

Physics 750: Exercise 13

Tuesday, October 31, 2017

A quantum particle moving freely in space is described by a wavefunction $\psi(x, t)$ that satisfies the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}.$$

Here, there is no external potential, and the Hamiltonian $\hat{H} = \hat{p}^2/2m$ consists of a kinetic term only. A complete set of solutions is provided by plane waves of the form $e^{i(kx - E_k t/\hbar)}$. The energy in each mode, $E_k = \hbar^2 k^2/2m$, is a quadratic function of the wavevector k .

An arbitrary wavefunction can be constructed from linear superpositions of such states,

$$\psi(x, t) = \int_{-\infty}^{\infty} dk w_k e^{i(kx - E_k t/\hbar)}.$$

At time $t = 0$, the equation above is just a Fourier transform. Hence, a weight $w_k \sim e^{-\sigma_0^2(k-k_0)^2 - ikx_0}$ leads to an initial Gaussian wave packet centred on x_0 :

$$\psi(x, 0) = \frac{1}{(\sqrt{2\pi}\sigma_0)^{1/2}} \exp\left(-\frac{(x-x_0)^2}{4\sigma_0^2} + ik_0 x\right).$$

At all subsequent times, the probability density has the form

$$|\psi(x, t)|^2 = \frac{1}{\sqrt{2\pi}\sigma(t)} \exp\left(-\frac{(x-x_0 - \hbar k_0 t)^2}{2\sigma(t)^2}\right),$$

where $\sigma(t)^2 = \sigma_0^2 + t^2/4\sigma_0^2$. In other words, the packet centre moves uniformly with group velocity $v_0 = (1/\hbar)\partial E_k/\partial k|_{k_0} = \hbar k_0/m$ while the packet of width $\sigma(t)$ spreads.

In this special Gaussian case, the solution can be derived analytically. Let's also solve it numerically by computing the eigenvalue problem $E\psi = \hat{H}\psi$. We proceed by discretizing the spatial derivative:

$$E\psi(x) = \hat{H}\psi(x) = \frac{\hbar^2}{2m} \frac{\psi(x + \Delta x) + \psi(x - \Delta x) - 2\psi(x)}{(\Delta x)^2}.$$

Then the matrix formulation of the problem on some finite line segment is

$$\frac{\hbar^2}{2m(\Delta x)^2} \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & \ddots & \ddots & \ddots \\ & & & 1 & -2 & 1 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{pmatrix}.$$

Numerical libraries will give us the eigenvectors $\{\phi_i^{(\alpha)}\}$ and their corresponding energies $\{E^{(\alpha)}\}$. The complete packet evolution is given by

$$\psi(\Delta x \cdot i, t) = \psi_i(t) = \sum_{\alpha=1}^N c^{(\alpha)} \phi_i^{(\alpha)} e^{-iE^{(\alpha)} t},$$

where

$$c^{(\alpha)} = \sum_i \phi_i^{(\alpha)*} \psi(x, 0)$$

For convenience, we'll work in simplified units where $\hbar = m = \Delta x = 1$.

1. Use the curl command to download from the class website everything you'll need for this exercise.

```
$ WEBPATH=http://www.phy.olemiss.edu/~kbeach/  
$ curl $WEBPATH/courses/fall2017/phys750/src/exercise13.tgz -O  
$ tar xzf exercise13.tgz  
$ cd exercise13
```

The make command will generate an executable packet that simulates a Gaussian wave packet in one and two spatial dimensions. The geometry is controlled by the variables Lx and Ly, which are set by the user through a command-line flag. The program can be run in one of three modes:

```
./packet  
Usage:  
packet -L=#,# dos  
packet -L=#,# evolution -k=#,# -w=#  
packet -L=#,# trajectory -w=#
```

2. Run the program with the evolution command line argument, and view the resulting time evolution with the provided gnuplot script.

```
$ ./packet -L=400 evolution -k=0.1,0 -w=15  
A linear mesh of 400 points  
Initial wavepacket has wavevector k=(0.1,0) and (half-max) width 15  
Diagonalizing the Hamiltonian ...  
t=0: 1  
t=24: 1  
t=48: 1  
.  
.  
t=11952: 1  
t=11976: 1  
$ gnuplot movie.gp  
Press return to start
```

The gnuplot animation shows the packet's motion alongside the exact analytical result. Try running the program with different values of the width. What happens when σ_0 is comparable to or smaller than the discretization length $\Delta x = 1$? Try various values of the wavevector and in particular $-k=1.57$ and $-k=3.14$. What happens to the group velocity? How does the motion differ from that of the continuum packet?

