PY 421/621 - Advanced Computing in Physics

Lecture notes.

Numerical experiments with the time dependent Schrödinger wave function.

These pages are a short guide to the numerical experiments you can perform with the program **wf** which calculates the solution to the time dependent Schrödinger equation in one dimension.

You start execution of the program by typing **wf** followed by the **Enter** key. You will be prompted to enter various parameters. You can enter the values you choose or simply press the enter key to accept the default values indicated within square brackets. After the last parameter a window will open that looks as the figure below.

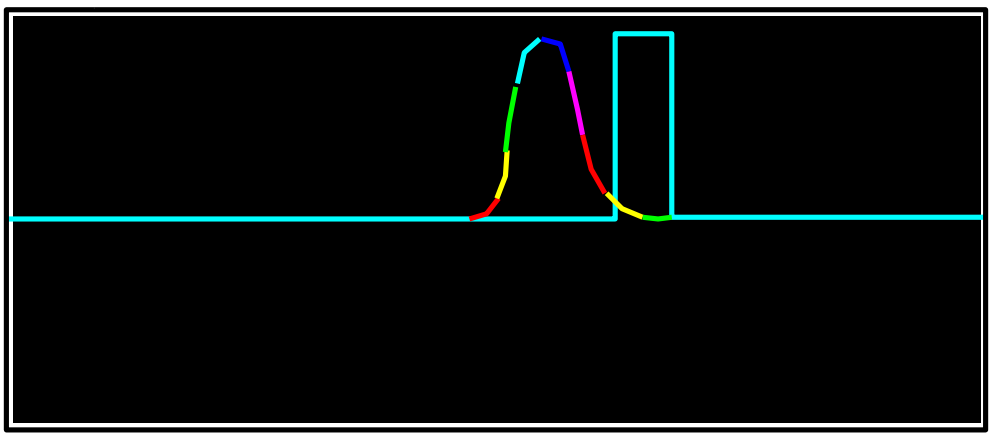

Figure 1: Wave function window.

At this point you should use the mouse to move the cursor over the window and click the left mouse button, keeping it pressed. This will cause the appearance of a pop up menu. While keeping the left mouse button still pressed, move it to a selection (that will be highlighted white). Move it to **start** to begin the animation, to **stop** to temporarily stop it (go again to **start** to resume), to **setup** to restart the animation with a new set of parameters (you will have to reenter the parameters or accept the default values again in the main window), or to **exit** to quit.

In the wave function window, the line with light blue color represents the profile of the potential energy $V(x)$, whereas the multicolored line represents the wave function $\psi(x)$. The height of this line is proportional to $|\psi(x)|^2$, that is to the probability density for finding the particle at x. The color of the line represents the complex phase $\varphi(x)$ of the wave function

$$\psi(x) = |\psi(x)|\, e^{\imath\varphi(x)}$$

As φ varies from 0 to 2π the color changes taking the colors of the rainbow, from red ($\varphi = 0$) to yellow ($\varphi = \pi/3$), green ($\varphi = 2\pi/3$), cyan ($\varphi = \pi$), blue ($\varphi = 4\pi/3$), purple ($\varphi = 5\pi/3$), and finally back to red for $\varphi = 2\pi$

1.) Free propagation of a Gaussian wave packet.

Enter the following parameters. **(Note that some differ from the default values.)**

Reduced Planck's constant	1.0000
Time step	0.0100
Imaginary component of the time step	0.0000
Name of the file with the potential	v.wall
Potential's height	0.0000
Initial position of the wave packet	-15.0000
Width	2.0000
Wavepacket's momentum	3.0000

Table 1: Parameters for numerical experiment 1.

Notice how the wave packet spreads out (dispersion).

Notice also that the phase velocity is smaller than the group velocity: the wave of colors also propagates forward, but with a velocity that is about one half the velocity of the whole wave packet. (Repeat the experiment if you missed this difference this the first time).

2.) and 3.) Dependence of rate of dispersion on the width.

Run the experiment with the following two sets of parameters. (You do not need to exit from the program and start it again. Just left click on the window and select **setup**.)

Only the initial width parameter is changed from the previous experiment.

Reduced Planck's constant	1.0000
Time step	0.0100
Imaginary component of the time step	0.0000
Name of the file with the potential	v.wall
Potential's height	0.0000
Initial position of the wave packet	-15.0000
Width	1.0000
Wavepacket's momentum	3.0000

Table 2: Parameters for numerical experiment 2.

