Homework 2, solutions

problem 1, solution

a) We have a hydrogen-like atom. The ground state wavefunction for a hydrogen-like atom is

$$\phi_0 = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a}\right)^{3/2} e^{-r/a}, \quad \text{where} \quad a_0 = \frac{\hbar^2}{\mu e^2}, \quad a = \frac{\mu}{\mu' Z} a_0 .$$

Here $Z = 2$, $\mu \approx m_e$ and $\mu' = \dfrac{3m_p m_\mu}{3m_p + m_\mu} \approx m_\mu = 207 m_e$.

b) $E_I' = E_I \dfrac{\mu'}{\mu} Z^2$. $E_I = \dfrac{e^2}{2a_0} = 13.6\,eV$. $E_I' = 13.6\,eV \times 207 \times 4 = 11260.8\,eV$.

The energy of the groundstate is $-11260.8\,eV$.

c) $$\langle r \rangle = 4\pi \int_0^\infty |\psi(r)|^2 r^3 dr = 4\pi N^2 \int_0^\infty e^{-2r/a} r^3 dr = 4\pi N^2 \left(\frac{a}{2}\right)^4 \int_0^\infty e^{-x} x^3 dx$$

$$= 4\pi N^2 \left(\frac{a}{2}\right)^4 6 = \frac{3}{2} a$$

$$\langle r^2 \rangle = 4\pi N^2 \int_0^\infty e^{-2r/a} r^4 dr = 4\pi N^2 \left(\frac{a}{2}\right)^5 24 = 3a^2.$$

$$\frac{\langle r \rangle_{(\mu^- + {}^3He^{++})}}{\langle r \rangle_H} = \frac{a}{a_0} = \frac{m_e}{2m_\mu} = \frac{1}{414}.$$

$$\frac{\langle r^2 \rangle_{(\mu^- + {}^3He^{++})}}{\langle r^2 \rangle_H} = \frac{a^2}{a_0^2} = \frac{1}{414^2}.$$

d) $P = |\langle \psi_{100_{after}} | \psi_{100_{before}} \rangle|^2$ (sudden approximation).

problem 2, solution

a) spherical coordinates:

$V(r) = \frac{1}{2}\mu\omega^2 r^2$ The eigenfunctions of H L^2 and L_z are of the form $R_{\kappa\ell}(r)\, Y_{\ell m}(\theta\phi) = \Psi_{\kappa\ell m}(\vec{r})$.

The radial function $R_{\kappa\ell}(r)$ satisfies

$$\left[-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{1}{2}\mu\omega^2 r^2 + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}\right]R_{\kappa\ell}(r) = E_{\kappa\ell}R_{\kappa\ell}(r).$$

Defining $R_{\kappa\ell}(r) = \frac{1}{r}U_{\kappa\ell}(r)$, $\varepsilon_{\kappa\ell} = \frac{2\mu}{\hbar^2}E_{\kappa\ell}$, $\beta = \sqrt{\frac{\mu\omega}{\hbar}}$,
we have

$$\left[\frac{d^2}{dr^2} - \beta^4 r^2 - \frac{\ell(\ell+1)}{r^2} + \varepsilon_{\kappa\ell}\right]U_{\kappa\ell}(r) = 0.$$

As $r\to\infty$ we have $\left[\frac{\partial^2}{\partial r^2} - \beta^4 r^2\right]U_{\kappa\ell}(r) = 0$, $U_{\kappa\ell}(r) \underset{r\to\infty}{\propto} e^{-\beta^2 r^2/2}$.

Let $U_{\kappa\ell}(r) = e^{-\beta^2 r^2/2}\, Y_{\kappa\ell}(r)$.

Then $Y_{\kappa\ell}$ satisfies

$$\frac{\partial^2}{\partial r^2}Y_{\kappa\ell} - 2\beta^2 r\frac{\partial}{\partial r}Y_{\kappa\ell} + \left(\varepsilon_{\kappa\ell} - \beta^2 - \frac{\ell(\ell+1)}{r^2}\right)Y_{\kappa\ell} = 0.$$

$Y_{\kappa\ell}(0) = 0$, $Y_{\kappa\ell}(r) \underset{r\to 0}{\propto} r^{\ell+1}$ are general results.

Trial solution: $Y_{\kappa\ell}(r) = r^{\ell+1}\sum_{q=0}^{\infty} a_q r^q$ $a_0 \neq 0$

Substituting this form into the differential equation and equating coefficients of the same power of q we find

$a_1 = 0$, $a_{q+2}(q+2)(q+2\ell+3) = a_q\left[(2q+2\ell+3)\beta^2 - \varepsilon_{\kappa\ell}\right]$.

