

Problem 1

For well:  $E_n = \frac{\hbar^2 \pi^2 n^2}{2m_e L^2}$ . Lowest energy transition is  $n=1 \rightarrow n=2$

$$\Rightarrow \Delta E = \frac{\hbar^2 \pi^2}{2m_e L^2} (2^2 - 1^2) = \frac{3\hbar^2 \pi^2}{2m_e L^2} = \frac{hc}{\lambda} \Rightarrow L^2 = \frac{3\hbar^2 \pi^2 \lambda}{2m_e hc} \Rightarrow$$

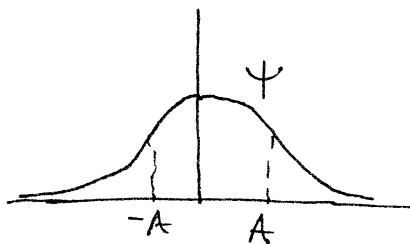
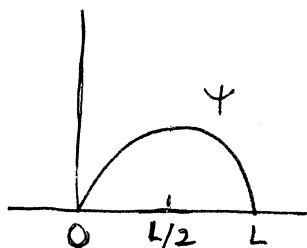
$$\Rightarrow L^2 = \frac{3\hbar^2 \pi^2 \lambda}{2m_e hc} = \frac{3}{2} \frac{\pi^2 \cdot 7.62 \cdot 1000}{12,400} \text{ \AA}^2 = 9.098 \text{ \AA}^2 \Rightarrow \boxed{L = 3.02 \text{ \AA}} \quad (a)$$

(b)  $E_n = \hbar\omega(n + \frac{1}{2}) \Rightarrow \Delta E = \hbar\omega = \frac{hc}{\lambda} = \frac{12,400}{1000} \text{ eV} = 12.4 \text{ eV}$

$\hbar\omega = 12.4 \text{ eV}$  Classical amplitude:  $\frac{1}{2} m\omega^2 A^2 = \frac{\hbar\omega}{2} \Rightarrow$

$$\Rightarrow A^2 = \frac{\hbar\omega}{m\omega^2} = \frac{\hbar}{m\omega} = \frac{\hbar^2}{m\hbar\omega} = \frac{7.62}{12.4} \text{ \AA}^2 = 0.615 \text{ \AA}^2 \Rightarrow \boxed{A = 0.78 \text{ \AA}}$$

(c)



For oscillator:  $\Psi_0(x) = C e^{-\frac{m\omega}{2\hbar} x^2} = C e^{-x^2/2A^2}$ ;  $\int dx \Psi_0^2 = 1 \Rightarrow$

$$\Rightarrow C^2 \sqrt{\pi A^2} = 1 \Rightarrow C = \frac{1}{\pi^{1/4} A^{1/2}} \Rightarrow \boxed{\Psi_0(x) = \frac{1}{\pi^{1/4} A^{1/2}} e^{-x^2/2A^2}}$$

$$\text{or } \boxed{\Psi_0(x) = \left(\frac{m\omega}{\pi \hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}}$$

$$\boxed{\Psi_0(0) = \frac{1}{\pi^{1/4} A^{1/2}} = 0.850 \text{ \AA}^{-1/2}}$$

For square well,  $\Psi_0(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L} \Rightarrow \boxed{\Psi_0\left(\frac{L}{2}\right) = \sqrt{\frac{2}{L}} = 0.814 \text{ \AA}^{-1/2}}$

So the probability is higher for the electron to be at the center in the harmonic oscillator case.

