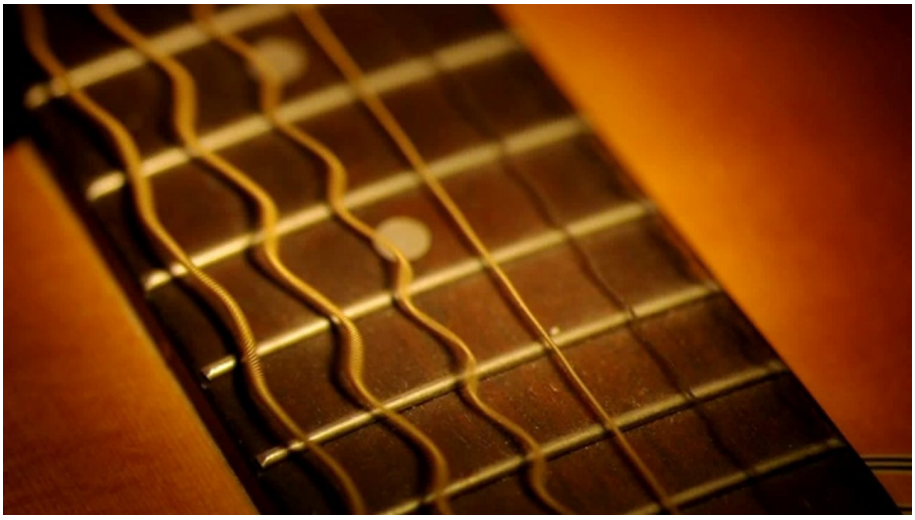
Playing around with the Schrödinger equation



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Contents

1 The time-dependent Schrödinger equation **5**

1.1 The wave function 5
1.2 Numerical Discretization 6
1.3 Exercise: The kinetic energy operator as a matrix 7
1.4 Exercise: The Crank-Nicolson propagator 7
1.5 Exercise: Wave propagation 8
1.6 Exercise: The Magnus propagator. 9
1.7 Exercise: Gaussian wave – once again 11
1.8 Exercise: Interference 11

2 Scattering **13**

2.1 Exercise: Scattering on a barrier 14
2.2 Exercise: The dynamics of a classical particle 15
2.3 Exercise: Tunneling 16
2.4 Exercise: Scattering on a double barrier 17

3 Dynamics **19**

3.1 Exercise: Magnus propagators of 1st and 2nd order 19
3.2 Exercise: Split-operators 20
3.3 Exercise: Some real dynamics 21

Chapter 1

The time-dependent Schrödinger equation

In generic form, the time-depenent Schrödinger equation reads

$$i\hbar\frac{\partial}{\partial t}\Psi(x;t) = \hat{H}\Psi(x;t) \quad , \tag{1.1}$$

where $\hat{H}$, the *Hamiltonian*, is a linear operator corresponding to the energy of the system in question. In our case, this system will be that of a single particle in one dimension. Moreover, for now, this system will not be exposed to any time-dependent interactions, in which case the Hamiltonian reads

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) = \hat{T} + V(x) \quad , \tag{1.2}$$

where the operator $\hat{T}$ correspodns to the kinetic energy of the particle. For convenience we will set $\hbar$ and m equal to unity. This is admissible as it simply corresponds to taking these constants as the unit of their respective quantities.

All in all, this is the partial differential equation we are to solve:

$$i\frac{\partial}{\partial t}\Psi(x;t) = -\frac{1}{2}\frac{d^2\Psi}{dx^2} + V(x)\Psi(x;t) \quad . \tag{1.3}$$

1.1 The wave function

The solution, Ψ, of Eq. 1.1 is called the *wave function*. Much could be said about it and how physical information is obtainable from it. We will keep it extremely short here: The absolute square of it, $|\Psi(x;t)|^2$ is the probability density that a popsition measurement at time t will provide result x. Or, put differently, the

probability of measuring the particle to be localized somewhere between $x = a$ and $x = b$ is

$$P(x \in [a,b];t) = \int_a^b |\Psi(x;t)|^2 \, dx \quad . \tag{1.4}$$

In other words, the result of a position measurement is a stochastical variable, and $|\Psi|^2$ is its distribution function. Consequently, it needs to normalize to 1,

$$\int_{-\infty}^{\infty} |\Psi(x;t)|^2 \, dx = 1 \tag{1.5}$$

at all times.

In addition, we require that both Ψ and its (spatial) dericative is continuous at all times.