All coefficients a_q, q = odd are zero.

All coefficients a_q, q = even are proportional to a_0.

As $q \to \infty$ we find

$$\frac{a_{q+2}}{a_q} \underset{q\to\infty}{\simeq} \frac{2\beta^2}{q} .$$

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots .$$

$$e^{\beta^2 r^2} = 1 + \beta^2 r^2 + \frac{(\beta^2 r^2)^2}{2!} + \frac{(\beta^2 r^2)^3}{3!} + \cdots = \sum_{q_{even}} c_q r^q , \quad c_q = \frac{\beta^q}{(q/2)!} .$$

$$\frac{c_{q+2}}{c_q} \underset{q\to\infty}{=} \frac{2\beta^2}{q} .$$

Therefore $\quad y_{k\ell}(r) \underset{r\to\infty}{\propto} e^{\beta^2 r^2} , \quad u_{k\ell}(r) \underset{r\to\infty}{\propto} e^{\frac{1}{2}\beta^2 r^2} ,$

$u_{k\ell}(r)$ blows up as $r \to \infty$. This is <u>not acceptable</u>, <u>the series must terminate.</u>

There exists an integer $q = k$ such that

$$(2k + 2\ell + 3)\beta^2 - \varepsilon_{k\ell} = 0 , \quad \varepsilon_{k\ell} = (2k + 2\ell + 3)\beta^2 .$$

$E_{k\ell} = \hbar\omega(k + \ell + 3/2)$, k = even, nonnegative integer $k = 0, 2, 4, \cdots$.

Define $n_r = k + \ell$, $k = n_r - \ell$, $\ell = 0, 1, 2, \cdots$. Then

<u>$E_{k\ell} = \hbar\omega(n_r + 3/2)$.</u>

$\psi_{k\ell m}(\vec{r}) = N \dfrac{e^{-\frac{1}{2}\beta^2 r^2}}{r} y_{k\ell}(r)\, Y_\ell^m(\theta\phi)$. The normalization constant N depends on the choice of a_0.

$$y_{k\ell}(r) = r^{\ell+1} \sum_{\substack{q=0 \\ q\ even}}^{k} a_q r^q \quad \text{with} \quad a_{q+2} = \frac{(2q+2\ell+3)\beta^2 - (2k+2\ell+3)\beta^2}{(q+2)(q+2\ell+3)} a_q .$$

For the wavefunction with the lowest energy we have $n_r = 0, \ell = 0, K = 0$,
$E = \frac{3}{2}\hbar\omega$.

$$\psi_{\substack{000\\ n\ell m}}(\vec{r}) = N e^{-\frac{1}{2}\beta^2 r^2} a_0 Y_0^0(\theta\phi) = \frac{N a_0}{\sqrt{4\pi}} e^{-\frac{1}{2}\beta^2 r^2} = \frac{N a_0}{\sqrt{4\pi}} e^{-\frac{m\omega}{2\hbar} r^2}.$$

$$\int |\psi_{000}(\vec{r})|^2 d^3r = 1 \implies \psi_{000}(\vec{r}) = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} e^{-\frac{m\omega}{2\hbar} r^2}.$$

The next higher energy level has $n_r = 1, \ell = 1, K = 0$.
$E = \frac{5}{2}\hbar\omega$ (3-fold degenerate, $m = 0, \pm 1$)

$$\psi_{01m}(\vec{r}) = N a_0 e^{-\frac{1}{2}\beta^2 r^2} r Y_1^m(\theta\phi).$$

$$\int |\psi_{01m}(\vec{r})|^2 d^3r = 1 \implies (Na_0)^2 \int r^4 e^{-\beta^2 r^2} dr = 1,$$

$$\frac{(Na_0)^2}{\beta^5} \times \frac{3}{2^3} \sqrt{\pi} = 1, \quad Na_0 = \frac{\beta^{5/2}}{\pi^{1/4}} \sqrt{\frac{8}{3}}.$$

b) cartesian coordinates:

In cartesian coordinates $H = H_x + H_y + H_z$.