## Problem 2

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \quad ; \quad \psi(x) = Cx e^{-x^2/2x_0^2}$$

$$\langle x \rangle = \int_{-\infty}^{\infty} dx \cdot x |\psi(x)|^2 = 0$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} dx x^2 |\psi(x)|^2 = \frac{\int_{-\infty}^{\infty} dx x^4 e^{-x^2/x_0^2}}{\int_{-\infty}^{\infty} dx x^2 e^{-x^2/x_0^2}}$$

$$\text{Use } \int_{-\infty}^{\infty} dx x^2 e^{-\lambda x^2} = \frac{1}{2} \sqrt{\frac{\pi}{\lambda^3}}, \quad \int_{-\infty}^{\infty} dx x^4 e^{-\lambda x^2} = \frac{3}{4} \sqrt{\frac{\pi}{\lambda^5}}$$

$$\Rightarrow \langle x^2 \rangle = \frac{\frac{3}{4} \sqrt{\pi} x_0^5}{\frac{1}{2} \sqrt{\pi} x_0^3} = \frac{3}{2} x_0^2 \Rightarrow \Delta x = \sqrt{\frac{3}{2}} x_0 = 1.22 x_0$$

$$(b) \quad P(x) = |\psi(x)|^2 = C^2 x^2 e^{-x^2/x_0^2} \quad ; \quad \text{maximize } P(x) \Rightarrow$$

$$P'(x) = 0 = 2x e^{-x^2/x_0^2} - \frac{2x^3}{x_0^2} e^{-x^2/x_0^2} = 0 \Rightarrow$$

$$\Rightarrow \boxed{x = x_0}$$

$$\frac{P(x=0.02x_0)}{P(x=0.01x_0)} \sim \frac{0.02^2}{0.01^2} = 4 \quad \boxed{\text{four times more likely}}$$

$$(e^{-x^2/x_0^2} \approx 1 \text{ for } x=0.01x_0 \text{ or } x=0.02x_0)$$

### Problem 3

$$\Psi(x) = C(1 + \cos(x/a)) ; V(x) = V_0 \frac{1 - \cos(x/a)}{1 + \cos(x/a)}$$

$$-\frac{\hbar^2}{2m_e} \frac{d^2\Psi}{dx^2} + V(x)\Psi = E\Psi$$

$$\frac{d\Psi}{dx} = -\frac{C}{a} \sin \frac{x}{a}, \quad \frac{d^2\Psi}{dx^2} = -\frac{C}{a^2} \cos \frac{x}{a} \Rightarrow$$

$$\frac{\hbar^2}{2m_e a^2} \cos \frac{x}{a} + V_0 \frac{1 - \cos x/a}{1 + \cos x/a} \cdot (1 + \cos x/a) = E(1 + \cos x/a) \Rightarrow$$

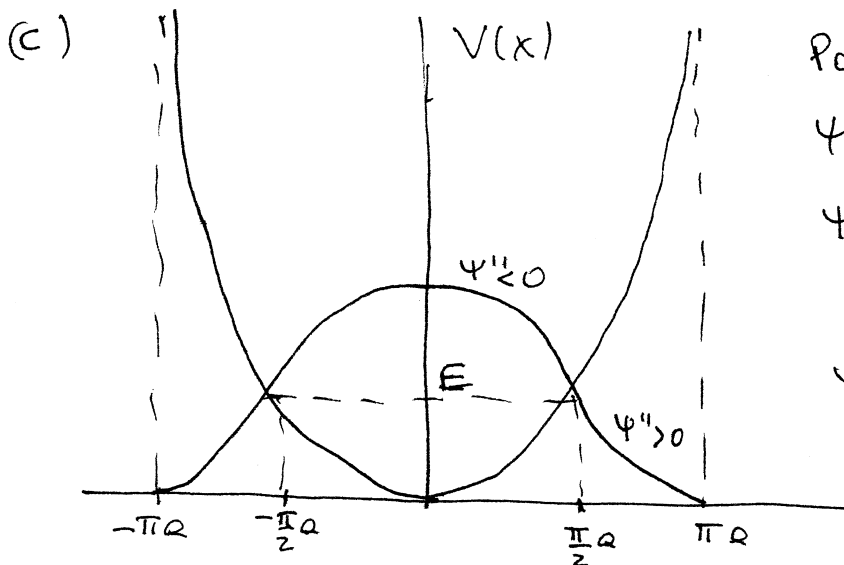
$$\cos \frac{x}{a} \left( \frac{\hbar^2}{2m_e a^2} - V_0 - E \right) + V_0 = E ; \text{ for this to be valid for}$$

