Problem set 4: Testing the postulates of quantum mechanics using Mathcad.

In this problem set you should make extensive use of Mathcad, as the mathematical manipulations would be lengthy otherwise. The purpose of the problem set is to give you insight in the nature of the postulates of quantum mechanics. In addition you will become more proficient in the use of Mathcad. It is often a little frustrating to get things to work, as computers are so picky. Be patient. We will go through things in the tutorial also.

In the problems below we will consistently use a box of size $L=2$, but formulate everything in terms of a variable $L$. I will not be concerned about units in this problem set. The normalized eigenfunctions of the Hamiltonian and the corresponding eigenvalues for the particle in the box are

$$
\phi_n(x) = \sqrt{\frac{2}{L}} \sin \left( \frac{n \pi x}{L} \right), \quad E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}.
$$

The problem sets can be treated independently, but you can also recycle a fair amount of things between problems. I think this may be a bit of a challenging problem set, as you need to get acquainted with Mathcad. You can work through the Metiu problem sets on the CD accompanying the book, as a good “warm up”.

1. Expectation values when measuring the energy on an arbitrary wave function.

Consider the unnormalized wave function $\Psi(x) = N x^2 (L-x)$, for $L=2$, and answer the following:

a) Normalize the function $\Psi(x)$, taking the integration interval $[0..L]$, i.e. determine the normalization constant $N$. Verify that the integral $\int_0^L \Psi(x) \Psi(x) dx = 1$. Here I used that $\Psi(x)$ is a real function.

b) Plot the normalized wave function $\Psi(x)$, on the integration interval $[0..L]$.
c) Calculate the expectation value of the kinetic energy in units of \( \frac{\hbar^2}{2m} \), i.e. evaluate \( \int_0^L \Psi(x)\left(-\frac{d^2\Psi}{dx^2}\right)dx \).

d) The wave function can be alternatively written as a linear combination of the eigenstates of the kinetic energy operator: \( \Psi(x) \approx \Phi(x) = \sum_{n=1}^{M} c_n \phi_n(x) \), where

\[
c_n = \int_0^L \phi_n(x)\Psi(x)dx .
\]

Evaluate the coefficients for \( n = 1..M \), where \( M = 50 \), say. What are the probabilities to measure \( E_n \) given an ensemble described by the function \( \Psi(x) \)? Clearly explain what you would expect to see in a hypothetical experiment where you would measure the energy.

e) Plot the original wave function \( \Psi(x) \) and the approximation \( \Phi(x) \) in a single plot (use the SUM feature in Mathcad). Also, plot the difference \( \Phi(x) - \Psi(x) \). Just for fun, you might plot the functions outside the region of interest ([0..L]). You will see agreement is only good inside the box!

f) The probabilities to find the kinetic energy \( E_n \) are given by \( P_n = c_n^2 \) (as the \( c_n \) are real). Hence the average value of the kinetic energy is given by \( \bar{E} = \sum_{n=1}^{M} P_n E_n \).

Evaluate the energy in units of \( \frac{\hbar^2}{2m} \). You should find that this way of calculating the average kinetic energy agrees with part c). You can easily play around with the above, and repeat questions d..f using a different value of \( M \), e.g. use \( M = 10, 20, 30, 40, 50 \). You should see that you get progressively better agreement with the exact result as you include more terms in the sum.
2. Verifying the Heisenberg uncertainty relation for a particle in the box.

Consider once again the eigenfunctions $\phi_n(x) = \sqrt{\frac{2}{L}} \sin \left( \frac{n\pi x}{L} \right)$ of the kinetic energy operator for a particle confined to the interval $[0..L]$, taking $L=1$ this time. Questions.

a) Calculate the expectation values $\langle \hat{X} \rangle, \langle \hat{X}^2 \rangle, \langle \hat{P_x} \rangle, \langle \hat{P^2}_x \rangle$, for the functions $\phi_n(x)$, expressed as a function of $n$. Simplify the Mathcad formulas, using that $n$ is an integer.

b) Tabulate the values of $\Delta(\hat{X}), \Delta(\hat{P}_x), \Delta(\hat{X}) \Delta(\hat{P}_x)$ as a function on $n$, for $n = 1..10$, and verify that the Heisenberg uncertainty relation, $\Delta(\hat{X}) \Delta(\hat{P}_x) \geq \hbar^2 / 4$ is satisfied for every state. For what state is the product of the variances the lowest?

c) Consider the state $\Psi(x) = N x^5 (L - x)$. Normalize the function and plot the normalized function over the interval $[0..L]$. You can expect the spread in the value for $x$ to be small. Conversely this must mean that the spread in the momentum must be large. Let us check. Calculate $\langle \hat{X} \rangle, \langle \hat{X}^2 \rangle, \langle \hat{P}_x \rangle, \langle \hat{P^2}_x \rangle$ for this function, and then $\Delta(\hat{X}), \Delta(\hat{P}_x), \Delta(\hat{X}) \Delta(\hat{P}_x)$. Comment on your findings. You can make the power in the function $\Psi_n(x) = N x^n (L - x)$ even higher, to make the distribution more peaked. It is all easy to do in Mathcad!
3. Analysing the time-dependent Schrödinger equation for the perpetual particle in the box. Animations in Mathcad.

