iI) =$ Range$(A + iI) = \mathscr{H}$.*

This last theorem even states criteria for both essential self-adjointness and self-adjointness of operators.

Theorem A.13. *Suppose that A is a symmetric operator on $\mathscr{H}$ and that $\langle \psi, A\psi \rangle \geq 0$ for all $\psi \in$ Dom(A). Then A is essentially self-adjoint if and only if $A + I$ has dense range. Equivalently, A is essentially self-adjoint if and only if $A^* + I$ is injective.*

The disadvantage of this theorem is that it is only applicable when A is positive-semidefinite, which means $\langle \psi, A\psi \rangle \geq 0$ has to hold for all $\psi \in \mathrm{Dom}(A)$.

We will now work towards the proof of this theorem. For this we will first give two propositions, which we will also prove.

Proposition A.14. *If A is an unbounded operator on $\mathscr{H}$, then*

$$(\mathrm{Range}(A))^{\perp} = \ker(A^*). \tag{A.2.3}$$

Proof. We will first show that $\text{Dom}(A) \neq \{0\}$, then we will use this to show that $(\text{Range}(A))^\perp \subset \ker(A^*)$ and then we will show that $(\text{Range}(A))^\perp \subset \ker(A^*)$, which will imply that $(\text{Range}(A))^\perp = \ker(A^*)$.

Since A is an unbounded operator, we know that there exists no constant C such that $||A\psi|| = C||\psi||$ for all $\psi \in \text{Dom}(A)$. So if $\text{Dom}(A) = \{0\}$, then $||A\psi|| = 0$ for all $\psi \in \text{Dom}(A)$, so every constant C would suffice and A would be bounded. So we find that for the unbounded operator A, we know that $\text{Dom}(A) \neq \{0\}$.

We will now take $\phi \in (\text{Range}(A))^\perp$, then ϕ is perpendicular to the Range of A, so for all $\psi \in \text{Dom}(A)$ we find that $\langle \phi, A\psi \rangle = 0$. Since $\langle \phi, A \cdot \rangle = 0$, it is clearly bounded, so by using Definition A.2 we find that $\phi \in \text{Dom}(A^*)$. This means that we can write $\langle \phi, A\psi \rangle = 0$ as $\langle \phi, A\psi \rangle = \langle A^*\phi, \psi \rangle = 0$ for all $\psi \in \text{Dom}(A)$. Since $\text{Dom}(A) \neq \{0\}$, this can only hold for all $\psi \in \text{Dom}(A)$ if $A^*\phi = 0$. As $A^*\phi = 0$, we know that $\phi \in \ker(A^*)$. So for all $\phi \in (\text{Range}(A))^\perp$ we find that $\phi \in \ker(A^*)$, so $(\text{Range}(A))^\perp \subset \ker(A^*)$.

We will now take $\phi \in \ker(A^*)$, then $\phi \in \text{Dom}(A^*)$ and $A^*\phi = 0$. For all $\psi \in \text{Dom}(A)$, we will find by using Definition A.2 that $\langle \phi, A\psi \rangle = \langle A^*\phi, \psi \rangle = 0$. Since $\text{Dom}(A) \neq \{0\}$, we know that ϕ must be perpendicular to $A\psi$ for all $\psi \in \text{Dom}(A)$, so it must hold that $\phi \in (\text{Range}(A))^\perp$. So for all $\phi \in \ker(A^*)$, we know that $\phi \in (\text{Range}(A))^\perp$, so $(\text{Range}(A))^\perp \supset \ker(A^*)$.

Since we have found that $(\text{Range}(A))^\perp \subset \ker(A^*)$ and that $(\text{Range}(A))^\perp \supset \ker(A^*)$ we indeed find that $(\text{Range}(A))^\perp = \ker(A^*)$. ■

The second proposition we want to look at before the proof of Theorem A.13 is the following. For this we take the domain of $A - \lambda I$ equal to the domain of A.

Proposition A.15. *Let A be a closed operator and λ an element of $\mathbb{C}$. Suppose that there exists an $\varepsilon > 0$ such that*

$$||(A - \lambda I)\psi|| \geq \varepsilon ||\psi|| \tag{A.2.4}$$

for all $\psi \in Dom(A)$. Then the range of $A - \lambda I$ is a closed subspace of $\mathscr{H}$.

Proof. To prove that the range of $A - \lambda I$ closed is, we will take a converging sequence ϕ_n, with $\phi_n \in \text{Range}(A - \lambda I)$ for all $n \in \mathbb{N}$. Now this sequence converges in $\mathscr{H}$ to some ϕ, if we can show that $\phi \in \text{Range}(A - \lambda I)$ we know that this range is closed in $\mathscr{H}$.

