22.101   Fall 2003   Professor Sow-Hsin Chen   Due: Oct.15 / 03
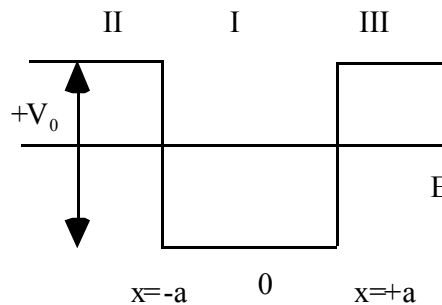
Problem Set No.3

1.   Consider a particle of mass m bound in a potential well of depth V_0 and width 2a, as illustrated in the following figure.

Solve the one-dimensional Schrödinger equation.

$$\frac{d^2u}{dx^2} + \frac{2m}{\hbar^2}(E - V)u = 0 \tag{1}$$

in regions I, II and III. Match the boundary conditions at $x = -a$ and $x = a$ to obtain the following   condition,

$$\tan\left[2a\sqrt{\frac{2mE}{\hbar^2}}\right] = \frac{2\sqrt{E(V_0 - E)}}{2E - V_0} \tag{2}$$

The roots of this equation can be determined by graphical means. It is found that there is a finite number of allowed discrete energies $E_1, E_2, E_3, \ldots\ldots$ These are quantized energy levels of the bound particle.

Take the particle to have the electron mass m = 9.108×10^{-28} gr. and $V_0 = 6$ eV, $2a = 9.6$ Å. It is convenient to use a dimensionless parameter $\eta = 2ma^2 V_0/\hbar^2 = 36$. Show that there are only four allowed states. Find these energy eigen values. Plot the wave functions of the first two states. It can be shown in general that the ground state (the lowest energy state) has no node and the first excited state has one node and the second excited state has two nodes, etc. in the region of the

potential well.

2. Use the condition derived in the deuteron problem

$$\chi b \cot \chi b = -\alpha b \tag{3}$$

and the fact that $\alpha = \sqrt{MB/\hbar^2} = 0.232 \ (fm)^{-1}, \quad b \leq 3 \ fm$ to show that there is no excited state in the deuteron -problem.

3. The Hamiltonian function of a one-dimensional harmonic oscillator is:

$$H = T + V = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 . \tag{4}$$

The ground state wave function and energy are given by:

$$\psi_0(x) = \left(\frac{\beta}{\pi}\right)^{1/4} e^{-\frac{1}{2}\beta x^2} ; \text{ where } \beta = \frac{m\omega}{\hbar} ; E_0 = \frac{1}{2}\hbar\omega . \tag{5}$$

Show that for this state, the expectation values of the kinetic and potential energies are equal,

$$\langle T \rangle = \langle V \rangle = \frac{1}{2} E_0 . \tag{6}$$

4. A hydrogen-like atom has a Hamiltonian function:

$$H = T + V = \frac{p^2}{2m} - \frac{Ze^2}{r} . \tag{7}$$

The ground state wave function and energy are:

$$\psi_0(x) = \sqrt{\frac{Z^3}{\pi a_b^3}} e^{-\frac{Zr}{a_b}} ; \text{ where } a_b = \frac{\hbar^2}{me^2} ; E_0 = -\frac{Z^2 me^4}{\hbar^2} . \tag{8}$$

Show that: $\langle T \rangle = -E_0 = -\frac{1}{2}\langle V \rangle .$

5. In polar coordinate, (r, ϑ, φ), the components of momentum may be written as, $(p_r, p_\vartheta, p_\varphi)$. In operator form one can write

$$\hat{p}_r \psi = -i\hbar \frac{1}{r} \frac{\partial}{\partial r} (r\psi) . \tag{9}$$

(a) Show that this operator satisfies the commutation relation $\left[\hat{r}, \hat{p}_r\right] = i\hbar$ and its square operator is

$$\hat{p}_r^2 \psi = -\hbar^2 \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial \psi}{\partial r}) . \tag{10}$$

(b) From these results and the hydrogen atom ground state wave function given in the last problem show directly by integration that the average kinetic energy is given by:

$$\langle \hat{T} \rangle = -\frac{\hbar^2}{2m} \int_0^\infty \psi_0(r) \frac{1}{r^2} \frac{d}{dr} (r^2 \frac{d\psi_0}{dr}) 4\pi r^2 dr = \frac{me^4}{2\hbar^2} , \qquad (Z=1) \tag{11}$$

(c) Show that the uncertainty relation for this ground state is given by: $\sqrt{\overline{(\Delta r)^2} \ \overline{(\Delta p_r)^2}} = \frac{\hbar}{2}\sqrt{3}$.

6. Consider a bound-state problem of a particle of mass m moving in a spherically symmetric potential well of a width a and a depth $-U_0$,

$$U(r) = \begin{cases} 0 & \text{if } r \le a \\ -U_0 & \text{if } r > a \end{cases} .$$

(a) Write down the Schrödinger equation, neglecting the orbital angular momentum (namely putting $\ell = 0$).

(b) Making a transformation of the wave function R(r) to a new radial wave function u(r) by a relation, R(r) = u(r)/r, and show that the equation for the function u(r) reduces to a simple form

$$\frac{d^2 u}{dr^2} + \frac{2m}{\hbar^2}(E - U)u = 0$$

(c) Since we are looking for bound states, put $E = -\varepsilon$, and write down the appropriate solutions in the two regions, inside and outside the well. By matching the two respective solutions at the boundary a, derive a consistency equation,

$$\alpha a \cot \alpha a = -\beta a$$

where

$$\alpha^2 = \frac{2m}{\hbar^2}(U_0 - \varepsilon) > 0, \quad \text{and} \quad \beta^2 = \frac{2m}{\hbar^2}\varepsilon > 0.$$

(d) Rewrite the consistency equation as :

$$\eta = -\xi \cot \xi$$

and note that

$$\xi^2 + \eta^2 = (\alpha^2 + \beta^2)a^2 = \frac{2mU_0a^2}{\hbar^2}.$$

Carry out the graphical solution of the pair of equations given above in the ξ, η plane to show the validity of the following theorem.

If $U_0a^2 \leq \frac{\pi^2\hbar^2}{8m}$, there is no bound state.

If $\frac{\pi^2\hbar^2}{8m} \leq U_0a^2 \leq \frac{9\pi^2\hbar^2}{8m}$, there is one bound state. Give the bound state energy.

If $\frac{9\pi^2\hbar^2}{8m} \leq U_0a^2 \leq \frac{25\pi^2\hbar^2}{8m}$, there are two bound states. Give the bound state energies.