Problem 1 | | Problem Set 7

For $f(x) = \epsilon x^2 + bx + c$, the roots are:

$$x_\pm = \frac{-b \pm \sqrt{b^2 - 4\epsilon c}}{2\epsilon} \qquad (*)$$

if we use $x = x_0 + \epsilon x_1$, we have:

$$f(x) = \epsilon(x_0^2 + 2\epsilon x_0 x_1 + \epsilon^2 x_1^2) + b(x_0 + \epsilon x_1) + c = 0$$

collecting in powers of ϵ:

$$\epsilon^0: \ bx_0 + c = 0 \Rightarrow x_0 = -c/b$$

$$\epsilon^1: \ x_0^2 + bx_1 = 0 \Rightarrow x_1 = -x_0^2/b = -c^2/b^3$$

so we get 1 approximate root: $x \approx -c/b - c^2/b^3 \cdot \epsilon$

Taylor expanding $(*)$ gives $x_\pm \approx -\frac{b}{2\epsilon} \pm \frac{b\left(1 - 2\frac{\epsilon c}{b^2} - 2\frac{\epsilon^2 c^2}{b^4}\right)}{2\epsilon}$

so

$x_+ \approx -c/b - \epsilon c^2/b^3$ matching what we got from perturbation.

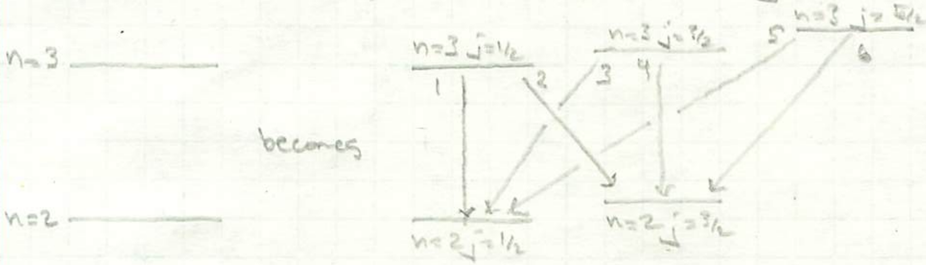
but

$x_- \approx -b/\epsilon + \ldots$ the leading order term goes like $1/\epsilon$, not captured by our perturbation assumption.

Problem 2 (7.21) (see attached notebook for calculations)

For (Bohr) hydrogen: $\Delta E = E_0/3^2 - E_0/2^2 = -E_0(5/36)$, $\Delta E = h\nu \Rightarrow \nu = \Delta E/h \approx 4.57 \times 10^{14}\ 1/s$, $\lambda = hc/\Delta E \approx 656$ nm (see attached notebook).

Fine structure correction: $E'_{fs} = \frac{(E_n^0)^2}{2mc^2}\left(3 - \frac{4n}{j+1/2}\right)$ – the $n=2$ states have $l = 0, 1$, so $j = l + 1/2 = 1/2, 3/2$, & $n=3$ has $l = 0, 1, 2$, so $j = l + 1/2 = 1/2, 3/2, 5/2$.



transitions: $(n_1, j_1) \to (n_2, j_2)$

1. $(3, 1/2) \to (2, 1/2)$
2. $(3, 1/2) \to (2, 3/2)$
3. $(3, 3/2) \to (2, 1/2)$
4. $(3, 3/2) \to (2, 3/2)$
5. $(3, 5/2) \to (2, 1/2)$
6. $(3, 5/2) \to (2, 3/2)$

transition energy diff.s: 1. 36.4×10^{-6} eV, 2. -8.8×10^{-6} eV, 3. 49.8×10^{-6} eV, 4. 4.6×10^{-6} eV, 5. 54.2×10^{-6} eV, 6. 9.1×10^{-6} eV, w/ freq.s 1. 8.8×10^9 Hz $= \nu_1$, 2. -2.1×10^9 Hz $= \nu_2$, 3. 12×10^9 Hz $= \nu_3$, 4. 1.1×10^9 Hz $= \nu_4$, 5. 13×10^9 Hz $= \nu_5$, 6. 2.2×10^9 Hz $= \nu_6$

ordering is: $\nu_2, \nu_4, \nu_6, \nu_1, \nu_3, \nu_5$ so the spacings are: $\nu_4 - \nu_2 \approx 3.2 \times 10^9$ Hz,

