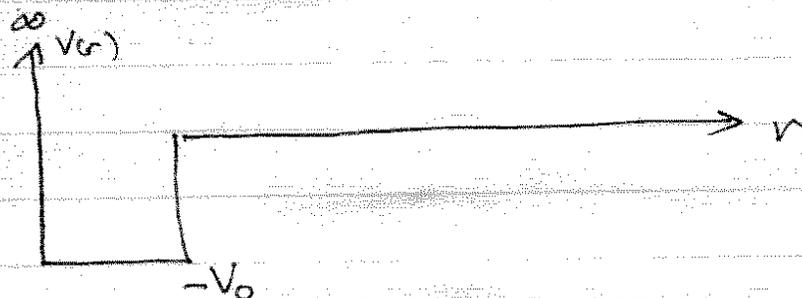


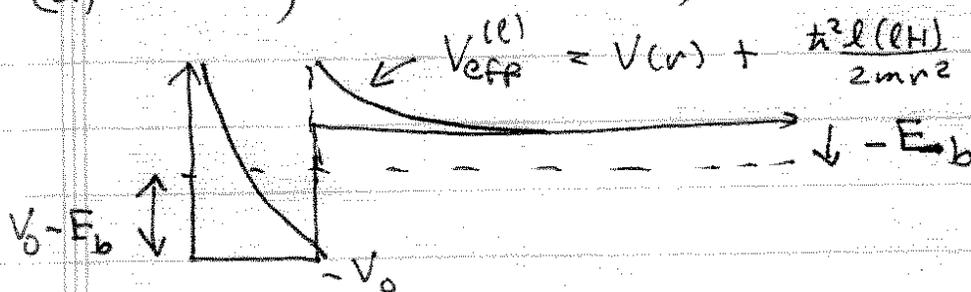
Physics 522: Problem Set #5 Solutions

Problem 1: The Finite Spherical Well

$$V(r) = \begin{cases} -V_0 & 0 < r < a \\ 0 & r > a \end{cases}$$



(a)  $E < 0$ , Bound state, let  $E = -E_b$



In each region we have a constant potential where the solution is generally

$$R_l(r) = A j_l(kr) + B n_l(kr)$$

or

$$= C h_l^{(1)}(kr) + D h_l^{(2)}(kr)$$

where  $k = \sqrt{\frac{2m}{\hbar^2} (E - V(r))}$   
 constant in the region

The coefficients  $A, B$  or  $C, D$  are set by the boundary conditions and normalization.

• For  $0 < r < a$ , we must have  $R_l(r=0)$  finite

$$\Rightarrow R_l^{(I)}(r) = A j_l(qr) \quad (B = 0)$$

$$\text{where } q = \sqrt{\frac{2m}{\hbar^2}(-E - V_0)} = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

• For  $a < r < \infty$  we must have  $\lim_{r \rightarrow \infty} R_l \rightarrow 0$

$$\text{Now } h_l^{(2)}(kr) = j_l(kr) \pm i n_l(kr) \propto e^{\pm ikr}$$

$$\text{In region II } k = \sqrt{\frac{2mE}{\hbar^2}} = \sqrt{\frac{-2mE_0}{\hbar^2}} = iK$$

(classically forbidden) Pure imaginary

$$\Rightarrow R_l^{(II)}(r) = C h_l^{(1)}(iKr) \quad \text{where } K = \sqrt{\frac{2mE_0}{\hbar^2}}$$

Finally using continuity of the wave function

$$R_l^{(I)}(a) = R_l^{(II)}(a) \Rightarrow C h_l^{(1)}(ika) = A j_l(qa)$$

$$\Rightarrow C = A j_l(qa) / h_l^{(1)}(ika)$$

$$\Rightarrow R_l(r) = \begin{cases} A j_l(qr) & 0 < r < a \\ \frac{A j_l(qa)}{h_l^{(1)}(ika)} h_l^{(1)}(iKr) & a < r < \infty \end{cases}$$

A. determined by normalization

(b) We now have two unknowns:  $A$  and  $E_b$

- $A$  is set by normalization
- $E_b$  is set by the remaining b.c.

$$\frac{d u_e^{(I)}(a)}{dr} = \frac{d u_e^{(II)}(a)}{dr}$$

where  $u_e(r) = r R_e(r)$  is the reduced radial wave function

$$\Rightarrow A \frac{d}{dr} (r j_l(qr)) \Big|_a = A \frac{j_l(qa)}{h_l^{(1)}(ika)} \frac{d}{dr} (r h_l^{(1)}(ikr)) \Big|_a$$

$$\Rightarrow \boxed{\frac{d}{dr} (r j_l(qr)) \Big|_a = \frac{d}{dr} (r h_l^{(1)}(ikr)) \Big|_a \frac{j_l(qa)}{h_l^{(1)}(ika)}}$$