Reduced Planck's constant	1.0000
Time step	0.0100
Imaginary component of the time step	0.0000
Name of the file with the potential	v.wall
Potential's height	0.0000
Initial position of the wave packet	-15.0000
Width	4.0000
Wavepacket's momentum	3.0000

Table 3: Parameters for numerical experiment 3.

Observe how a narrower wave packet spreads out faster, while a broader wave packet disperses more slowly.

4.) Going classical.

Let us change the value of $\hbar$. (Ask any experimental physicist if she/he can do this!!)

Enter 0.25 for $\hbar$ and set the initial width back to 2.

Reduced Planck's constant	0.2500
Time step	0.0100
Imaginary component of the time step	0.0000
Name of the file with the potential	v.wall
Potential's height	0.0000
Initial position of the wave packet	-15.0000
Width	2.0000
Wavepacket's momentum	3.0000

Table 4: Parameters for numerical experiment 4.

Notice that the dispersion is almost absent. (There is still a tiny amount of dispersion, because we have reduced $\hbar$ only by a factor of 4. On the other hand we cannot make $\hbar$ much smaller without introducing an appreciable discretization error, because if we reduce $\hbar$ further the de Broglie wave length becomes comparable to the lattice spacing used for the numerical solution of the equation. See also the following observation.)

Notice how the wave length decreases when $\hbar$ is reduced. Remember that the classical limit is the one where the wave length goes to zero. Notice also that the phase velocity is still one half of the group velocity.

5.) Tunneling.

We reset $\hbar = 1$ and enter 4 for the height of the square potential wall. Enter -5 for the initial position of the wave packet. The particle has mass 1. Let us give it momentum 2.7, which would correspond to a kinetic energy of approximately 3.6 (exercise: calculate the actual quantum mechanical expectation vale of the kinetic energy for our Gaussian wave packet). The particle thus does not have sufficient energy to overcome the barrier ...

Reduced Planck's constant	1.0000
Time step	0.0100
Imaginary component of the time step	0.0000
Name of the file with the potential	v.wall
Potential's height	4.0000
Initial position of the wave packet	-5.0000
Width	2.0000
Wavepacket's momentum	2.7000

Table 5: Parameters for numerical experiment 5.

... but, as you can see from the experiment, part of the wave function actually makes it through the barrier.

If you let the evolution continue long enough, the transmitted and reflected packets meet each other (because the system is defined with periodic boundary conditions, i.e. the x-axis wraps around) and you can observe the phenomenon of quantum interference.

6.) No classical tunneling.

Run the same experiment as before, but with $\hbar = 0.25$.

Reduced Planck's constant	0.2500
Time step	0.0100
Imaginary component of the time step	0.0000
Name of the file with the potential	v.wall
Potential's height	4.0000
Initial position of the wave packet	-5.0000
Width	2.0000
Wavepacket's momentum	2.7000

Table 6: Parameters for numerical experiment 6.

The behavior becomes more classical and there no longer is any appreciable tunneling.

7.) and 8.) A smoother potential.

The ripples you observed when the particle hits the barrier in experiments 5. and 6. are due to the sharp edge in the potential, which temporarily excites high Fourier components (components with large momentum) in the wave function. They go away when the particle leaves the wall. With the smoother potential defined in the file "v.hill" there are no more ripples in the wave function when it hits the barrier.

Redo the tunneling experiments with $\hbar = 1$ and 0.25. Enter **v.hill** when prompted for the name of the file with the potential.

Reduced Planck's constant	1.0000
Time step	0.0100
Imaginary component of the time step	0.0000
Name of the file with the potential	v.hill
Potential's height	4.0000
Initial position of the wave packet	-5.0000
Width	2.0000
Wavepacket's momentum	2.7000

Table 7: Parameters for numerical experiment 7.

Reduced Planck's constant	0.2500
Time step	0.0100
Imaginary component of the time step	0.0000
Name of the file with the potential	v.hill
Potential's height	4.0000
Initial position of the wave packet	-5.0000
Width	2.0000
Wavepacket's momentum	2.7000

Table 8: Parameters for numerical experiment 8.