$$\text{all } x, \text{ we need: } V_0 = E ; \quad \frac{\hbar^2}{2m_e a^2} - V_0 - E = 0 = \frac{\hbar^2}{2m_e a^2} - 2V_0 \Rightarrow$$

$$\Rightarrow \boxed{V_0 = \frac{\hbar^2}{4m_e a^2} = E = \frac{1}{4} \cdot 7.62 \frac{\text{eV}\text{\AA}^2}{1\text{\AA}^2} = 1.905 \text{eV}}$$

$$(b) \text{ Region where } V(x) < E \Rightarrow V_0 \frac{1 - \cos x/a}{1 + \cos x/a} < V_0 \Rightarrow 1 - \cos x/a < 1 + \cos x/a$$

$$\Rightarrow \cos x/a > 0 \Rightarrow \frac{|x|}{a} < \frac{\pi}{2} \Rightarrow \boxed{-\frac{\pi a}{2} < x < \frac{\pi a}{2}}$$



Potential diverges at  $x = \pm \pi a$

$$\Psi(x = \pi a) = \Psi(x = -\pi a) = 0$$

$$\Psi'' < 0 \text{ for } -\frac{\pi}{2} a < x < \frac{\pi}{2} a$$

= region where  $E > V(x)$

$$\Psi'' > 0 \text{ for } \frac{\pi}{2} a < |x| < \pi a$$

## Problem 4

For a harmonic oscillator,  $\langle E \rangle = \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}$ ,  $k_B = \frac{1}{11,600} \frac{\text{eV}}{\text{K}}$

For  $N$  three-dimensional harmonic oscillators,

$$\langle E \rangle_N = 3N \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}$$

For very high  $T$ ,  $e^{\hbar\omega/k_B T} \approx 1 + \frac{\hbar\omega}{k_B T} \Rightarrow \langle E \rangle_N = 3N k_B T \Rightarrow C_V = 3N k_B$

(a) At  $T = 100 \text{ K}$

$$\frac{\hbar\omega}{k_B T} = \frac{0.02 \text{ eV} \times 11,600 \text{ K}}{100 \text{ K} \times \text{eV}} = 2.32$$

$$\langle E \rangle = \frac{\hbar\omega}{e^{2.32} - 1} = \frac{\hbar\omega}{k_B T} \frac{1}{e^{2.32} - 1} k_B T = 0.253 k_B T$$

$$\Rightarrow \boxed{\langle E \rangle_N = 3N \times 0.253 k_B T = 0.759 N k_B T}$$

(b) at  $T = 1000 \text{ K}$

$$\frac{\hbar\omega}{k_B T} = 0.232$$

$$\langle E \rangle = \frac{0.232}{e^{0.232} - 1} k_B T = 0.888 k_B T$$

$$\boxed{\langle E \rangle_N = 2.665 N k_B T}$$

(c) at  $T = 10,000 \text{ K}$ ,  $\frac{\hbar\omega}{k_B T} = 0.0232$

$$\langle E \rangle = \frac{0.0232}{e^{0.0232} - 1} k_B T = 0.988 k_B T$$

$$\boxed{\langle E \rangle_N = 2.965 N k_B T}$$

### Problem 5

$$\psi(r, \theta, \phi) = Cr e^{-r/a_0} \cos \theta$$

(a) exponential dependence is  $e^{-zr/a_0}$

since  $\psi \propto r \Rightarrow \boxed{n=2}$  ; since  $\psi \propto e^{-r/a_0} \Rightarrow \boxed{z=2}$