$\nu_6 - \nu_4 \approx 1.1 \times 10^9$ Hz, $\nu_1 - \nu_6 \approx 6.6 \times 10^9$ Hz, $\nu_3 - \nu_1 \approx 3.2 \times 10^9$ Hz, $\nu_5 - \nu_3 \approx 1.1 \times 10^9$ Hz

```
In[ ]:= E0 = -2.17987224752 × 10^(-18); (* Ground state energy in Joules *)
        c = 3 × 10^8; (* Speed of light in m/s *)
        h = 6.62607015 × 10^(-34); (* Planck's constant in Js *)
        m = 9.11 × 10^(-31); (* electron mass in kilograms *)

In[ ]:= nu = -(5 / 36) E0 / h
Out[ ]=
```

4.56922×10^{14}

Frequency in hertz.

```
In[ ]:= Lambda = -(36 / 5 h c / E0) 10^9
Out[ ]=
        656.567
```

This is the wavelength in nanometers.

```
In[ ]:= E0 = -13.6; (* Ground state energy in eV *)
        mc2 = 511 803; (* m c^2 for the electron in eV *)

In[ ]:= Ef[n_, j_] := (E0 / n^2)^2 / (2 mc2) (3 - 4 n / (j + 1 / 2))
```

The six energy differences are:

```
In[ ]:= DeltaE1 = (Ef[3, 1 / 2] - Ef[2, 1 / 2])
Out[ ]=
        0.0000363899

In[ ]:= DeltaE2 =  (Ef[3, 1 / 2] - Ef[2, 3 / 2])
Out[ ]=
```

-8.78376×10^{-6}

```
In[ ]:= DeltaE3 =  (Ef[3, 3 / 2] - Ef[2, 1 / 2])
Out[ ]=
        0.0000497746

In[ ]:= DeltaE4 =  (Ef[3, 3 / 2] - Ef[2, 3 / 2])
Out[ ]=
```

4.60102×10^{-6}

```
In[ ]:= DeltaE5 =  (Ef[3, 5 / 2] - Ef[2, 1 / 2])
Out[ ]=
        0.0000542362

In[ ]:= DeltaE6 =  (Ef[3, 5 / 2] - Ef[2, 3 / 2])
Out[ ]=
```

9.06261×10^{-6}

```
In[ ]:= h = 4.136 × 10^(-15); (* Planck's constant in eV s *)

In[ ]:= nu1 = DeltaE1 / h
Out[ ]=
```

8.79832×10^{9}

In[ ]:= nu2 = DeltaE2 / h

Out[ ]= -2.12373×10^{9}

In[ ]:= nu3 = DeltaE3 / h

Out[ ]= 1.20345×10^{10}

In[ ]:= nu4 = DeltaE4 / h

Out[ ]= 1.11243×10^{9}

In[ ]:= nu5 = DeltaE5 / h

Out[ ]= 1.31132×10^{10}

In[ ]:= nu6 = DeltaE6 / h

Out[ ]= 2.19115×10^{9}

In[ ]:= nu4 - nu2

Out[ ]= 3.23617×10^{9}

In[ ]:= nu6 - nu4

Out[ ]= 1.07872×10^{9}

In[ ]:= nu1 - nu6

Out[ ]= 6.60717×10^{9}

In[ ]:= nu3 - nu1

Out[ ]= 3.23617×10^{9}

In[ ]:= nu5 - nu3

Out[ ]= 1.07872×10^{9}

Problem 3 (7.33)

The full potential we want to use here is: (using R for "b")

$$U(r) = U_0\Theta(R-r) + U_c(r)\Theta(r-R)$$

w/ $U_0 = \frac{-e^2}{4\pi\epsilon_0 R}$ & $U_c(r) = \frac{-e^2}{4\pi\epsilon_0 r}$.