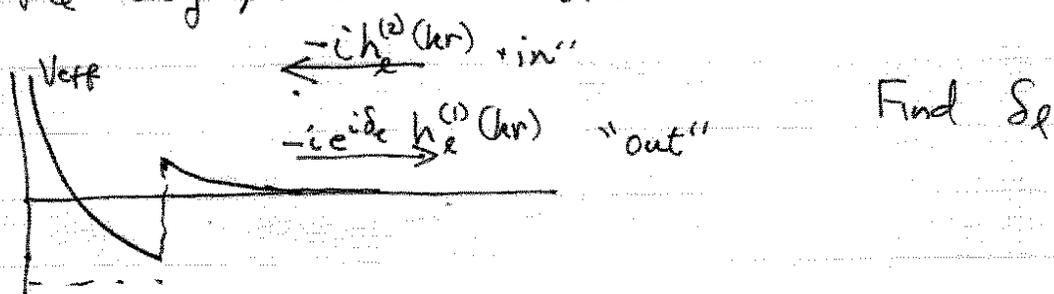
Check: for  $l=0$ ,  $V_{\text{eff}}^{(l=0)} = V(r)$ .

$$\text{Recall } j_0(qr) = \frac{\sin qr}{qr} \quad h_0^{(1)}(ikr) = -\frac{e^{-kr}}{kr}$$

$$\Rightarrow \frac{d}{dr} (r j_0(qr)) \Big|_a = \frac{\cos(qa)}{a}, \quad \frac{d}{dr} (r h_0^{(1)}(ikr)) \Big|_{r=a} = \frac{e^{-ka}}{a}$$

$$\xrightarrow{l=0} \Rightarrow \frac{q \cos(qa)}{\sin(qa)} = -K \Rightarrow \boxed{K = -q \cot(qa)}$$

We now consider the unbound energy eigenstates.  
 We seek the scattering phase shift according to the asymptotic conditions



• For  $r > a$   $R_l(r) = -i (h_l^{(2)}(kr) + e^{i\delta_l} h_l^{(1)}(kr))$

Note  $h_l^{(2)}(kr) = j_l(kr) \pm i n_l(kr)$

$\Rightarrow r > a$   $R_l(r) = -i(1 + e^{i\delta_l}) j_l(kr) + (-1 + e^{i\delta_l}) n_l(kr)$

$$R_l(r) = -2i e^{i\delta_l/2} \left[ \cos \frac{\delta_l}{2} j_l(kr) - \sin \frac{\delta_l}{2} n_l(kr) \right]$$

• For  $0 < r < a$   $R_l(r) = A j_l(kr)$  (to remain regular at origin)

Logarithmic derivative:

$$\left( \frac{1}{R_l} \frac{dR_l}{dr} \right) \Big|_{r=a}^{\text{I}} = \left( \frac{1}{R_l} \frac{dR_l}{dr} \right) \Big|_{r=a}^{\text{II}}$$

$$\Rightarrow \frac{j_l(ka)}{j_l' \frac{dj_l}{dr} \Big|_{ka}} = \frac{\cos \frac{\delta_l}{2} j_l(ka) - \sin \frac{\delta_l}{2} n_l(ka)}{k \left[ \cos \frac{\delta_l}{2} \frac{dj_l}{dr} \Big|_{ka} - \sin \frac{\delta_l}{2} \frac{dn_l}{dr} \Big|_{ka} \right]}$$

Alternatively we can use the reduced equation

$$\left. \frac{r j_l(qr)}{\frac{d}{dr}(r j_l(qr))} \right|_{r=a} = \left. \frac{(r \cos \frac{\delta_l}{2} j_l(kr) - r \sin \frac{\delta_l}{2} n_l(kr))}{\frac{d}{dr} [r \cos \frac{\delta_l}{2} j_l(kr) - r \sin \frac{\delta_l}{2} n_l(kr)]} \right|_{r=a}$$