So we have a sequence $\phi_n \in \text{Range}(A - \lambda I)$ for all $n \in \mathbb{N}$. This tells us that for each ϕ_n, there is some ψ_n, such that we can write $\phi_n = (A - \lambda I)\psi_n$. We know that these $\psi_n \in \text{Dom}(A)$, since we took the domain of A to be equal to the domain of $A - \lambda I$. Now we can use this to write $\phi_n - \phi_m = (A - \lambda I)\psi_n - (A - \lambda I)\psi_m = (A - \lambda I)(\psi_n - \psi_m)$. We now also find that $(\psi_n - \psi_m) \in \text{Dom}(A)$, since we took equal domains. We can now use Equation (A.2.4) to get that there exists an $\varepsilon > 0$ such that

$$||\phi_n - \phi_m|| = ||(A - \lambda I)(\psi_n - \psi_m)|| \geq \varepsilon ||\psi_n - \psi_m||. \tag{A.2.5}$$

We can rewrite this equation to get that $||\psi_n - \psi_m|| \leq \frac{1}{\varepsilon}||\phi_n - \phi_m||$. Since $\phi_n \to \phi$ for $n \to \infty$, we find that $||\phi_n - \phi_m|| \to 0$ for $n, m \to \infty$. We thus get that $\frac{1}{\varepsilon}||\phi_n - \phi_m|| \to 0$ for $n, m \to \infty$. This tells us that $||\psi_n - \psi_m|| \to 0$ for $n, m \to \infty$, or that the sequence ψ_n is Cauchy. If we assume $\text{Dom}(A)$ to be complete, we find that ψ_n is convergent, so there exists some ψ such that $\psi_n \to \psi$ for $n \to \infty$. We know that A is closed, so we also find that $\psi \in \text{Dom}(A)$.

Now we know that $\phi_n = (A - \lambda I)\psi_n$ so we get that $A\psi_n = \lambda\psi_n + \phi_n$. Now we also know that $\lambda\psi_n + \phi_n \to \lambda\psi + \phi$ for $n \to \infty$. We thus find that $A\psi_n \to \lambda\psi + \phi$ for $n \to \infty$. We thus find that $A\psi_n$ also converges as n goes to infinity. Since we already found that $\psi \in \mathrm{Dom}(A)$ we get that $A\psi = \lambda\psi + \phi$, which we can rewrite to $\phi = (A - \lambda I)\psi$, with $\psi \in \mathrm{Dom}(A)$. This tells us that $\phi \in \mathrm{Range}(A - \lambda I)$. So we found that for a converging sequence $\phi_n \in \mathrm{Range}(A - \lambda I)$ the limit ϕ is also in the range of $(A - \lambda I)$, which tells us that $\mathrm{Range}(A - \lambda I)$ is closed. ■

Proof of Theorem A.12. Our proof will consist of two steps. The first will be to show that if A is essentially self-adjoint that $A + I$ has dense range and that $A^* + I$ is injective. The second step will be to show that if $A + I$ has dense range or if $A^* + I$ is injective that A is essentially self-adjoint. Then by using both steps, we will have proved both statements.

Now if A is essentially self-adjoint we know that A^{cl} is self-adjoint and thus that the closure of A is equal to its adjoint and that the domain of the closure and its adjoint are equal. Since we know that $\langle\psi, A\psi\rangle \geq 0$ for all $\psi \in \mathrm{Dom}(A)$ and since A^{cl} is self-adjoint and densely defined, we can see that A^{cl} is positive definite, so $\langle\psi, A^{cl}\psi\rangle > 0$ for all $\psi \neq 0$. Since A^{cl} is self-adjoint, by using Proposition A.9 we find that $(A+I)^* = A^*+I^* = A^*+I = A^{cl}+I$. This tells us that $\langle\psi, (A^{cl}+I)\psi\rangle = \langle\psi, \psi\rangle + \langle\psi, A^{cl}\psi\rangle > \langle\psi, \psi\rangle$ for $\psi \neq 0$. Since $\langle\psi, A^{cl}\psi\rangle > 0$ for all $\psi \neq 0$, we know that $\ker(A^{cl}) = \{0\}$, so we know that A^{cl} is injective. Since A^{cl} is injective and since I is clearly injective, we find that $A^{cl} + I$ is injective. We have already seen that $(A+I)^* = A^* + I = A^{cl} + I$, so $(A+I)^*$ is also injective. Here we can note that we have now already seen that the essential self-adjointness of A implies that $A^* + I$ is injective. Now since $(A + I)^*$ is also injective, we know that $\ker((A + I)^*) = \{0\}$. We can now use Proposition A.14 to find that $(\mathrm{Range}(A+I))^\perp = \{0\}$, which shows us that $(A+I)$ must have a dense range in $\mathscr{H}$, since the only element perpendicular to it is $\{0\}$. Now we have shown that if A is essentially self-adjoint that $A + I$ has dense range and that $A^* + I$ is injective, as we wanted to show in step 1.

