PH 204: Quantum Mechanics II
Mid semester examination
16.02.2018
2:00- 5:00 pm
Total Marks: 200

1. Let us consider the Hydrogen atom problem. The Hamiltonian is

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} \tag{1}$$

In spherical coordinates we can write the Schrödinger equation as:

$$\left\{ -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{l(l+1)}{r^2}\right] - \frac{e^2}{4\pi\epsilon_0 r^2}\right\} R(r) = ER(r) \tag{2}$$

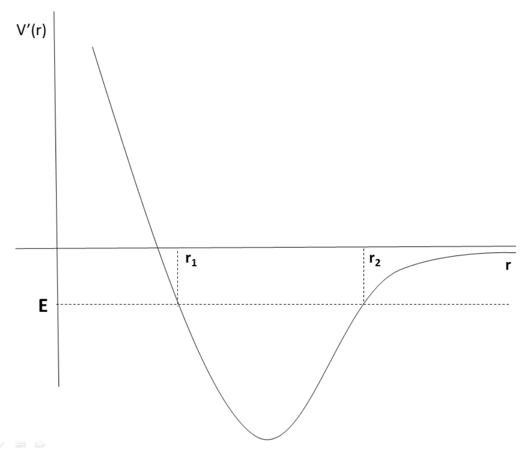
where $R(r)$ is he radial part of the wave function. We can define the linear momentum operator $p(r)$, which depends only on the r coordinate as

$$p(r) = -\hbar^2 \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) \tag{3}$$

Then the Schrödinger equation becomes,

$$\left[\frac{p^2(r)}{2m} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} - \frac{e^2}{4\pi\epsilon_0 r}\right] R(r) = ER(r) \tag{4}$$

In what follows, we can treat $V'(r) = \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} - \frac{e^2}{4\pi\epsilon_0 r}$ as a new potential and the corresponding kinetic energy is $\frac{p^2(r)}{2m}$. The plot of $V'(r)$ gives



(a) (10 points) Show that r_1 and r_2 follows the relation

$$r_1 + r_2 = -\frac{e^2}{4\pi\epsilon_0 E}$$

$$r_1 r_2 = -\frac{\hbar^2}{2m}\frac{l(l+1)}{E}$$

[Hence $E < 0$ for a stable orbit to form.]

(b) (10 points) Let us assume that $V'(r)$ varies slowly enough such that one can use WKB approximation. From equation (4) can you estimate the condition of validity of this approximation?

(c) (30 points) Use the Bohr-Sommerfeld quantisation condition

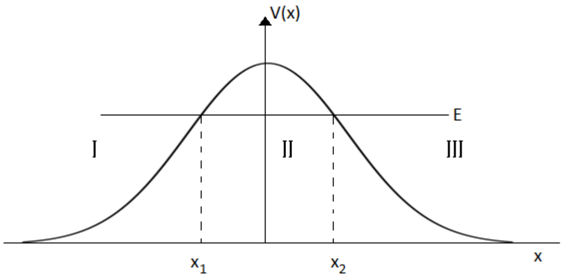
$$\int_{r_1}^{r_2} p(r)dr = \left(n - \frac{1}{2}\right)\hbar\pi \tag{5}$$

to show that the energy levels are approximately of the form

$$E_{nl} \approx \frac{E_0}{[(n-1/2)+\sqrt{l(l+1)}]^2}$$

where $E_0 = -\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2 = -13.6$ eV.
This formula is valid in the limit of $n >> l$ and $n >> \frac{1}{2}$
[useful integral: $\int_a^b \frac{1}{x}\sqrt{(x-a)(x-b)}dx = \frac{\pi}{2}(\sqrt{b}-\sqrt{a})^2$]

2. Penetration through a potential barrier:



We assume $V(r)$ varies slowly enough to have the WKB approximation applicable.
Using WKB approximation and correction formula we obtain the wave function in the three regions as

Region III:

$$\Psi_{\rm III}(x > x_2) = \frac{A}{\sqrt{p(x)}} \exp\left[\frac{\mathrm{i}}{\hbar}\int_{x_2}^{x} p(x')dx' - \frac{\mathrm{i}\pi}{4}\right] \tag{1}$$

Note that we could absorb the phase $e^{\mathrm{i}\pi/4}$ with the constant A but we keep it for our own convenience.

Region II: In region II, we can either start from x_2 to x, or from x_1 to x for $x_1 < x < x_2$. Therefore we can have two equivalent solutions written as

$$\Psi_{\rm II}(x < x_2) = -\frac{\mathrm{i}A}{\sqrt{|p(x)|}} \exp\left[\frac{1}{\hbar}\int_{x}^{x_2} |p(x')|dx'\right] \tag{2}$$

or

$$\Psi_{\rm II}(x > x_1) = -\frac{\mathrm{i}A}{\sqrt{|p(x)|}} e^{\hbar\lambda} \exp\left[-\frac{1}{\hbar}\int_{x_1}^{x} |p(x')|dx'\right] \tag{3}$$

where $\hbar\lambda$ is to be determined below.

Region I:

$$\Psi_{\rm II}(x < x_1) = -\frac{2\mathrm{i}A}{\sqrt{|p(x)|}} e^{\hbar\lambda} \cos\left[-\frac{1}{\hbar}\int_{x_1}^{x} |p(x')|dx' - \frac{\pi}{4}\right] \tag{4}$$

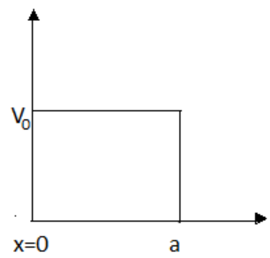
(a) (15 points) Find λ in terms of momentum $p(x)$.