Now check:  $l=0$   $r j_0(qr) = \frac{1}{q} \sin(qr)$

$$r n_0(qr) = -\frac{1}{q} \cos qr$$

$$\Rightarrow \frac{\sin qa}{q \cos(qa)} = \frac{\cos \frac{\delta_0}{2} \sin(ka) + \sin \frac{\delta_0}{2} \cos(ka)}{k(\cos \frac{\delta_0}{2} \cos(ka) - \frac{\sin \delta_0}{2} \cos(ka))}$$

$$\Rightarrow \frac{1}{q} \tan(qa) = \frac{\sin(ka + \frac{\delta_0}{2})}{k \cos(ka + \frac{\delta_0}{2})} = \frac{1}{k} \tan(ka + \frac{\delta_0}{2})$$

$$\Rightarrow \boxed{\frac{\delta_0}{2} = \tan^{-1}\left(\frac{k}{q} \tan(qa)\right) - ka}$$

## Problem 2: The 3D Isotropic SHO

The Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(\vec{r})$$

$$\hat{V}(\vec{r}) = \frac{1}{2} m \omega^2 (x^2 + y^2 + z^2) \\ = \frac{1}{2} m \omega^2 r^2$$

(a) This problem is separable in Cartesian coordinates. The energy eigenkets are

$$|n_x, n_y, n_z\rangle = |n_x\rangle \otimes |n_y\rangle \otimes |n_z\rangle \quad \begin{matrix} \text{(Product of three)} \\ \text{1D oscillators} \end{matrix}$$

With energy eigenvalues  $E_n = \hbar \omega (n + 3/2)$  where  $n = n_x + n_y + n_z$

The degeneracy of the states with energy  $E_n$  is as follows

We showed in class that the degeneracy of a 2D isotropic SHO with eigenvalues  $E = \hbar \omega (n_x + n_y + 1)$  is  $n_x + n_y + 1$

If we fix  $n_z$  then  $n_x + n_y = n - n_z \Rightarrow$  Degeneracy  $n - n_z + 1$

Thus, as we allow  $n_z$  to range over all possible values for a given  $n$  (i.e.  $0 \leq n_z \leq n$ ), the total degeneracy is

$$g_n^{3D} = \sum_{n_z=0}^n g_{n-n_z}^{2D} = \sum_{n_z=0}^n (n+1-n_z) = (n+1)^2 - \sum_{n_z=0}^n n_z$$

$$\left( \text{Aside: } \sum_{i=0}^N i = \frac{N(N+1)}{2} \right)$$

$$\Rightarrow \text{Degeneracy } g_n^{3D} = (n+1)^2 - \frac{n(n+1)}{2} = (n+1) \left( n+1 - \frac{n}{2} \right)$$

$$\Rightarrow \boxed{g_n^{3D} = \frac{(n+1)(n+2)}{2}}$$

The first few degenerate energy levels with cartesian quantum numbers are shown below

$n=2$ ( $g_2=6$ )	$12,0,0$	$10,2,0$	$10,0,2$	$11,1,0$	$11,0,1$	$10,1,1$
$n=1$ ( $g_1=3$ )	$11,0,0$	$10,1,0$	$10,0,1$			
$n=0$ ( $g_0=1$ )	$10,0,0$					

• these states are denoted by  $|n_x, n_y, n_z\rangle$

(b) Because of the rotational symmetry we can seek eigenstates of the complete set of commuting operators

$$\{H, L^2, L_z\}$$

Separating in spherical coordinates with the eigenfunction written the usual way:

$$\psi_{n_r, l, m}(r, \theta, \phi) = R_{n_r, l}(r) Y_{l, m}(\theta, \phi)$$

where  $R_{n_r, l}(r) = \frac{u_{n_r, l}(r)}{r}$  ← Reduced radial wavefunction

The radial equation for  $u_{n_r, l}(r)$  is

$$\left( -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + \frac{1}{2} m \omega^2 r^2 \right) u_{n_r, l}(r) = E_{n_r, l} u_{n_r, l}(r)$$

Defining the usual dimensionless variables  $\bar{r} \equiv \frac{r}{r_c}$ ,  $\epsilon \equiv \frac{E}{\hbar \omega}$  where the characteristic radius is  $r_c = \sqrt{\frac{\hbar}{m\omega}}$

$$\Rightarrow \left( -\frac{1}{2} \frac{d^2}{d\bar{r}^2} + \frac{l(l+1)}{2\bar{r}^2} + \frac{1}{2} \bar{r}^2 \right) u(\bar{r}) = \epsilon u(\bar{r})$$

Since  $\hat{V}(r)$  does not blow up at the origin, the centrifugal barrier dominates there and we expect the asymptotic form:

$$u(r) \sim r^{l+1} \quad \text{as } r \rightarrow 0$$

For  $r \rightarrow \infty$ , the potential blows up and dominates over the centrifugal barrier and the E.U. term

$$\Rightarrow \text{As } r \rightarrow \infty \quad \frac{d^2}{dr^2} u - r^2 u = 0$$