$$= \underbrace{(U_0 - U_c(r))\Theta(R-r)}_{\text{treat this as the perturbation}} + U_c(r)$$

Coulomb potential as it appears in the Bohr Hamiltonian

The ground state wave function is: $\psi_{100} = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$

& we want:

$$E^1 = \langle\psi_{100}|(U_0-U_c(r))\Theta(R-r)|\psi_{100}\rangle = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \frac{e^{-2r/a}}{\pi a^3}\left(U_0+\frac{e^2}{4\pi\epsilon_0 r}\right)\Theta(R-r)\, r^2\sin\theta\, dr\, d\theta\, d\phi$$

$$= \frac{4}{a^3}\int_0^R e^{-2r/a}\left(U_0 + \frac{e^2}{4\pi\epsilon_0 r}\right)r^2\, dr$$

$$= \frac{4}{a^3}\left[\frac{U_0 a}{4}\left(a^2 - e^{-2R/a}(a^2+2aR+2R^2)\right) + \frac{e^2 a^2\left(1-e^{-2R/a}(1+2R/a)\right)}{16\pi\epsilon_0}\right]$$

$$= -\frac{e^2}{4\pi\epsilon_0 a^2 R}\left(a^2 - e^{-2R/a}(a^2+2aR+2R^2)\right) + \frac{e^2}{4\pi\epsilon_0 a}\left(1-e^{-2R/a}(1+2R/a)\right)$$

let $R/a = \delta$, then $a = R/\delta$, & the above can be written:

$$\approx \frac{e^2}{4\pi\epsilon_0 a}\left[-\frac{1}{\delta} + \left(1-2\delta+2\delta^2-\tfrac{1}{3}4\delta^3\right)\left(\frac{1}{\delta}+2+2\delta\right) + \left(2\delta^2 - \tfrac{8}{3}\delta^3\right)\right]$$

$$\approx \frac{e^2}{4\pi\epsilon_0 a}\left[\frac{2}{3}\delta^2 \underbrace{- \frac{4}{3}\delta^3 + \frac{8}{3}\delta^4}_{\text{drop, to leading order}}\right] \approx \frac{e^2}{4\pi\epsilon_0 a}\cdot\frac{2}{3}\left(\frac{R}{a}\right)^2$$

the hydrogen (Bohr) ground state energy is: $E_0 = -\frac{1}{2a}\frac{e^2}{4\pi\epsilon_0}$, so

$\frac{E^1}{E_0} \approx -\frac{4}{3}\left(\frac{R}{a}\right)^2$, for $a \approx 5\times10^{-11}$ m, $R \approx 10^{-15}$ m, $(R/a)^2 \approx 4\times10^{-10}$

so $\frac{E^1}{E_0} \approx -5.3\times10^{-11}$ fine structure corrections are of order $\frac{13.6}{500000} \approx 2.7^{-5}$

Problem 4 (8.2)

For $\psi(x) = \dfrac{A}{x^2+b^2}$, normalization requires: $\displaystyle\int_{-\infty}^{+\infty}\left(\frac{A}{x^2+b^2}\right)^2 dx = \frac{A^2\pi}{2b^3} = 1$

so $A = \sqrt{2b^3}/\sqrt{\pi}$, the Hamiltonian is $\hat{H} = \dfrac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2x^2$, so

$$\hat{H}\psi = -\frac{\hbar^2}{2m}\left(\frac{8Ax^2}{(b^2+x^2)^3} - \frac{2A}{(b^2+x^2)^2}\right) + \frac{1}{2}m\omega^2x^2\left(\frac{A}{x^2+b^2}\right)$$

$$\langle\hat{H}\rangle = -\frac{\hbar^2}{2m}A^2\underbrace{\int_{-\infty}^{+\infty}\left(\frac{8x^2}{(b^2+x^2)^3} - \frac{2}{(b^2+x^2)^2}\right)\frac{1}{x^2+b^2}dx}_{=-\frac{\pi}{4b^5}} + \frac{A^2}{2}m\omega^2\underbrace{\int_{-\infty}^{+\infty}\frac{x^2}{(x^2+b^2)^2}dx}_{=\frac{\pi}{2b}}$$

