Quantum Physics I (8.04) Spring 2016
Assignment 6

MIT Physics Department
March 17, 2016

Due Friday April 1, 2016
12:00 noon

Reading: Griffiths section 2.6. For the following week sections 2.5 and 2.3.

Problem Set 6

1. **Particle in a square well.** [10 points] A particle of mass m moves in an infinite square well of width a. Its wavefunction at time $t = 0$ is

$$\Psi(x, 0) \;=\; \frac{1}{\sqrt{3}}\sqrt{\frac{2}{a}}\sin\frac{2\pi x}{a} + \sqrt{\frac{2}{3}}\sqrt{\frac{2}{a}}\sin\frac{3\pi x}{a}\,.$$

   (a) Is Ψ in an energy eigenstate? Find $\Psi(x, t)$.

   (b) What are the probabilities that a measurement of the energy at time t gives each of the following values

$$\frac{\hbar^2\pi^2}{2ma^2}\,, \quad \frac{4\hbar^2\pi^2}{2ma^2}\,, \quad \frac{9\hbar^2\pi^2}{2ma^2}\,.$$

   (c) What is the expectation value of x at time t?

   (d) What is the expectation value of p at time t ?

2. **Non-degeneracy of bound states in one dimension** [10 points]

   Griffiths Problem 2.45, p. 87.

3. **Infinite rectangular well in the plane** [10 points]

   Consider a particle of mass m moving in the x, y plane with potential that is zero inside the rectangular box comprised of all points (x, y) for which

$$0 \le x \le L_x\,, \quad 0 \le y \le L_y\,,$$

   and is infinite elsewhere.

   (a) Use the two-dimensional Schrödinger equation to find the energy eigenstates. Give the energies and the normalized eigenfunctions.

(b) Consider the case $L_x = L_y = L$. You will see that there are degeneracies in the energy spectrum. Some degeneracies have a simple symmetry explanation; identify them and state why they occur. Some degeneracies are accidental; they seem to be random. Display some examples. [Hint: 49+ 1 = 25 + 25].

(c) Show that whenever $(L_x/L_y)^2$ is irrational there are no degeneracies.

4. **An infinite square well with a step** [10 points]

A particle of mass m is moving in one dimension, subject to the potential $V(x)$:

$$V(x) = \begin{cases} \infty\,, & \text{for } x < 0, \\ 0, & \text{for } 0 < x < a\,, \\ V_0\,, & \text{for } a < x < 2a\,, \quad (V_0 > 0) \\ \infty\,, & \text{for } \ x > 2a\,. \end{cases}$$

(a) Find the equations that determine the stationary states with energies $0 < E < V_0$. For this we define

$$k^2 \equiv \frac{2mE}{\hbar^2}\,, \quad \kappa^2 \equiv \frac{2m(V_0 - E)}{\hbar^2}\,, \quad z_0^2 = \frac{2ma^2V_0}{\hbar^2}\,, \quad \eta \equiv ka\,, \quad \xi \equiv \kappa a\,.$$

(We use k for classically allowed regions and κ for classically forbidden regions).Your equations should be possible to write in terms of ξ, η, and z_0.

(b) As a numerical application, consider $z_0 = 2\pi$. How many states do you get with $E < V_0$? Find the possible values of the energy E in terms of V_0 (use at least 4 significant digits).

5. **Shooting method and application** [15 points]

For a particle in a quartic potential $V(x) \sim x^4$, after rescaling of x into a unit-free variable u, the Schrödinger equation takes the form

$$-\frac{1}{2}\frac{d^2\psi}{du^2} + (u^4 - e)\psi \ = \ 0\,,$$

where e is a unit-free measure of the energy eigenvalue. The Mathematica instructions that allow you to find the values of e for the even solutions of this potential are given below. These instructions produce a plot for the solution $\psi(u)$, for $u \in [0, 3.5]$ with some suitable initial conditions and for the chosen value of the energy e.

```
Clear[e, psi]

v[x_]:= x^4

e=0.65;

psi = psi/. NDSolve[{-(1/2)psi''[u] + (v[u]-e)psi[u]==0, psi[0]==1,
```

```
  psi'[0]==0}, psi, {u, 0, 3.5}][[1]];
Plot[psi[u], {u, 0, 3.5}]
```

After executing these instructions, if you write `psi[0.5]`, for example, the program will return the value of ψ at $u = 0.5$.

Play with this to familiarize yourself. The initial value of e set above is 0.65 but the ground state energy, as you can find out by trial and error, is a little bit higher.

We now revisit the previous problem: a particle of mass m on an infinite square well with a step. Again, we take $z_0 = 2\pi$. You found two bound states with $E < V_0$:

$$E_1 = 0.\#\#436\, V_0\,, \quad E_2 = 0.\#\#747 V_0\,.$$

(a) Use $x = au$, with $u \in [0, 2]$ unit free, and write $V = V_0 f(u)$ for a suitably defined $f(u)$ to obtain a differential equation for the energy eigenstates in which no units appear and the energy eigenvalue is encoded by the pure number $e = E/V_0$.

Test your differential equation with the shooting method to recover the above values of E_1 and E_2. Find the next two energy levels E_3 and E_4.

(b) We discussed in lecture the fact that for slowly varying potentials the amplitude of the wavefunction is roughly proportional to the square root of the 'local' de Broglie wavelength. Our potential, having a step, is not really slowly varying, but we can still see numerically to what degree this property holds.

Construct the energy eigenstate with 8 nodes (the eighth excited state) and determine its energy. Let A_L and A_R denote the amplitudes of your wavefunction on the left and right sides of the square well. Read the ratio A_L/A_R from your wavefunction and compare with the prediction for this ratio using the de Broglie wavelength.

6. **Hydrogen ion using the square well model.** [10 points]

Last time you modeled the hydrogen atom size and ground state energy

$$a_0 = \frac{\hbar^2}{me^2}\,, \quad E_0 = -\frac{e^2}{2a_0} = -13.6 \text{ eV},$$

using the square well potential

$$V(x) = \begin{cases} -V_0, & \text{for } |x| < a_0, \quad V_0 > 0\,, \\ 0\,, & \text{for } |x| > a_0\,. \end{cases}$$

You previously found that this well has

$$z_0 = 1.3192, \quad \text{and} \quad V_0 = z_0^2|E_0| = 1.7402|E_0| = 23.67\text{eV}\,.$$

The square well potential mimics the potential created by the proton and the ground state energy is the energy of the electron in this potential.

To simulate the *hydrogen ion* H_2^+ (2 protons 1 electron) we will construct an *even* potential with two identical square well models of hydrogen separated by a small distance $2\gamma\, a_0$ where γ is a small positive unit-free constant. The potential is therefore

$$V(x) = \begin{cases} 0 & \text{for} \quad |x| < \gamma a_0\,, \\ -V_0, & \text{for} \quad \gamma a_0 < |x| < (2+\gamma)a_0, \quad V_0 > 0\,, \\ 0\,, & \text{for} \quad |x| > (2+\gamma)a_0\,. \end{cases}$$

For definiteness work with $\gamma = 0.2$.

(a) Use the shooting method to find the energy of the lowest energy eigenstate, namely, the bound state energy of an electron shared by the two protons. Show the wavefunction of the electron from the plot of your solution.

(b) The *binding* energy of the ion is obtained by adding the positive energy due to the repulsion of the two protons to the above ground state energy. What binding energy do you get? How does it compare with the experimental value?