No  $\phi$  angular dependence  $\Rightarrow \boxed{l=1, m=0}$

(b) Most probable  $r$ :

$$P(r) = r^2 R^2(r) = Cr^4 e^{-2r/a_0}$$

$$P'(r) = 0 \Rightarrow 4r^3 - \frac{2r^4}{a_0} = 0 \Rightarrow \boxed{r_m = 2a_0}$$

(c) Average of  $1/r$ :

$$\left\langle \frac{1}{r} \right\rangle = \int dr P(r) \frac{1}{r} = \frac{\int_0^\infty dr r^3 e^{-2r/a_0}}{\int_0^\infty dr r^4 e^{-2r/a_0}}$$

Use  $\int_0^\infty dr r^s e^{-\lambda r} = \frac{s!}{\lambda^{s+1}} \Rightarrow \int_0^\infty dr r^3 e^{-2r/a_0} = \frac{3!}{\left(\frac{2}{a_0}\right)^4} = \frac{6}{2^4} a_0^4$

$$\int_0^\infty dr r^4 e^{-2r/a_0} = \frac{4!}{\left(\frac{2}{a_0}\right)^5} = \frac{24}{2^5} a_0^5 \Rightarrow \left\langle \frac{1}{r} \right\rangle = \frac{6 \cdot 2^4 \cdot a_0^4}{2^4 \cdot 24 \cdot a_0^5} = \frac{1}{2a_0}$$

$$\Rightarrow \boxed{\left\langle \frac{1}{r} \right\rangle = \frac{1}{2a_0} = \frac{1}{r_m}}$$

(d) In Bohr atom,  $r_n^{\text{Bohr}} = \frac{a_0}{z} n^2 = \frac{a_0 \cdot 2^2}{2} = 2a_0$  for  $z=2, n=2$

hence  $\boxed{r_m = r_2^{\text{Bohr}}, \left\langle \frac{1}{r} \right\rangle = \frac{1}{r_2^{\text{Bohr}}}}$

## Problem 6

The electron energy is

$$E_p = \frac{\hbar^2 \pi^2}{2m_e \cdot 1\text{\AA}^2} = 3.81 \pi^2 \text{ eV} = 37.6 \text{ eV}$$

Tunneling probability:

$$T \approx e^{-2 \sqrt{\frac{2m}{\hbar^2} (V-E)} \Delta x} = e^{-2 \sqrt{\frac{1}{3.81} (90 - 37.6)} \cdot 6}$$
$$= e^{-44.50} = 4.71 \times 10^{-20}$$

Velocity of electron in well is given by

$$v = \frac{p}{m_e}, \quad p = \hbar \pi \Rightarrow \frac{v}{c} = \frac{\hbar \pi}{m_e c} = \frac{\hbar c \pi}{m_e c^2} \Rightarrow$$

$$\Rightarrow \frac{v}{c} = 0.0121 \Rightarrow v = 0.0121 \times 3 \times 10^8 \frac{\text{\AA}}{\text{s}} = 3.64 \times 10^{16} \frac{\text{\AA}}{\text{s}}$$

the probability per second that the particle will escape: since it travels  $2 \times 1\text{\AA} = 2\text{\AA}$  each time it bounces against the barriers, per second it hits the barrier  $1.82 \times 10^{16}$  times  $\Rightarrow$  since  $T =$  escape prob,

$$\text{prob escape per second} = \frac{1}{\tau} = \frac{1.82 \times 10^{16}}{\text{s}} \times T = \frac{8.57 \times 10^{-4}}{\text{s}}$$

$$\Rightarrow \tau = 1,167 \text{ s} = 19.5 \text{ minutes}$$

# Problem 7

$n=3, l=1$ . Can make transitions to  $n=2, l=0$  or  $n=1, l=0$ .