1.2 Numerical Discretization

We will start out by choosing a certain domain for our wave function Ψ to "live" in. Assuming that $\Psi(x;t)$ vanish for $x < a$ and $x > b$ at all times, vi may disregard the parts of space beyond these points. Moreover, we will *discretize* the resulting interval so that our wave function may be represented by a set of points. Effectively, our approximate wave function becomes a column vector in $\mathbb{C}^{n+1}$:

$$\Psi(x;t) \to \boldsymbol{\Psi}(t) = \begin{pmatrix} \Psi(x_0;t) \\ \Psi(x_1;t) \\ \vdots \\ \Psi(x_n;t) \end{pmatrix} \quad , \tag{1.6}$$

where $x_i = a + ih$ and $h = (b-a)/n$ as before. Please do not confuse the numerical parameter h with the Planck constant.

The approximation of Eq. 1.6 is, of course, a tremendous reduction in complexity. The wave function can in principle be *any* complex function which is finite, differentiable and normalizable on $\mathbb{R}$, while in Eq. 1.6 it is reduced to a simple vector.

When imposing discretization like this, it is absolutely crucial that we check for convergence; our results may certainly not depend significantly on our choices for the numerical parameters a, b and n. We *must* increase the span of our interval $[a,b]$ and reduce our step size h (increase n) until our numerical predictions are no longer affected by such modifications. Then, and only then, we may reasonably assume that the discretized representation $\boldsymbol{\Psi}(t)$ is a decent approximation to the true wave function $\Psi(x;t)$.

In the following we will, for convenience, skip writing out the time-dependence of the wave function explicitly.

Now, with a proper numerical discretization of Ψ we may apply numerical differentiation methods to it. The most straight forward approach would be that of *finite difference schemes*. We may, for instance, apply the symmetric three point rule or the symmetric five point rule for the double derivative in the Hamiltonian,

$$f''(x) = \frac{f(x-h) - 2f(x) + f(x+h)}{h^2} + \mathcal{O}(h^2) \quad \text{and} \tag{1.7a}$$

$$f''(x) = \frac{-f(x-2h) + 16f(x-h) - 30f(x) + 16f(x+h) - f(x+2h)}{12h^2} + \mathcal{O}(h^4) \quad , \tag{1.7b}$$

respectively.

1.3 Exercise: The kinetic energy operator as a matrix

With Ψ given on vector form as in Eq. 1.6, we may write the action of $\hat{T}$ on Ψ as a matrix multiplication. For the above choices, Eqs. 1.7, what will the corresponding matrices be? Assume that $\Psi(x) = 0$ for $x \notin [a,b]$ and that it falls off smoothly towards these edges.

With our wave fuction approximated by a column vector and our Hamiltonian represented by a square matrix, the numerical solution of the Schrödinger equation may be approximated. Effectively, this has turned Eq. 1.1, which is a partial differential equation, into a coupled set of ordinary differential equations.

In order to solve it, we need an initial condition, $\Psi_0 = \Psi(x; t = 0)$, and some scheme numerical scheme for the time evolution. One option for doing this could be the backward-forward Euler method, or the Crank-Nicolson method, which it is also refered to. It approximates the solution of the initial value problem

$$y'(t) = F(t,y), \quad y(t_0) = y_0 \tag{1.8}$$

by

$$y(t+\Delta t) - y(t) = \frac{\Delta t}{2}\left(F(t,y(t)) + F(t+\Delta t, y(t+\Delta t))\right) + \mathcal{O}(\Delta t^3) \quad . \tag{1.9}$$

1.4 Exercise: The Crank-Nicolson propagator

Show that, in our case, with our discretized representation, it may be written out explicitly:

$$\boldsymbol{\Psi}(t+\Delta t) \approx \left[I + iH\Delta t/2\right]^{-1}\left[I - iH\Delta t/2\right]\boldsymbol{\Psi}(t) \quad , \tag{1.10}$$

where I is the identity matrix and the matrix H is our numerical appoximation to the Hamiltonian.

Since our Hamiltonian has no time-dependence, the equation is *autnomous*, Eq. 1.10 is, in fact, unchanged in time. That means that you only need to contruct it once and then use it repeateldy to arrive at some final solution $\Psi(T)$, where $T = N_{dt}\Delta t$.

We will do just that.