(b) (25 points) Find the transmission coefficient T in terms of λ, for a particle moving from region I to region III through the barrier.

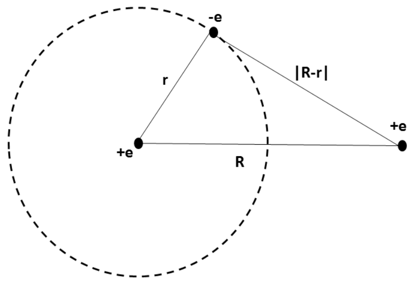
(c) (10 points) Using the equation obtained in part(b) above, show that the transmission coefficient becomes simply

$$T \approx \frac{16E(V_0 - E)}{V_0^2} e^{-2\kappa a}$$

where $\kappa = \frac{1}{\hbar}\sqrt{2m(V_0 - E)}$ for a rectangular potential of the form



3. Suppose we bring a positive charge $+e$ close to a Hydrogen atom from infinity upto a distance R from the proton. Will the positive charge be attracted or repelled by the H-atom? That is, will there be a ground state of this system, whose energy is less than the total energy of the inidividual systems?



This problem can be solved via variational method. The problem is described as follows:

The Hamiltonian for the problem is

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} - \frac{e^2}{4\pi\epsilon_0 (R-r)} + \frac{e^2}{4\pi\epsilon_0 R} \quad (1)$$

Let us assume $R >> a$ where a is the Bohr radius, such that the last term can be neglected. So we are left with

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} - \frac{e^2}{4\pi\epsilon_0 (R-r)} \quad (2)$$

Then we can solve the above problem by assuming a trial wave function of the electron with a variaional parameter and try to find if there is a ground state energy which is negative for an optimum distance of R.

To construct the trial wavefunction, we can approach this way.
The electron has equal probability of forming Hydrogen atom with the proton 1 (original Hydrogen atom's proton) or with proton 2 (which is the inserted positive charge). The hydrogen

atom's wavefunction is

$$\psi(r) = \frac{1}{\sqrt{\pi a^3}} e^{-\frac{r}{a}} \tag{3}$$

where a is the Bohr-radius.

(a) (10 points) Under the above assumption, what will be a valid trial wavefunction among the two choices given below and why?
(i) $\psi(r,R) = A\psi(r)\psi(|\vec{R}-\vec{r}|)$
(ii) $\psi(r,R) = A[\psi(r) + \psi(|\vec{R}-\vec{r}|)]$
Give valid physical reasoning.

(b) (30 points) With your choice of proper trial wavefunction, estimate the expectation value of the Hamiltonian.

$$E_g = \langle \psi(r,R)| H(r,R) |\psi(r,R)\rangle \tag{4}$$

Hint: Assume $r^{'} = |\vec{R}-\vec{r}|$ and use the integrals
$\int d^3r\, e^{-\frac{(r+r^{'})}{a}} = \pi a^3 e^{-\frac{R}{a}}[1 + \frac{R}{a} + \frac{1}{3}(\frac{R}{a})^2]$
$\int d^3r\, \frac{1}{r} e^{-\frac{2r^{'}}{a}} = \pi a^2[\frac{a}{R} - (1+\frac{a}{R})e^{-\frac{2R}{a}}]$
$\int d^3r\, e^{-\frac{(r+r^{'})}{a}} \frac{1}{r^{'}} = \pi a^2 e^{-\frac{R}{a}}[1+\frac{R}{a}]$

Hydrogen atom's ground state energy is $E_0 = \frac{-e^2}{4\pi\epsilon_0}\frac{1}{2a} = -13.6eV$
where Bohr radius $a = \frac{4\pi\epsilon_0\hbar^2}{me^2} = 0.529 \times 10^{-10}m$

(c) (10 points) The final result can be expressed in units of E_0 as

$$F(x) = -\frac{E_g}{E_0} = -1 + \frac{2}{x}[\frac{(1-\frac{2x^2}{3})e^{-x} + (1+x)e^{-2x}}{1+(1+x+\frac{x^2}{3})e^{-x}}]$$

What is the variational parameter here? Do you think the ground state energy has a minimum negative value for an optimum value of the variational parameter? Show steps and argument. Exact evaluation of the optimum value of the parameter is tedious.

4. Wigner- Eckart Theorem

(a) (10 points) Let us assume we have a spinless system whose Hamiltonian is rotationally invariant. For this system what are the vector operators which can be written in terms of the proper angular momentum operator using Wigner- Eckart theorem? (Derivation is not required)

(b) Now, let us assume a system of spin-$\frac{1}{2}$ particles in the ground state of the hydrogen atom. In such a system, let us assume $\vec{A_1}$ and $\vec{A_2}$ are two vectors operators which follow the condition in (a) above.

i. (15 points) Can you write $\vec{A_1}$ and $\vec{A_2}$ in terms of three Pauli matrices $\vec{\sigma}$?

ii. (10 points) Find a relation between $\vec{A_1}$ and $\vec{A_2}$.
[Useful identity, $\vec{V} = \frac{< \vec{J}.\vec{V} >}{j(j+1)\hbar^2}\vec{J}$]

iii. (15 points) We assume there are two spin-$\frac{1}{2}$ particles in the ground state of the hydrogen atom. Show that the g-factor of the total spin $\vec{S} = \vec{S_1} + \vec{S_2}$, is $g_s = \frac{3}{2}$.