Or, first to  $n=2$ , then  $n=2 \rightarrow n=1$ .

$$E_n = -\frac{E_0}{n^2}, \quad E_0 = 13.6 \text{ eV}$$

$$\Delta E_{31} = E_3 - E_1 = E_0 \left(1 - \frac{1}{9}\right) = \frac{8}{9} E_0 = 12.0889 \text{ eV} = \frac{hc}{\lambda_{31}}$$

$$\Delta E_{32} = E_3 - E_2 = E_0 \left(\frac{1}{4} - \frac{1}{9}\right) = \frac{5}{36} E_0 = 1.8889 \text{ eV} = \frac{hc}{\lambda_{32}}$$

with  $hc = 12,400 \text{ eV}\text{\AA}$

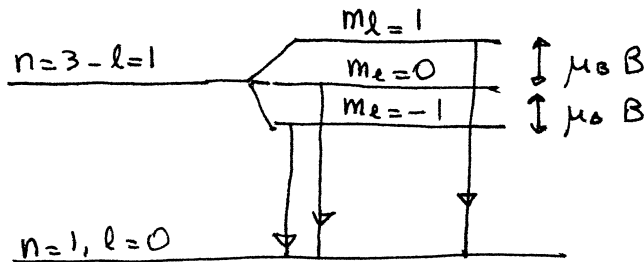
$$\Delta E_{21} = E_2 - E_1 = E_0 \left(1 - \frac{1}{4}\right) = \frac{3}{4} E_0 = 10.2 \text{ eV} = \frac{hc}{\lambda_{21}}$$

$$\Rightarrow \lambda_{31} = 1025.73 \text{ \AA} \quad ; \quad \lambda_{32} = 6564.67 \text{ \AA} \quad ; \quad \lambda_{21} = 1215.69 \text{ \AA}$$

(b) With magnetic field,  $\Delta E = -\vec{\mu} \cdot \vec{B} = -\mu_z B$  for  $B$  in the  $z$  direction

$$\mu_z = -\frac{e}{2m_e} L_z = -\frac{e\hbar}{2m_e} m_l = -\mu_B m_l \Rightarrow \Delta E(m_l) = \mu_B \cdot B \cdot m_l$$

So energies of  $n=3, l=1$  states are split



$$\mu_B B = 5.79 \times 10^{-3} \text{ eV}$$

$$\begin{aligned} \Delta E_{31}(m_l=1) &= 12.0889 \text{ eV} + 5.79 \times 10^{-3} \text{ eV} = 12.0947 \text{ eV}, & \lambda_{31}(m_l=1) &= 1025.24 \text{ \AA} \\ \Delta E_{31}(m_l=0) &= \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} & \lambda_{31}(m_l=0) &= 1025.73 \text{ \AA} \\ \Delta E_{31}(m_l=-1) &= \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} & \lambda_{31}(m_l=-1) &= 1026.23 \text{ \AA} \end{aligned}$$

## Problem 7 (cont.)

Spin-orbit coupling: the internal magnetic field  $B_{eff}$  couples to the spin magnetic moment, giving rise to energy shift

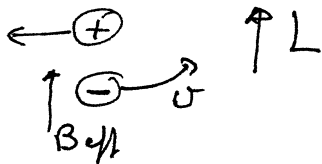
$$\Delta E_{spin} = -\vec{\mu}_s \cdot \vec{B}_{eff}$$

$$\mu_s = -m_s g_s \mu_B = \begin{cases} -\mu_B & \text{for } m_s = +1/2 \\ +\mu_B & \text{for } m_s = -1/2 \end{cases} \quad (g_s = 2)$$

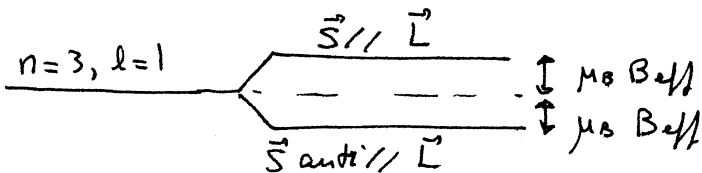
$$\Rightarrow \Delta E = +\mu_B B_{eff} \quad \text{for } m_s = +1/2$$

$$\Delta E = -\mu_B B_{eff} \quad \text{for } m_s = -1/2$$

$B_{eff}$  is parallel to orbital angular momentum



So energy level  $n=3, l=1$  splits:



$\vec{J} = \vec{L} + \vec{S} = \text{total angular momentum.}$

$$\text{For } \vec{S} \parallel \vec{L}, \quad J = 3/2 \longrightarrow \Delta E_{s.o.} = +\mu_B B_{eff} = +2.895 \times 10^{-6} \text{ eV}$$

$$\text{For } \vec{S} \nparallel \vec{L}, \quad J = 1/2 \longrightarrow \Delta E_{s.o.} = -\mu_B B_{eff} = -2.895 \times 10^{-6} \text{ eV}$$

$J = 3/2$  gives higher energy than  $J = 1/2$ .



# Problem 8

$\Psi(x, y)$  is wavefunction. Assume  $\Psi(x, y) = \Psi_1(x) \Psi_2(y)$

$$-\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \Psi_1(x) \Psi_2(y) +$$

$$+ \frac{1}{2} K(x^2 + y^2) \Psi_1(x) \Psi_2(y) = E \Psi_1(x) \Psi_2(y) \Rightarrow$$

$$\Rightarrow \underbrace{-\frac{\hbar^2}{2m} \Psi_2(y) \frac{\partial^2 \Psi_1(x)}{\partial x^2} + \frac{1}{2} K x^2 \Psi_2(y)}_{\text{depends on } x} + \underbrace{-\frac{\hbar^2}{2m \Psi_1(x)} \frac{\partial^2 \Psi_2(y)}{\partial y^2} + \frac{1}{2} K y^2 \Psi_1(x)}_{\text{depends on } y} = E$$

$= \text{constant} = C_1$ 
 $= \text{constant} = C_2$

$E = C_1 + C_2$ ,  $C_1$  and  $C_2$  are energies for 1 dim harmonic oscillator.

(b) Ground state wave function:

$$\Psi_0(x, y) = \Psi_{10}(x) \Psi_{20}(y) = C e^{-\frac{m\omega}{2\hbar}(x^2 + y^2)}$$

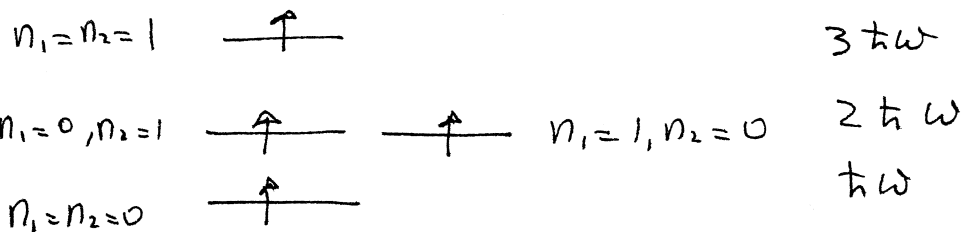
(c) For 1d oscillator,  $E_n = \hbar\omega(n + \frac{1}{2})$ , for  $n \geq 0$ ,

$$E_{n_1, n_2} = \hbar\omega(n_1 + \frac{1}{2}) + \hbar\omega(n_2 + \frac{1}{2}) = \hbar\omega(n_1 + n_2 + 1)$$

First excited state is  $n_1 = 0, n_2 = 1$  or  $n_1 = 1, n_2 = 0$

$$\Rightarrow E = \hbar\omega(1 + 1) = 2\hbar\omega, \text{ degeneracy} = 2.$$

(d) For 4 fermions



$$\text{Total energy} = \hbar\omega + 4\hbar\omega + 3\hbar\omega = \boxed{8\hbar\omega}$$