And in doing so, it is convenient to let our initial state, Ψ_0, be a Gaussian, as it will remain a Gaussian with analytically known form in that case. Specifically, with your normalized state at time $t = 0$ being

$$\Psi(x,t=0) = \sqrt{\frac{\sqrt{2}\sigma_p}{\sqrt{\pi}(1-2i\sigma_p^2\tau)}}\exp\left[-\frac{\sigma_p^2(x-x_0)^2/\hbar^2}{1-2i\sigma_p^2\tau/(\hbar m)} + ip_0x/\hbar\right] \quad , \tag{1.11}$$

then the absolute square of our wave function at time t is

$$|\Psi(x;t)|^2 = |N|^2\exp\left[-\frac{2}{\hbar^2}\frac{\sigma_p^2(x-x_0-p_0t/m)^2}{1+4\sigma_p^4(t-\tau)^2/(m\hbar)^2}\right] \tag{1.12}$$

with the time-dependent normalization factor

$$|N|^2 = \sqrt{\frac{2}{\pi}}\frac{\sigma_p/\hbar}{\sqrt{1+4\sigma_p^4(t-\tau)^2/(m\hbar)^2}} \quad .$$

Here x_0 is the particle's mean position initially, τ is the time at which the wave packet is at its narrowest, p_0 is the mean momentum and σ_p is the width of the momentum distribution.

1.5 Exercise: Wave propagation

In this exercise we are going to simulate a Gaussian wave packet which is not exposed to any potential $V(x)$. With $V = 0$, the Hamiltonian is simply the kinetic energy operator, $\hat{H} = \hat{T} = -\hbar^2/2m\,\mathrm{d}^2/\mathrm{d}x^2$. This system serves well for checking the accuracy of our numerical approximations since the exact solution is known analytically, Eq. 1.12.

For starters, you can choose the following set of parameters:

x_0	σ_p	p_0	τ
-20	0.2	3	5

Also, let your domain be $[a,b] = [-L/2, L/2]$ with $L = 100$. Choose an initial number of grid points n, and let your initial time be $t = 0$.

Let the mass m and $\hbar$ be unity in your implementation.

a) For our two approximations to the kinetic energy operator, the finite difference approximations of Eqs. 1.7, simulate the evolution of the wave function according to Eq. 1.10 and compare the numerical estimate to the exact one, Eq. 1.12. Specifically, for a set of times $t_0 = 0$, t_1, t_2, ... where $t_{i+1} = t_i + \Delta t$, plot $|\Psi(x;t_i)|^2$ at each time step t_i. Preferably, do this with all three versions of the wave function – the two numerical approximations and the exact, analytical one – simultaneously as an animation.

   Chose a reasonably small Δt so that when you iterate over time as $t \to t + \Delta t$ and update your plot repeatedly, it renders a reasonably smooth animation.

b) Play around with the numerical parameter n. For numerical estimates, how large n do you need for your estimate to, more or less, coincide with the analytical exact solution? Which implementation seems to be the most precise one? Is the wave function in fact at its narrowest when $t = \tau$?

c) What happens to the wave function when they hit the boundary at $x = \pm L/2$?

Perhaps you found it somewhat odd to introduce the Crank-Nicolson propagater here at all. In fact, with a time-independent Hamiltonian, the exact time evolution is given by

$$\Psi(x;t) = \exp[-i\hat{H}\Delta t/\hbar]\Psi(x;t=0) \quad . \tag{1.13}$$

Albeit trivial in this case, this is an example of a so-called *Magnus propagator*.

1.6 Exercise: The Magnus propagator.

a) How does it make sense to exponentiate an operator or a matrix?

b) Prove that Eq. 1.13 actually *is* a solution of the (time-dependent) Schrödinger equation, Eq. 1.1.

c) Modify your implementation from Exercise 1.5 where you replace Eq. 1.10 with

$$\boldsymbol{\Psi}(t + \Delta t) = e^{-iH\Delta t/\hbar}\boldsymbol{\Psi}(t) \quad , \tag{1.14}$$

   Note that the approximation sign in Eq. 1.10 is replaced by equality. Note that you will find ready made implementations for matrix exponentials in Python[1]

[1] In the SciPy library.

and MATLAB.

We will not settle for improving our time discretization scheme. Although our improvement will not result in any exact solution this time, we can do better when it comes to the double spatial derivative.

There are, of course, several other methods to estimate differentiation of various orders numerically. A particularly convenient one is provided by the Fourier transform, which is defined as

$$\Phi(k) = \mathscr{F}\{\Psi(x)\}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} \Psi(x)\, \mathrm{d}x \quad . \tag{1.15}$$

This shifts our position-dependent wave function into another function which depends on the wave number k instead. We may transform this one back into the original x-dependent function again by the inverse Fourier transform, $\mathscr{F}^{-1}$:

$$\Psi(x) = \mathscr{F}^{-1}\{\Phi(k)\}(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{+ikx} \Phi(k)\, \mathrm{d}k \quad . \tag{1.16}$$