3. Take a look at the code listing for packet.cpp. Read through the subroutines build_Hamiltonian and eigensolve, both of which are called in the first few lines of main. Be sure you understand how the Hamiltonian matrix is organized in "packed" storage format and sent to LAPACK's DSEPV routine for diagonalization. (Notice that we have left all the elements on the main diagonal empty. This just amounts to an energy shift of 1 in the one-dimensional case and 2 in the two-dimensional case.) Write additional code in eigensolve to verify that the resulting eigenvectors obey the orthonormality conditions

$$\sum_{\alpha=1}^N \phi_i^{(\alpha)} \phi_j^{(\alpha)} = \delta_{i,j} \quad \text{and} \quad \sum_{i=1}^N \phi_i^{(\alpha)} \phi_i^{(\beta)} = \delta^{\alpha,\beta}.$$

4. Observe the two-dimensional problem.

```

./packet -L=40,40 evolution -k=1.57,1.57 -w=3
A rectangular 40x40 mesh of 1600 points
Initial wavepacket has wavevector k=1.57 and (half-max) width 3
Diagonalizing the Hamiltonian ...
t=0: 1
t=0.152866: 1
.
.
t=76.2803: 1
t=76.4331: 1
$ gnuplot movie.gp

```

What difference do you notice when you run it again with $k=1.57, 0$?

5. Run the program with the `dos` command line argument. This will cause the program to dump a histogram of the density of states

$$g(E) = \sum_{\alpha} \delta(E - E^{(\alpha)})$$

to a file named `dos.dat`. In one dimension, the exact result is

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} \delta(E - E_k) = \int_0^{\infty} \frac{dk}{\pi} \delta(E + 1 - k^2/2) = \frac{1}{\pi\sqrt{2(1+E)}}.$$

Try making the comparison in `gnuplot`.

```

$ ./packet -L=400 dos
$ gnuplot
> plot "dos.dat" with lines, 1/sqrt(2*(1+x))/pi

```

Increase the mesh size up from 400 until the plot looks smooth. Use `gnuplot` to convince yourself that what you're actually generating is

$$\frac{1}{\pi\sqrt{(1+E)(1-E)}},$$

which is symmetric about $E = 0$. What's going on here?

6. The exact density of states in two dimensions is a constant, independent of E . Try systematically changing the aspect ratio from $L_x = 400, L_y = 1$ to $L_x = 20, L_y = 20$ (or larger).

```

$ ./packet -L=400,1 dos
$ ./packet -L=200,2 dos
$ ./packet -L=100,4 dos
$ ./packet -L=80,5 dos
.
.
$ ./packet -L=20,20 dos

```

Does the density of states flatten out?

7. Complete the body of the function `ave_position` so that its last two arguments are assigned the position expectation values

$$\langle x(t) \rangle = \int dx dy |\psi(x, y, t)|^2 x,$$

$$\langle y(t) \rangle = \int dx dy |\psi(x, y, t)|^2 y.$$

The trajectory mode shows how the semi-classical trajectory ($\langle x(t) \rangle - x_0, \langle y(t) \rangle - y_0$) changes with the choice of initial wavevectors.

```

./packet -L=400 trajectory -w=5
A linear mesh of 400 points
Diagonalizing the Hamiltonian ...
Computing k=0
Computing k=0.261799
Computing k=0.523599
Computing k=0.785398
Computing k=1.0472
Computing k=1.309
Computing k=1.5708
Computing k=1.8326
Computing k=2.0944
Computing k=2.35619
Computing k=2.61799
Computing k=2.87979
Computing k=3.14159
$ gnuplot
> plot "traj.dat" u 2:3 w l
> plot "traj.dat" i 1 u 2:3, 0.261799*x
> plot "traj.dat" i 2 u 2:3, 0.523599*x
> f(x) = a*x
> fit f(x) "traj.dat" i 1 u 2:3 via a
> print a
0.257528127931512
> fit f(x) "traj.dat" i 2 u 2:3 via a
> print a
0.497505902926639

```

Extract the slopes of these curves and plot them versus their wavevector. The continuum result is $\partial E_k / \partial k = k$. Convince yourself that the numerical result is actually $\partial E_k / \partial k = \sin k$ (and with the units, $\partial E_k / \partial k = \sin(k\Delta x) / \Delta x$).