$$= \frac{\hbar^2\cdot\frac{2b^3}{\pi}\pi}{8mb^5} + \frac{m\omega^2\,2b^3}{4b\pi}\pi = \frac{\hbar^2}{4mb^2} + \frac{m\omega^2b^2}{2}$$

$$\frac{d\langle\hat{H}\rangle}{db} = -\frac{\hbar^2}{2mb^3} + m\omega^2b = 0 \Rightarrow b^4 = \frac{\hbar^2}{2m^2\omega^2} \Rightarrow b^2 = \frac{\hbar}{\sqrt{2}m\omega}$$

& then $$\langle\hat{H}\rangle = \frac{\hbar^2}{4m\frac{\hbar}{\sqrt{2}m\omega}} + \frac{m\omega^2}{2}\cdot\frac{\hbar}{\sqrt{2}m\omega} = \frac{\sqrt{2}\hbar\omega}{4} + \frac{\hbar\omega}{2\sqrt{2}} = \frac{1}{\sqrt{2}}\hbar\omega \simeq .707\hbar\omega$$

(compare w/ $\frac{1}{2}\hbar\omega$)

Problem 5 (8-16b)

For $\psi = Ax^p(a-x)$, $\displaystyle\int_0^a \psi^2 dx = \frac{A^2a^{3+2p}}{3+11p+12p^2+4p^3} = 1 \Rightarrow A^2 = \left[\frac{3+11p+12p^2+4p^3}{a^{3+2p}}\right]$

$$\hat{H}\psi = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = -\frac{\hbar^2A}{2m}\left(p(p-1)(a-x)x^{p-2} - 2px^{p-1}\right)$$

$$\langle\hat{H}\rangle = -\frac{\hbar^2}{2m}\left[\int_0^a\left(p(p+1)x^{2p} + a^2p(p-1)x^{2p-2} - 2ap^2x^{2p-1}\right)dx\right]$$

$$= -\frac{\hbar^2}{2m}\left[\frac{p(p+1)x^{2p+1}}{2p+1} + \frac{a^2p(p-1)}{2p-1}x^{2p-1} - \frac{2ap^2x^{2p}}{2p}\right]\Bigg|_{x=0}^{a}$$

to get a well-defined value at the lower, $x=0$, limit, we must have $2p-1 \geq 0$ or $p \geq \frac{1}{2}$.

Then $$\langle\hat{H}\rangle = -\frac{\hbar^2}{2m}\frac{a^{2p+1}A^2}{1-4p^2} = -\frac{\hbar^2}{2m}\frac{a^{2p+1}}{1-4p^2}\cdot\frac{(3+11p+12p^2+4p^3)}{a^{3+2p}}$$

$$\frac{d\langle\hat{H}\rangle}{dp} = 0 \Longrightarrow p = \frac{1}{6}\left[-1 + \frac{16}{(17+i9\sqrt{47})^{1/3}} + (17+i9\sqrt{47})^{1/3}\right] \simeq 1.04307$$

used Mathematica! to solve the cubic

& $\langle\hat{H}\rangle_p \simeq \dfrac{4.98964\hbar^2}{ma^2}$ compare w/ $\dfrac{\pi^2}{2}\dfrac{\hbar^2}{ma^2}$ $\simeq 4.9348$

Problem 6

If you found $\psi(x)$ w/ $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \frac{\alpha}{x^2}\psi = E_0\psi$

let $y = \sigma x$, then $\frac{d^2\psi}{dx^2} = \frac{d^2\psi}{\sigma^{-2}dy^2}$, so

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dy^2}\cdot\sigma^2 - \frac{\alpha}{y^2}\sigma^2\psi = \sigma^2\underbrace{\left[-\frac{\hbar^2}{2m}\frac{d^2\psi}{dy^2} - \frac{\alpha}{y^2}\psi\right]}_{=E_0\psi} = \sigma^2 E_0\psi$$

so whatever E_0 is, we can multiply by the arbitrary σ^2 to make the new energy $\sigma^2 E_0$ smaller, but it's the same state.