Within the "k-space", differentiations are trivial[2]:

$$\frac{\mathrm{d}^n}{\mathrm{d}x^n}\Psi(x) = \frac{\mathrm{d}^n}{\mathrm{d}x^n} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \Phi(k)\, dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\frac{\mathrm{d}^n}{\mathrm{d}x^n} e^{ikx} \right) \Phi(k)\, dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx}\, (ik)^n\, \Phi(k)\, dk = \mathscr{F}^{-1}\{(ik)^n \Phi(k)\}(x) \quad . \tag{1.17}$$

That means that differentiation may be performed by first Fourier-transforming Ψ into "k-space", multiply this transformed wave function by ik to the proper power and then transform it back into the x-representation. The action of the kinetic energy operator, for instance, may be calculated as

$$\hat{T}\Psi = -\frac{\hbar^2}{2m} \mathscr{F}^{-1}\left\{(ik)^2 \mathscr{F}\{\Psi\}\right\} = \frac{\hbar^2}{2m} \mathscr{F}^{-1}\left\{k^2 \mathscr{F}\{\Psi\}\right\} \quad . \tag{1.18}$$

In terms of numerical implementation, this is really good news because discrete numerical Fourier transforms may be done extremely quickly, and standard

[2]Actually, quantum physics may also be formulated in "k-space" or *momentum space* rather than position space. In this case, the $\hat{x}$ and $\hat{p}$ operators change roles, so to speak, and the momentum wave function, $\Phi(k)$, gives the momentum distribution in the same manner as $\Psi(x)$ gives the position distribution. The momentum variable p and the wave number k are related by $p = k\hbar$, which means that they are the same in our convenient units.

implementations for the *Fast Fourier Transform*, FFT, are easily found within all frameworks.

In discrete "k-space", the discrete x vector, $(x_0, x_1, ..., x_n)$ is replaced by a k vector. The maximum magnitude of k is inversely proportional to the numerical step size h; $k_{\max} = \pi/h$. The k-vector corresponding to the Fourier transformed wave function extends from $-k_{\max}$ to (almost) $k_{\max}$ in n steps of length $\Delta k = 2\pi/L$, where $L = b - a$ is the size of the domain. Note, however, that FFT implementations typically distort this k-vector in a somewhat non-intuitive manner; when n is even, it typically starts from zero and reaches $(n/2-1)\cdot\Delta k$ and then continues from $-n/2\cdot\Delta k$ to $-1\cdot\Delta k$. Check the documentation of your FFT implementation of choice in order to work this out.

1.7 Exercise: Gaussian wave – once again

Within the same implemntation as before, add to your finite difference approximation to the kinetic enery operator $\hat{T}$ with a FFT approximation. In doing so, the number of grid points should be of the form 2^k with k being an integer. In other words, you should have, say, 128, 512, 1024, ... grid points.

Remember that since we are dealing with linear matrix transformation, the matrix representation of $\exp(-iH\Delta t/\hbar)$ in Eq. 1.14 can be constructing from each of the columns of the identity matrix I.

With your new implementation, repeat Exercise 1.5 with all three numerical approximation and compare with the exact solution once more. What happens to the FFT approximation when it hits the wall at $b = L/2$?

Witht his framework in place, we are able to study various fundamental quantum phenomena. One such phenomena is that of *interference*.

1.8 Exercise: Interference

Construct an initial wave packet of the form

$$\Psi(x, t=0) = \frac{1}{\sqrt{2}}\left(\psi_1(x) + \psi_2(x)\right) \quad , \tag{1.19}$$

where each of the two functions ψ_1 and ψ_2 is of the form Eq. 1.11. The parameters should not be the same, make sure to choose values for the mean momentum and initial positions such that the two Gaussians travel towards each other. Also, make sure that the two initial Gaussians have negligible overlap initially. If so, the pre-factor $1/\sqrt{2}$ above ensures normalization.

Now, as in Exercise 1.5, simulate the evolution according to the Schrödinger equation for the system – still without any potential. In this case, just use the FFT-version. What happens?

Also plot the real and imaginary parts of the wave function separately in this case, not just the absolute value squared.

While interference phenomena are interesting enough, simulations such as these are rather boring since the moving wave function never actually hits anything ...

Chapter 2

Scattering

With our quantum particle behaving as a wave, as opposed to a massive *ball* or anything similar, it exhibits behaviour which we really woundt expect from matter. We will study a few of them by appying the framework we developed in Chapter 1.

Before we do that, we introduce a potential, V, in the Hamiltonian. For simplicity, we will let this potential be a rectangular one, centered at the middle of the grid:

$$V(x) = \begin{cases} V_0, & |x| \leq w/2 \\ 0, & |x| > w/2 \end{cases} \tag{2.1}$$

The value V_0 can be positive, in which case the potential is a barrier, or negative, in which case it may confine our quantum particle. For now we will address the former case.