For the following step we assume that $A + I$ is dense. We can use that A is symmetric, that $\langle\psi, A\psi\rangle \geq 0$ for all $\psi \in \mathrm{Dom}(A)$ and since A is symmetric, we know that it is closable, so its closure A^{cl} exists. Now since we know that $\langle\psi, (A^{cl} + I)\psi\rangle = \langle\psi, \psi\rangle + \langle\psi, A^{cl}\psi\rangle \geq \langle\psi, \psi\rangle$, we find that $A^{cl} + I$ is injective, since its kernel can only contain the element 0. Now since $\langle\psi, (A^{cl}+I)\psi\rangle \geq \langle\psi, \psi\rangle$ we find that $\langle(A^{cl}+I)\psi, (A^{cl}+I)\psi\rangle = \langle A^{cl}\psi, (A^{cl}+I)\psi\rangle + \langle\psi, (A^{cl} + I)\psi\rangle \geq \langle\psi, (A^{cl} + I)\psi\rangle \geq \langle\psi, \psi\rangle$. If we now take $\varepsilon = 1$ and $\lambda = -1$, we find that we can use Proposition A.15 for A^{cl} to find that $\mathrm{Range}(A^{cl} + I)$ is closed in $\mathscr{H}$. Since we know that $A + I$ has dense range, we know that $A^{cl} + I$ also has dense range. So since the range of $A^{cl} + I$ is dense and closed in $\mathscr{H}$, we know that it must be equal to $\mathscr{H}$.

By using Proposition A.9 we find that $A^* = A^{cl,*}$. Since both A and thus A^{cl} are symmetric, by using Proposition A.6 we find that on the domain of A^{cl} it holds that $A^{cl} = A^{cl,*}$ and thus that $A^{cl} = A^*$. If we now can show that the domain of A^* and A^{cl} are equal, we know that A^{cl} is equal to its adjoint and thus that A is essentially self-adjoint. Since we know that A^* is an extension of A^{cl}, we know that $\mathrm{Dom}(A^*) \supset \mathrm{Dom}(A^{cl})$.

We will now assume that the domain of A^* is strictly larger than the domain of A^{cl}. This will lead to a contradiction, which will tell us that the domains must be equal.

Now we assume that the domain of A^* is strictly larger than the domain of A^{cl}. We already know that the range of $A^{cl} + I$ is equal to $\mathscr{H}$, so $A^{cl} + I$ is surjective, since its range

is the whole space we are working on. This means that every element of $\mathscr{H}$ has at least one original in $\mathrm{Dom}(A^{cl}+I)$. Since we assume that $\mathrm{Dom}(A^{cl}) \subsetneq \mathrm{Dom}(A^*)$ we also know that $\mathrm{Dom}(A^{cl}+I) \subsetneq \mathrm{Dom}(A^*+I)$. We thus know that $\mathrm{Dom}(A^*+I)$ contains more elements than $\mathscr{H}$, so $A^*+I=(A+I)^*$ cannot be injective. Since $(A+I)^*$ is not injective, its kernel must contain more elements than only 0, so it will be non-trivial. By using Proposition A.14 again, we find that $\mathrm{Range}(A+I)$ must be non-trivial, so the range of $A+I$ cannot be dense. Since we started this second step with the assumption that $A+I$ is dense, this is a contradiction.

We thus know that the domain of A^* cannot be strictly larger than the domain of A^{cl}. Since A^* is an extension of A^{cl} this must mean that their domains are equal. This tells us that the closure of A is equal to its adjoint and that their domains are equal. So the closure of A is self-adjoint and we thus find that A is essentially self-adjoint when $A+I$ has dense range, since we already know that both A and its closure are symmetric.

Now if we would have started this second step with the assumption that A^*+I is injective, we would have already seen the contradiction sooner. Now the other steps could have remained the same, so we would also have seen that A is essentially self-adjoint when A^*+I is injective. ■

We will now look at an example, to see how some of the definitions and theorems can be used.

Example A.16. *Suppose that A is a symmetric operator on the Hilbert space $\mathscr{H}$ that has an orthonormal basis of eigenvectors, given by $\{e_j\}$. Since A is on $\mathscr{H}$, we know that we can get $Ae_j=\lambda_j e_j$ for some real numbers λ_j. Then A is essentially self-adjoint.*

Proof. First of all, we know that any λ_j for which $Ae_j=\lambda_j e_j$ has to be real, since A is a symmetric operator. If we now, for any j, take $(A-iI)e_j$, we get $(A-iI)e_j=\lambda_j e_j - ie_j = (\lambda_j - i)e_j$. We know that λ_j is real, so for all j we know that $\lambda_j - i \neq 0$, so we find that $(\lambda_j - i) \in \mathrm{Range}(A-iI)$. Since this holds for all j, we find that this range is dense in $\mathscr{H}$.

We will now use the same steps, while taking $(A+iI)e_j$. We then get $(A+iI)e_j = \lambda_j e_j + ie_j = (\lambda_j + i)e_j$. We know that λ_j is real, so for all j we know that $\lambda_j + i \neq 0$. So for all j, we find that $(\lambda_j + i) \in \mathrm{Range}(A+iI)$. This thus tells us that this range is also dense in $\mathscr{H}$.

Now since we know that $\mathrm{Range}(A-iI)$ and $\mathrm{Range}(A+iI)$ are dense in $\mathscr{H}$ and since we have a symmetric operator A, we can use Theorem A.10 to find that A is essentially self-adjoint. ■

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