$$\psi_{n_x n_y n_z}(\vec{r}) = \phi_{n_x}(x)\,\phi_{n_y}(y)\,\phi_{n_z}(z), \qquad E_{n_x n_y n_z} = (n_x + n_y + n_z + \tfrac{3}{2})\hbar\omega,$$

where $\phi_{n_x}(x) = \left(\frac{\beta^2}{\pi}\right)^{1/4} \frac{1}{\sqrt{2^n n_x!}} e^{-\beta^2 x^2/2} H_n(\beta x)$, and similarly for $\phi_{n_y}(y)$ and $\phi_{n_z}(z)$.

$$\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar} x^2}$$

The wave function with the lowest energy $E_{000} = \frac{3}{2}\hbar\omega$ is

$$\psi_{\substack{000\\ n_x n_y n_z}}(\vec{r}) = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} e^{-\frac{m\omega}{2\hbar} r^2}. \qquad \psi_{\substack{n\ell m\\ 000}}(\vec{r}) = \psi_{\substack{n_x n_y n_z\\ 000}}(\vec{r}).$$

The next higher energy level is $E = \frac{5}{2}\hbar\omega$.

It is threefold degenerate.

The three eigenfunctions of H_x, H_y, and H_z are

$\psi_{\underset{1\ 0\ 0}{n_x n_y n_z}}(\vec{r})$, $\psi_{\underset{0\ 1\ 0}{n_x n_y n_z}}(\vec{r})$ and $\psi_{\underset{0\ 0\ 1}{n_x n_y n_z}}(\vec{r})$.

$$\phi_1(x) = \left[\frac{4}{\pi}\left(\frac{m\omega}{\hbar}\right)^3\right]^{1/4} \times e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2} = \left[\frac{4}{\pi}\beta^6\right]^{1/4} \times e^{-\beta x^2/2}.$$

$$\psi_{\underset{1\ 0\ 0}{n_x n_y n_z}}(\vec{r}) = \left(\frac{\beta^2}{\pi}\right)^{1/2}\left(\frac{4}{\pi}\beta^6\right)^{1/4} \times e^{-\frac{\beta r^2}{2}} = \frac{\beta^{5/2}}{\pi^{3/4}}\sqrt{2} \times e^{-\frac{\beta r^2}{2}}.$$

c) Let us express $\psi_{\underset{0\,1\,0}{k\ell m}}(\vec{r})$ in terms of the eigenfunctions of H_x, H_y and H_z.

$$\psi_{\underset{0\,1\,0}{k\ell m}}(\vec{r}) = \frac{\beta^{5/2}}{\pi^{1/4}}\sqrt{\frac{8}{3}}\, e^{-\beta^2 r^2/2}\sqrt{\frac{3}{4\pi}}\, z = \frac{\beta^{5/2}}{\pi^{3/2}}\sqrt{2}\, z\, e^{-\beta r^2/2}$$

$$= \psi_{\underset{0\ 0\ 1}{n_x n_y n_z}}(\vec{r})$$

$$\psi_{\underset{0\,1\,1}{k\ell m}}(\vec{r}) = \frac{-\beta^{5/2}}{\pi^{1/4}}\sqrt{\frac{8}{3}}\, e^{-\beta^2 r^2/2}\sqrt{\frac{3}{8\pi}}\, r\sin\theta(\cos\phi + i\sin\phi)$$

$$= \frac{-\beta^{5/2}}{\pi^{3/4}} e^{-\beta^2 r^2/2}(x+iy) = \frac{-1}{\sqrt{2}}\left(\psi_{\underset{1\ 0\ 0}{n_x n_y n_z}} + i\,\psi_{\underset{0\ 1\ 0}{n_x n_y n_z}}\right).$$

$$\psi_{\underset{0\,1\,-1}{k\ell m}}(\vec{r}) = \frac{\beta^{5/2}}{\pi^{1/4}}\sqrt{\frac{8}{3}}\, e^{-\beta^2 r^2/2}\sqrt{\frac{3}{8\pi}}\, r\sin\theta(\cos\phi - i\sin\phi)$$

$$= \frac{\beta^{5/2}}{\pi^{3/4}} e^{-\beta^2 r^2/2}(x-iy) = \frac{1}{\sqrt{2}}\left(\psi_{\underset{1\ 0\ 0}{n_x n_y n_z}} - i\,\psi_{\underset{0\ 1\ 0}{n_x n_y n_z}}\right).$$

problem 3, solution

$$\langle T\rangle = \langle H - V\rangle = \langle H\rangle - \langle V\rangle = E_n - \langle V\rangle$$

