Physics 3220 – Quantum Mechanics 1 – Fall 2008
Problem Set #4

Due Wednesday, September 17 at 2pm

Problem 4.1: Stationary state in the infinite square well. (20 points)

The infinite square well has the potential

$$\begin{aligned} V(x) &= 0\,, \quad 0 \le x \le a\,, && (1) \\ &= \infty \quad \text{otherwise}\,, && (2) \end{aligned}$$

and the (normalized) stationary states were found to be

$$\psi_n(x) = \sqrt{\frac{2}{a}}\, \sin\left(\frac{n\pi x}{a}\right)\,, \tag{3}$$

with energies

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}\,. \tag{4}$$

a) If a wavefunction at time $t = 0$ is $\Psi(x, 0) = \psi_n(x)$, write down $\Psi(x, t)$ at all times.

b) Calculate the expectation values $\langle x\rangle$, $\langle x^2\rangle$, $\langle p\rangle$ and $\langle p^2\rangle$ for the n^{th} stationary state. Briefly describe the physical meaning of the $\langle x\rangle$ and $\langle p\rangle$ results.

c) Calculate the standard deviations σ_x and σ_p, called "uncertainties" in quantum mechanics. One grows much more rapidly than the other as n increases; can you make physical sense of why they behave differently? Think about the values that x and p may take.

d) Heisenberg's Uncertainty Principle states that for any physical wavefunction Ψ, the uncertainties σ_x and σ_p will always obey

$$\sigma_x\sigma_p \ge \frac{\hbar}{2}\,. \tag{5}$$

Check Heisenberg's Uncertainty Principle in the case of the stationary states. Which stationary state is closest to the lower bound of the inequality?

Now that we know about how to check expectation values for momentum, it's time to get some practice, while getting acquainted with the infinite square well and its stationary states. The Uncertainty Principle will appear more later.

Problem 4.2: Non-stationary state in the infinite square well. (20 points)

Using the same conventions for the infinite square well as the previous problem, a wavefunction at time $t = 0$ is

$$\Psi(x, 0) = A\left(\psi_2(x) + \psi_3(x)\right) . \tag{6}$$

a) Normalize $\Psi(x, 0)$. There is an easy way and a less easy way: the easy way is to exploit the orthonormality of the $\psi_n(x)$.

b) Determine $\Psi(x, t)$ and $|\Psi(x, t)|^2$, and write the latter in an explicitly real form (no i's anywhere). What is the angular frequency ω of oscillation of $|\Psi(x, t)|^2$, and how is it related to the stationary state energies?

c) Calculate $\langle x\rangle$ and $\langle p\rangle$ as functions of time and express them in terms of ω. *Hint:* once you have $\langle x\rangle$ as a function of time, there is a shortcut to calculating $\langle p\rangle$.

d) If you measured the energy of this particle, what are the values you might get, and what is the probability of each of them? Find the expectation values $\langle H\rangle$ and $\langle H^2\rangle$, which are the same thing as $\langle E\rangle$ and $\langle E^2\rangle$, and the uncertainty in the energy σ_E.

Not all states are stationary states, even though all states can be built from stationary states, and in fact non-stationary states are much more interesting — where by "interesting" we mean "something actually happens".

Problem 4.3: Expanding infinite square well and time evolution. (30 points)

For times $t < 0$, a particle is sitting in the ground state of an infinite square well of length $1/2$, $0 \le x \le 1/2$. At $t = 0$, the experimenter causes the well to be doubled in size to occupy $0 \le x \le 1$.

This problem requires some numerical work, with software such as Mathematica or Matlab. Posted on the web site are two sample Mathematica notebooks you may find useful if you don't know much about it, but you are free to use other software if you wish.

a) Assume that the change in the size of the well does not affect the wavefunction at the instant $t = 0$; write down the wavefunction $\Psi(x, t = 0)$. (Think carefully about what is happening in different ranges of x.)

b) The wavefunction can be written as a linear combination of stationary states *of the larger well*, $\Psi(x, t = 0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$, where ψ_n are the stationary states of the well of size 1. Determine a formula for the c_n. To check that this infinite series is approximating $\Psi(x, t = 0)$, plot the terms up to $n = 5$ and compare the result to the exact graph. (Going to higher n should make the comparison better, but $n = 5$ will be good enough for us.)