Actually, for numerical simulations we will, instead of the purely rectangular potential above, use a smoother version:

$$V_s(x) = \frac{V_0}{e^{s(|x|-w/2)}+1} \quad . \tag{2.2}$$

This one is a bit more convenient to work with numerically. The parameter s fixes the smoothness; in the limit $s \to \infty$ we reproduce the sharp corners of the potential in Eq. 2.1. The potentials are plotted in Fig. 2.1.

In solving these exercises, use the FFT approximation to the kinetic energy operator consistently. As for time evolution, use the maxtrix exponential formulation, Eq. 1.13. Since this is exact, there is no need for doing any time-stepping; you can just jump straight to the final time T you may be interested in. However, it could also be interesting to see the evolution of the wave as it goes along ...

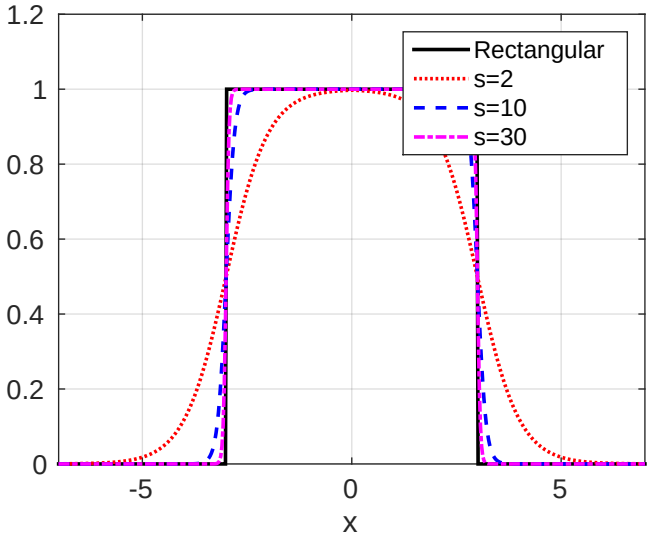

Figure 2.1: This figure shows the rectangular potential in Eq. 2.1 – along with the "smooth" version of Eq. 2.2 for three different values of s. Here $V_0 = 1$ and $w = 6$.

2.1 Exercise: Scattering on a barrier

In this exercise you do not get to choose the parameters yourself – at least not initially. In the implementation from Exercise 1.5, again with the initial state as in Eq. 1.12, you impose a potential of the above shape, Eq. 2.2. This is easy, you just augment your Hamiltonian with the potential V, which becomes a diagonal matrix in our representation:

$$\mathrm{diag}(V(x_0), V(x_1), V_(x_2), ...) = \begin{pmatrix} V(x_1) & 0 & 0 & \\ 0 & V(x_2) & 0 & \cdots \\ 0 & 0 & V(x_2) & \\ & \vdots & & \ddots \end{pmatrix} \quad , \qquad (2.3)$$

before you perform the exponentiation, Eq. 1.14. Again, we suggest you use the FFT representation of kinetic energy.

Use the following parameters:

L	n	σ_p	p_0	x_0	τ	V_0	w	s
200	512	0.2	1	-20	0	3	2	5

As in Exercise 1.5, make an animation/simulation where your wave packet hits the barrier. You may want to indicate the position of the barrier somehow in your simulation.

What happens?

After the wave packet has collided with the barrier, what is the final probability for the wave function to remain on the left side of the barrier ($x < 0$)? And what is the probability that it has passed into the right side of it ($x > 0$)? The former is called *reflection probability*, and the latter is called *transmission probability*.

Rerun the scattering process playing around with the parameters. How is reflection and transmission probabilities affected by the height and the width of the barrier?

Finally, replace the hight of the barrier V_0 with a negative one – so that the barrier becomes a pit instead. Will our quantum particle, with some probability, fall into the pit and get trapped? Do we still get reflection with a negative V_0 in the potential?

We suppose the answer to the last question is affirmative. Would a classical particle – a particle which follows Newton's laws – behave this way?

Actually, let's see (in case the answer is not obvious):

2.2 Exercise: The dynamics of a classical particle

It could be interesting to compare the wave function with the position that a classical particle would have. If we include this in the same simulation as in Exercise 2.1, this will serve to illustrate some of the profound differences between classical physics and quantum physics.