As before, consider a box of length L (L = 2), and the normalized eigenfunctions of the Hamiltonian \( \phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \). We are interested in the time dependence of the general function, which at time \( t = 0 \) is given by \( \Psi(x, 0) = \sum_{n=1}^{M} c_n \phi_n(x) \). The coefficients \( c_n \) will be determined shortly. Given the coefficients, the wave function at time \( t \) is given by

\[
\Psi(x, t) = \sum_{n=1}^{M} c_n \phi_n(x) e^{-iE_n t / \hbar} = \sum_{n=1}^{M} c_n \phi_n(x) e^{-\frac{n^2 \pi^2 \hbar^2}{2mL^2} t / \hbar}
\]

Let us make our life a little easier and define \( \frac{\pi^2 \hbar^2}{2mL^2} t / \hbar = 2\pi \tau \rightarrow \tau = \frac{2mL^2}{\pi^2 \hbar (2\pi)} t \) and evaluate

\[
\Psi(x, \tau) = \sum_{n=1}^{M} c_n \phi_n(x) e^{-i2\pi n^2 \tau} = \sum_{n=1}^{M} c_n \phi_n(x) \cos(2\pi n^2 \tau) - i \sum_{n=1}^{M} c_n \phi_n(x) \sin(2\pi n^2 \tau)
\]

where I have explicitly indicated the real and imaginary parts of \( \Psi(x, t) \):

\[
\Psi^R(x, \tau) = \sum_{n=1}^{M} c_n \phi_n(x) \cos(2\pi n^2 \tau)
\]

\[
\Psi^I(x, \tau) = -i \sum_{n=1}^{M} c_n \phi_n(x) \sin(2\pi n^2 \tau)
\]

The probability density as a function of the “time” variable \( \tau \) is given by

\[
\rho(x, \tau) = (\Psi^R(x, \tau))^2 + (\Psi^I(x, \tau))^2
\]

All functions will be periodic in \( \tau \) over a period \([0..1]\).
Questions: for the three different initial states

\[ \Psi_1(x) = N \sin\left(\frac{\pi x}{L}\right) + \sin\left(\frac{2\pi x}{L}\right) \]
\[ \Psi_2(x) = N \sin\left(\frac{\pi x}{L}\right) \]
\[ \Psi_3(x) = N x^3 (L - x) \]

do the following, where I use the name \( \Psi(x) \) for either one of the initial states:

a) Normalize \( \Psi(x) \)

b) Calculate the expansion coefficients \( c_n = \int_0^L \phi_n(x) \Psi(x) dx \). Take \( M=50 \), or set the range of \( n \) to be \( n = 1..50 \).

c) Define the time-dependent functions \( \Psi^R(x, \tau), \Psi^I(x, \tau), \rho(x, \tau) \).

d) Plot the above time-dependent functions for time \( \tau = 0 \), and compare to the exact initial state \( \Psi(x) \). This should match nicely. It is a check of your program.

e) Plot the time dependent functions \( \Psi^R(x, \tau), \Psi^I(x, \tau), \rho(x, \tau) \) for time \( \tau = 1 \). You should see the same result as under d). This is another check!

f) We can now plot the wave function pieces for different times, e.g. \( \tau = 0.05, 0.1, 0.2, 0.3 \). Plot the functions \( \Psi^R(x, \tau), \Psi^I(x, \tau) \) in one plot, and plot in an adjacent picture \( \rho(x, \tau), \rho(x, 0) \). This will give you a good idea, of what is going on in time-dependent quantum mechanics.

g) Now we can even do something much neater, and perform a simulation, or make a movie. In Mathcad, type \( \tau := 0.01 \times \text{FRAME} \), above the plots you wish to make a movie of. Also keep a record of the time, by including “\( \tau = \)” below the plots. Then go to Tools/Animate/Record and set the “To” box to 9 to try things out. Then select the parts of the file you wish to make a movie of, e.g. select the plots and the FRAME line. Click “Animate” in the pop up box. This calculation will take a little time. When it is done, Mathcad pops up a window and you can play the movie instantly, by clicking the lower let “play” button. You can adjust the speed of the movie, by selecting the button to the right of the play button. You can also save it as a Video for Windows, a “.avi” file, which
you can play as a movie on your computer. You can repeat the exercise, once everything is working properly, and Record another movie, but with more frames by setting the “To” box to 100. This will perform the simulation for one entire period. I was quite proud when I could get it all to work. Give it a shot!

h) You can repeat steps a … g for each of the three functions listed in the beginning. This should be very easy to set up in Mathcad. Just change the initial state. Try it out, and digest what you see. Can you make sense of it?