In the classical case try also with an initial momentum of 3.3, which sufficiently large to make the initial kinetic energy larger than the barrier height, but not by much. Notice how the packet slows down as it climbs up the hill.

9.) and 10.) The double wall.

Redo the tunneling experiments with the double wall potential defined in the file "v.doublew"

Enter **v.doublew** when prompted for the name of the file with the potential. Also, set the initial position of the particle at 0, in the middle between the two walls.

Remember to reset the initial momentum to 2.7, in case you experimented with a larger momentum.

Reduced Planck's constant	1.0000
Time step	0.0100
Imaginary component of the time step	0.0000
Name of the file with the potential	v.doublew
Potential's height	4.0000
Initial position of the wave packet	0.0000
Width	2.0000
Wavepacket's momentum	2.7000

Table 9: Parameters for numerical experiment 9.

Reduced Planck's constant	0.2500
Time step	0.0100
Imaginary component of the time step	0.0000
Name of the file with the potential	v.doublew
Potential's height	4.0000
Initial position of the wave packet	0.0000
Width	2.0000
Wavepacket's momentum	2.7000

Table 10: Parameters for numerical experiment 10.

11.) The harmonic oscillator.

The harmonic oscillator potential is very special. The motion of the packet is in some sense classical for all values of $\hbar$.

Enter **v.hosc** when prompted for the name of the file with the potential. Set the potential height to 25 (otherwise the particle falls out at the end of the axis.)

Reduced Planck's constant	1.0000
Time step	0.0100
Imaginary component of the time step	0.0000
Name of the file with the potential	v.hosc
Potential's height	25.0000
Initial position of the wave packet	0.0000
Width	2.0000
Wavepacket's momentum	3.0000

Table 11: Parameters for numerical experiment 11.

Experiment for a few different values of the initial momentum and of $\hbar$. Let the motion continue for some amount of time. Notice how the oscillations seem to go on forever unchanged.

Can you find the ground state wave function? You know that it is a Gaussian, that it is centered at 0 and that it must have 0 momentum. So the only parameter is the width. Experiment with various widths until you find a wave function whose profile does not change. The color will be uniform, but it will change with time, going gradually through the colors of the rainbow. Can you explain why? (Remember the time dependence $\exp(-\imath Et/\hbar)$ of the eigenstates of energy.)

12.) Decay to the ground state.

It is possible to make the wave function evolve towards the ground state by giving a small, negative imaginary component to the time step. We recall that the energy eigenfunctions $\psi_n(x,t)$ evolve according to

$$\psi_n(x,t) = e^{-\frac{\imath E_n t}{\hbar}} \psi_n(x,0)$$

Adding a small (negative) imaginary component to the time step, $dt \to dt - \imath\epsilon\, dt = (1 - \imath\epsilon)\, dt$ the above equation becomes

$$\psi_n(x,t) = e^{-\frac{\imath E_n (1-\imath\epsilon) t}{\hbar}} \psi_n(x,0) = e^{-\frac{\imath E_n t}{\hbar}} \psi_n(x,0) e^{-\frac{E_n \epsilon t}{\hbar}}$$

We see that all energy components of the wave function decay to 0, with a rate proportional to the energy eigenvalues. For large t the component with lowest energy will dominate over all other components. If we constantly renormalize the wave function to its original norm, the evolution will approach the ground state wave function.

Experiment with the harmonic oscillator and an imaginary component of the time step equal to 0.01. Notice that we can start with a wave packet with momentum different from 0 and the evolution will still converge to the ground state.

Reduced Planck's constant	1.0000
Time step	0.0100
Imaginary component of the time step	0.0100
Name of the file with the potential	v.hosc
Potential's height	25.0000
Initial position of the wave packet	0.0000
Width	2.0000
Wavepacket's momentum	3.0000

Table 12: Parameters for numerical experiment 12.

Notice again the fact that the ground state wave function has uniform color (see the comment at the end of the previous experiment).

13.) Ground state in the square well.

Find the ground state wave function with a square well potential. Enter **v.well** as name of the file with the potential and use a height equal to 4.

Reduced Planck's constant	1.0000
Time step	0.0100
Imaginary component of the time step	0.0100
Name of the file with the potential	v.well
Potential's height	4.0000
Initial position of the wave packet	0.0000
Width	2.0000
Wavepacket's momentum	3.0000

Table 13: Parameters for numerical experiment 13.