Simulate numerically the trajectory of a classical particle, $x(t)$, with the initial conditions given by the mean position and mean momentum of the initial Gaussian wave packet; set $x(t = 0) = x_0$ and let the initial velocity be $v(t = 0) = p_0/m$. The classical evolution is dictated by Newton's second law in one dimension:

$$mx''(t) = -V'(x) \quad . \tag{2.4}$$

It may be useful to formulate it as a first order ordinary differential equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} v \\ -V'(x)/m \end{pmatrix} \quad , \tag{2.5}$$

and solve it by some standard scheme for ordinary differential equation such as Runge Kutta. The differentiation of the potential could be done, for instance, by

the midpoint rule,

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + \mathcal{O}(h^3) \quad , \tag{2.6}$$

or it could be done using paper and pencil.

Once implemented, indicate the position of the classical particle along with the evolution of the quantum wave that you implemented in Exercise 2.1.

Now, suppose a ball is rolling uphill with an initial velocity of $v_0 = 4$ m/s. The top of the hill is $H = 1$ m above the ball's initial position. Why can we be absolutely certain that the ball will *not* make it to the other side of the hill?

-Because energy conservation prohibits it. It would take the ball with mass $m = 1$ kg an energy of $mgH \approx 10$ J to reach the top of the hill, while it only has $1/2mv_0^2 = 8$ J to spend. Thus, for sure, the classical ball will roll down again on the same side; there is absolutely no way we would retrieve the ball on the other side.

Let's have a look at the same process within the quantum world:

2.3 Exercise: Tunneling

We start out in the same scenario as in Exercise 2.1 with the same parameters – except for one thing: This time, let $V_0 = 1$.

Again: Run the simulation and see what happens. And, again, calculate the reflection probability and transmission probability. What is the probability for this quantum physical "ball" to make it to the other side of the hill?

Finally, rerun you collision between particle and barrier with various widths w and heights V_0. How does these quantities affect the propability of encountering the quantum particle on the other side of the barrier?

When running your simulations, feel free to include the corresponding classical simulation, the one from Exercise 2.2, as well.

So, despite the fact that our quantum ball has a mean energy of about $p_0^2/2m = 0.5$ in our units, it still has a significant probability to be found on the other side of a "hill" it would take an energy of $V_0 = 1$ units to climb. Isn't that rather odd?

Well, you could argue that 0.5 is only the *mean* energy of the particle – more or less. Since the wave that is a quantum particle typically has a *distribution* in momentum, rather than a specific one, it also has a distribution in energy. And this distribution may very well contain some higher energy components which

could make it over the barrier. If we think of the particle as a wave in water, parts of it could "splash" over, so to speak.

This is, indeed, a bona fide argument. However, in the case corresponding to the parameters above, the probability of measuring an energy beyond 1 is actually just 1.6%[1]. As seen in the exercise, the probability of turning up on the other side of the barrier is considerably higher than this. So, the oddity remains.

It does not get any less weired when we replace our barrier with a double barrier:

2.4 Exercise: Scattering on a double barrier

Now, we will replace the barrier with two narrow barriers, symmetrically placed on either side of $x = 0$. This can be achieved with this potential:

$$V(x) = V_s(x-d) + V_s(x+d) \quad , \tag{2.7}$$

where V_s refers Eq. 2.2. Here the separation d must be significantly larger than the width w of the barriers. You could choose the parameters $V_0 = 3$, $d = 1$ and $s = 5$ for the potential, Eqs. 2.7 and 2.2. As for the initial wave packet, you can set $\sigma_p = 0.1$ for all calculations.

Let your initial wave function be your initial Gaussian, and set x_0 so that virtually all of the wave is located to the left of double barrier initially.

Now, for several choices of the mean momentum p_0, solve the Schrödinger equation in order to determine the transmission and relfection probabilites. You don't need to simulate the wave packet on the fly; it is enough that you determine the wave packet at some final time T. This time should be long enough for the collision with the double well to be over and small enough to avoid collisions with the walls at $x = \pm L/2$. A reasonable choice could be to set T so that a classical particle with initial position x_0 and velocity p_0/m will have reached $x = L/4$ at $t = T$.

You can determine $\Psi(x,T)$ either by construcing the full exponential, Eq. 1.13, for each choice of p_0, or by repeated use of Eq. 1.14 for a reasonably small Δt. The former requires a full exponentiation for each choice of p_0, while the latter leads to several somewhat tedious matrix multiplications.

Make a plot of the relfection and/or transmission probabilities as functions of p_0, $R(p_0)$ and $T(p_0)$. It's not very monotonic, is it?

Suppose that you remove the rightmost barrier in the above exercise and redo it. The resulting transmission probability changes quite a bit, doesn't it? Isn't

[1] We will get back to how to determine such probabilities.

that rather odd? Remeber that the quantum particle is entirely located to the left initially. And almost nothing penetrates the first barrier at low energies. Yet, it makes all the difference in the world that there is another barrier behind the first one – despite the fact that our quantum particle hardly sees it?