(Note: the coefficient c_2 for $n = 2$ is finite, but depending on how it is evaluated a math program may think it is infinite; you may have to treat it carefully.)

c) Define the time constant $t_0 \equiv 2ma^2/\hbar\pi^2$; for an electron in a 1D well the size of an atom, what is the numerical value of t_0? We will find it convenient to measure time in units of t_0; why is this a useful standard of time to use? Working with the dimensionless variable $\tau \equiv t/t_0$, consider the probability density $|\Psi(x,\tau)|^2$, again using the terms up to $n = 5$. Plot the results at $\tau = 0.3, 0.7, 1.0$ and 2.0, and look at a few other values in between. Describe in words what the probability density is doing as time goes on.

Here we get an idea what happens if you set up a particle in a highly non-stationary state and watch it go. Numerical work can be invaluable for plotting and watching the evolution of physical states that are too complicated to understand analytically. Even though we are watching the probability density instead of the actual particle as we would in classical mechanics, hopefully the overall motion can still be discerned.

Problem 4.4: Order of magnitude estimate. (10 points)

Before the neutron was discovered by Chadwick in 1932, the masses of nuclei were very puzzling. Each nucleus has a positive charge $q = Ze$ (we use conventions where $e > 0$), where Z is called the atomic number, and a mass approximately $m = Am_p$, where m_p is the mass of the hydrogen nucleus (now known to be a single proton). A proton has charge e, and the fact that generally $A > Z$ meant that higher nuclei were not just built out of protons; we know now there are Z protons and $A - Z$ neutrons.

Before Chadwick's discovery, a different model was proposed. This model suggested that the nucleus contained *electrons* as well as extra protons; the electrons (which have charge $-e$) were supposed to cancel some of the protons' charge, giving the correct mass and net charge for the nucleus. For instance, the carbon-12 nucleus with $A = 12$ and $Z = 6$ would contain 12 protons and 6 electrons in this model, giving it the correct total charge and mass number.

In evaluating this model however, one other source of mass must be taken into account, a surprising one: the binding energy of the electrons that arises in confining them to the nucleus will act as an effective source of mass, via $E = mc^2$.

a) Let us make a very rough estimate of this energy and the corresponding mass in quantum mechanics: without knowing anything about the details of the confining potential, model it with a 1D infinite square well with a the size of a nucleus, about 10^{-15} m. What is the ground-state energy of the electron in this potential? What mass (using $E = mc^2$) does this ground-state energy correspond to? Give the mass in units of eV$/c^2$ and find the ratio to the mass of a proton. Does this seem like a good model of the nucleus? Explain.

Because the infinite square well is just a very rough guess, there is no *point* in trying to be totally precise about its consequences; we are just trying to answer the broad question, "How big an energy do we get squeezing an electron into something the size of the nucleus?" without pretending we have a precise model of nuclear dynamics. So in doing the calculation, just look for the order of magnitude: don't worry about factors of 2, and feel free to say things like $\pi^2 = 10$. Real nuclei are also three-dimensional, of course, but the difference turns out to be only a factor of three, which we can ignore for this order-of-magnitude estimate.

b) In determining the masses of things, we don't usually think to include mass from binding energy; this is because it is usually not very important. Repeat part a) for an electron confined within a well of size 10^{-10} m instead, which is the size of an electronic orbital in an atom instead of the size of a nucleus. (Of course the electron is really bound to the nucleus through electrostatic forces, which don't look much like a square well, but we are just making a very rough estimate here.) Find the ratio of the result again to the mass of a proton; does the binding energy of the electron in its atomic orbital correct the mass of the atom much?

Making an order-of-magnitude estimate is another valuable tool in your toolbox. Being able to make a rough-and-ready approximation to a solution you are interested in in just a couple minutes can be just as valuable as spending hours (or days....) solving it exactly. Sometimes more so. Knowing what kinds of approximations are fair game is not always easy, and takes practice.