$$= -\frac{\mu e^4}{2n^2\hbar^2} - \langle V\rangle .$$

$$\langle V\rangle = \left\langle \frac{e^2}{r}\right\rangle = -e^2\left\langle\frac{1}{r}\right\rangle .$$

$$\left\langle\frac{1}{r}\right\rangle = \alpha^3\frac{(n-\ell-1)!}{(n+\ell)!\,2n}\frac{1}{\alpha^2}\int(\alpha r)^{2\ell+1}e^{-\alpha r}\left(L^{2\ell+1}_{n-\ell-1}(\alpha r)\right)^2 d\alpha r$$

$$= \alpha^3\frac{(n-\ell-1)!}{(n+\ell)!\,2n}\frac{1}{\alpha^2}\frac{(n+\ell)!}{(n-\ell-1)!} = \frac{2}{n a_0}\frac{1}{2n} = \frac{1}{n^2 a_0} = \frac{\mu e^2}{n^2\hbar^2} .$$

$$\langle T\rangle = -\frac{\mu e^4}{2n^2\hbar^2} + \frac{\mu e^4}{n^2\hbar^2} = \frac{\mu e^4}{2n^2\hbar^2} = -E_n .$$

you can also use the virial theorem.

If $H = \frac{P^2}{2m} + V(\vec{R})$ and $V(\vec{R})$ is a homogeneous function of nth degree then $2\langle T\rangle = n\langle V\rangle$.

Here $V(r)$ is a homogeneous function of degree (-1).

Therefore $2\langle T\rangle = -\langle V\rangle \qquad \langle T\rangle = -\langle V\rangle - \langle T\rangle = -\langle H\rangle$

problem 4, solution

The radial equation for $U(r) = r R(r)$ is

$$\left[\frac{\partial^2}{\partial r^2} - \frac{\ell(\ell+1)}{r^2} + \frac{2\mu}{\hbar^2}\frac{e^2}{r}\left(1+\frac{\alpha}{r}\right) - \kappa_{k\ell}^2\right] U_{k\ell}(r) = 0 \quad \text{with } \kappa_{k\ell} = \sqrt{\frac{-2\mu E_{k\ell}}{\hbar^2}}.$$

We can write

$$\left[\frac{\partial^2}{\partial r^2} - \frac{C_\ell}{r^2} + \frac{2\mu}{\hbar^2}\frac{e^2}{r} - \kappa^2\right] U_{k\ell}(r) = 0 \quad \text{with } C_\ell = \ell(\ell+1) - \frac{2\mu e^2 \alpha}{\hbar^2}.$$

Changing to the variable $\rho = r/a$ with $a = \frac{\hbar^2}{\mu e^2}$ we have

$$\left[\frac{\partial^2}{\partial \rho^2} - \frac{C_\ell}{\rho^2} + \frac{2}{\rho} - \Lambda_{k\ell}^2\right] U_{k\ell}(\rho) = 0, \quad \text{with } \Lambda_{k\ell}^2 = \frac{-2a E_{k\ell}}{e^2}.$$

If we write $C_\ell = \ell'(\ell'+1)$, then this is the same equation we obtained for the hydrogen atom, with ℓ replaced by ℓ'.

For the hydrogen atom we have $\Lambda_{k\ell} = \frac{1}{k+\ell}$.

In this problem we therefore have $\Lambda_{k\ell} = \frac{1}{k+\ell'}$.

$$\ell'(\ell'+1) = \ell(\ell+1) - \frac{2\alpha}{a}, \quad \ell' = -\frac{1}{2} + \sqrt{\frac{1}{4} + \ell(\ell+1) - \frac{2\alpha}{a}} = -\frac{1}{2} + \sqrt{\left(\ell+\tfrac{1}{2}\right)^2 - \frac{2\alpha}{a}}.$$

(As $\rho \to 0$ $U(\rho) \to \rho^{\ell'+1}$. Only $\ell'+1 > 0$ is acceptable.)

Let $n = k+\ell$, $k = n-\ell$. Then $\Lambda_{k\ell} = \frac{1}{n + \sqrt{(\ell+\frac{1}{2})^2 - \frac{2\alpha}{a}} - (\ell+\frac{1}{2})} = \frac{1}{n + D(\ell)}$,

$$D(\ell) = \sqrt{\left(\ell+\tfrac{1}{2}\right)^2 - \frac{2\alpha}{a}} - \left(\ell+\tfrac{1}{2}\right).$$

$$E_{k\ell} = -\frac{e^2}{2a\,(n+D(\ell))^2}.$$