Chapter 3

Dynamics

As we have seen, resolving the time-evolution numerically does not induce any error in the case of a time-independent Hamiltonian – since we can determine it exactly by matrix exponentiation. Still, Eq. 1.14 may provide a decent approximation to the dynamics – at least with a small adjustment.

The evolution of the wave functon from a time t to a later time $t+\Delta t$ may be written as the action of an operator:

$$\Psi(t+\Delta t) = \hat{U}(t, t+\Delta t)\Psi(t) \quad . \tag{3.1}$$

This operator, $\hat{U}$, is referred to as a *propagator*[1].

3.1 Exercise: Magnus propagators of 1st and 2nd order

a) Show that the error in using Eq. 1.14 for the time evolution is proportional to Δt^2 at each time step. To this end, differentiate the Schrödinger equation, Eq. 1.1, in order to express the first three terms in a Tayor expansion of $\Psi(t+\Delta t)$ and compare it to the three first terms in an expansion of Eq. 1.14.

b) Show that if you replace $\hat{H}(t)\,\Delta t$ in Eq 1.14 by $\int_t^{t+\Delta t} \hat{H}(t')\,dt'$, the error is proportional to Δt^3.
Hint: Use Taylor expansion to approximate the integral as well – or the trapezoidal rule.

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[1] Unless you are doing quantum computing, in which case it is called a *gate*.

Let's summarize:

$$\Psi(t+\Delta t) = e^{-i/\hbar H(t)\Delta t}\Psi(t) + \mathscr{O}(\Delta t^2) \quad \text{and} \tag{3.2a}$$

$$\Psi(t+\Delta t) = e^{-i/\hbar \overline{H}(t)\Delta t}\Psi(t) + \mathscr{O}(\Delta t^3) \quad \text{where} \tag{3.2b}$$

$$\overline{H} \equiv \frac{1}{\Delta t}\int_t^{t+\Delta t} \hat{H}(t')\,\mathrm{d}t' \quad .$$

So we get a significant improvement in accuracy if we replace the Hamiltonian with its time-average over the interval in question. Since the (local) error is of third order, the time averaged Hamiltonian $\overline{H}$ may safely be approximated by the trapezoidal or midpoint rule,

$$\overline{H} \approx \frac{\hat{H}(t)+\hat{H}(t+\Delta t)}{2} \approx \hat{H}(t+\Delta t/2) \quad . \tag{3.3}$$

Propagators which are written as the exponential of some time-averaged Hamtilonian are called *Magnus propagators*. They are convenient in several respects. One advantage is that they are *explicit* – as opposed to implicit schemes in which you have to solve an equation in order to get to get from one time to the next. They are also convenient due to their norm-conserving property; although we introduce errors when using Eqs. 3.2 with finite Δt, the *norm* of the wave function is always perserved to machine accuracy.

There is a drawback with propagators of the form 3.2, however: Since the Hamiltonian now changes in time, we cannot exponentiate it once and then use it repeatedly as we did in Chapter 1. We must perform a full exponentiation at each time step. This is quite costly, we really don't want to do that. Luckily, there are ways arount it.

3.2 Exercise: Split-operators

a) While the relation $e^{a+b} = e^a e^b$ holds for any numbers a and b, why is this generally not the case with operators; $e^{\hat{A}+\hat{B}} \neq e^{\hat{A}}e^{\hat{B}}$?

b) Use Taylor expansion to prove that

$$e^{(\hat{A}+\hat{B})\Delta t} = e^{\hat{A}\Delta t/2}e^{\hat{B}\Delta t}e^{\hat{A}\Delta t/2} + \mathscr{O}(\Delta t^3) \quad . \tag{3.4}$$

When we want to implement a Magnus propagator, Eq. 3.4 may be very useful indeed as it allows us to treat the various parts of the exponentiation of the Hamiltonian independently – and yet maintain a reasonable degree of precision.

In many cases, the Hamiltonian may be split in a time-dependent and a time-independent part:

$$\hat{H} = \hat{H}_0 + \hat{H}'(t) \quad . \tag{3.5}$$

This is for instance the situation for a quantum particle exposed to a strong laser field: The time-independent part, $\hat{H}_0$, is just $\hat{T} + V$ as before while the laser interaction, in one dimension, may be written

$$\hat{H}'(t) = -qE(t)x \quad . \tag{3.6}$$

Here, q is the charge of the particle and $E(t)$ is the time-dependent strength of the electric field of the laser[2].

For instance, with the Hamiltonian in Eq. 3.5 (with $\hat{H}'$ time averaged) and $\hat{A} = -i/\hbar \hat{H}_0$ and $\hat{B} = -i/\hbar \overline{H'}$, we may estimate the wave function at next time as

$$\Psi(t+\Delta t) = e^{-i/\hbar \hat{H}_0 \Delta t/2} e^{-i/\hbar \overline{H'} \Delta t} e^{-i/\hbar \hat{H}_0 \Delta t/2} \Psi(t) + \mathcal{O}(\Delta t^3) \quad . \tag{3.7}$$

This means that the time-independent $\hat{H}_0$-part may be exponentiated initially – once and for all, while only the time dependent part, $\overline{H'}$, must be exponentiated on the fly. This is good news since the latter is often quite easily implemented. For instance, the interaction in Eq. 3.6 is diagonal in a position representation. Thus, exponentiating it is trivial – you just exponentiate the diagonal elements directly.

It should be mentioned that both Magnus propagators and split operator techniques of higher order than three in (local) error are well established. Third order will do for our purposes, however.

3.3 Exercise: Some real dynamics

The time is ripe to actually solve the time-dependent Schrödinger equation for a wave function with space dependence again. We will do so for a one-dimensional model for an atom exposed to a short, intense laser pulse:

$$E(t) = \begin{cases} E_0 \sin^2\left(\frac{\pi}{T} t\right) \sin(\omega t), & 0 \le t \le T \\ 0, & \text{otherwise} \end{cases} \quad . \tag{3.8}$$

We set the charge q in Eq. 3.6 to -1 in our own convenient units. Here E_0 is the maximum field strength, T is the duration of the pulse and ω is the central

[2]Here we have neglected the fact that the field **E** would also be space-dependent, not just time-dependent. Often this is admissible since the extension of the system in question, such as an atom or a molecule, is much smaller than the wavelength of the elecric field.

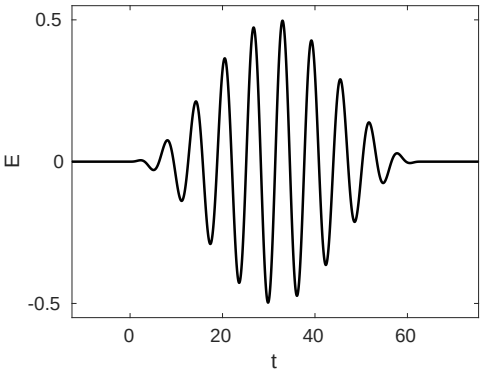

Figure 3.1: In Exercise 3.3 we expose our model atom to a time-dependent electric field with this shape. The amplitude E_0 is 0.5 and the angular frequency ω is 1 in our units. The pulse duration T corresponds to 10 so-called optical cycles, $T = 10 \cdot 2\pi/\omega$.

angular frequency of the laser[3] You can choose the field parameters $\omega = 1$, $E_0 = 0.5$ and $T = 10t_{\text{cycl}}$, where $t_{\text{cycl}} = 2\pi/\omega$ is a so-called *optical cycle*. See Figure 3.1 We also apply a static potential of form Eq. 2.2 with $V_0 = -1$, $s = 5$ and $w = 5$.

a) First of all, we need our initial condition – the state we start out in. We will take this to be the ground state of the system – the state with the lowest energy when the field is off, $E(t) = 0$. To make a long story short, you can find this by numerically determining the eigen values and eigen vectors of your numerical Hamiltonian approximation. Choose the eigen vector which corresponds to the lowest eingen value, and make sure that it is properly normalized. This would, in practice, mean multiplying it with $\sqrt{h}$, where h is the distance bewtween neighbouring points on your numerical spatial grid.

b) Implement the propagator in Eq. 3.7 and propagate your system for the entire duration of the laser pulse – and a bit beyond. With a grid extending from $-L/2$ to $L/2$, make sure to use an L large enough to contain the wave packet at all times and, as always, a number of grid points n which is high enough to ensure converged results.

   In the same spirit, redo your calculation with a smaller Δt to check that you have set it small enough.

   Why was this not crucial in the exercises we did in Chapter 1?

c) How much of your wave packet has actually left the region of the confining potential? Or in other words: What is the propabaility for our model atom to be *ionized* by the laser pulse?

[3] In addition to neglecting the spatial dependence of **E** we actually make one more simplificaton: We do not treat the field as a set of photons. This is admissible for strong fields.

What we just did is a rather direct approach to determining the ionization probability. It may seem inconvenient that we need to use a numerical domain of rather large extension L to include the full wave function, when all the action takes place in the vicinity of the confining potential ...