We can solve this diff'eqn by making the substitution  $y = r^2 \Rightarrow \frac{du}{dr} = \frac{dy}{dr} \frac{du}{dy} = 2r \frac{du}{dy}$

$$\Rightarrow \frac{d^2 u}{dr^2} = 2 \frac{du}{dy} + 4y \frac{d^2 u}{dy^2} = y u(y) \Rightarrow \frac{d^2 u}{dy^2} = \frac{-1}{2y} \frac{du}{dy} + \frac{1}{4} u(y)$$

We can neglect the second term in asymptote  $y \rightarrow \infty$

$$\Rightarrow \frac{d^2 u}{dy^2} - \frac{1}{4} u(y) = 0 \Rightarrow u(y) = A e^{-y/2} + B e^{+y/2}$$

$$\Rightarrow \text{As } r \rightarrow \infty \quad u(r) \sim e^{-r^2/2}$$

neglect since it diverges at  $\infty$

$\Rightarrow$  We expect the reduced radial wavefunction to have the form

$$u_{n,l}(r) = r^{l+1} e^{-r^2/2} F_{n,l}(r)$$

where  $F_{n,l}(r)$  is constant near the origin

and does not blow up faster than  $e^{r^2}$

c) Substitute the Ansatz into the radial equation

$$\left( \frac{d^2}{d\bar{r}^2} - \frac{l(l+1)}{\bar{r}^2} - \bar{r}^2 + 2\varepsilon \right) u_l(\bar{r}) = 0$$

$$u_l(r) = g(r) F_l(r) \quad \text{where} \quad g(r) = \bar{r}^{l+1} e^{-\frac{\bar{r}^2}{2}}$$

$$\frac{d^2}{d\bar{r}^2} u_l(\bar{r}) = \frac{d^2 g}{d\bar{r}^2} F_l + g \frac{d^2 F_l}{d\bar{r}^2} + 2 \frac{dg}{d\bar{r}} \frac{dF_l}{d\bar{r}}$$

After some algebra,

$$\frac{d^2}{d\bar{r}^2} u_l(\bar{r}) = \left\{ \left( \frac{l(l+1)}{\bar{r}^2} - (2l+3) + \bar{r}^2 \right) F_l(\bar{r}) + \left( \frac{2l+2}{\bar{r}} - 2\bar{r} \right) F_l'(\bar{r}) + F_l''(\bar{r}) \right\} \bar{r}^{l+1} e^{-\frac{\bar{r}^2}{2}}$$

$$\Rightarrow \frac{d^2 F_l}{d\bar{r}^2} + 2 \left( \frac{l+1}{\bar{r}} - \bar{r} \right) \frac{dF_l}{d\bar{r}} - (3+2l-2\varepsilon) F_l(\bar{r}) = 0$$

We can put this in the form of the Laguerre equation through a change of variables

$$\text{Let } x = \bar{r}^2. \quad \text{Define } F(\bar{r}) = G(x) \quad \Rightarrow \quad \frac{dF(\bar{r})}{d\bar{r}} = 2\bar{r} \frac{dG}{dx}, \quad \frac{d^2 F}{d\bar{r}^2} = 2 \frac{dG}{dx} + 4\bar{r}^2 \frac{d^2 G}{dx^2}$$

$$\left( 2 \frac{dG}{dx} + 4\bar{r}^2 \frac{d^2 G}{dx^2} \right) + 2 \left[ \frac{l+1}{\bar{r}} - \bar{r} \right] \left( 2\bar{r} \frac{dG}{dx} \right) = (3+2l-2\varepsilon) G(x)$$

$$\Rightarrow 4x \frac{d^2 G}{dx^2} + 4 \left[ l + \frac{3}{2} - x \right] \frac{dG}{dx} = (3+2l-2\varepsilon) G(x)$$

$$\Rightarrow \boxed{x \frac{d^2 G}{dx^2} + \left[ 1 + l + \frac{1}{2} - x \right] \frac{dG}{dx} = \frac{1}{2} \left( \frac{3}{2} + l - \varepsilon \right) G(x)}$$

This is the Laguerre equation  $x \frac{d^2 L_n^q}{dx^2} + [1 + q - x] \frac{dL_n^q}{dx} = -n L_n^q(x)$

where  $n_r = 0, 1, 2, \dots$  determines the order of the polynomial  $\Rightarrow F_{n_r, l}(\bar{r}) = L_{n_r}^{l+\frac{1}{2}}(\bar{r}^2)$

$$\Rightarrow n_r = \frac{1}{2} \left( \frac{3}{2} + l - 2\varepsilon \right) \Rightarrow \varepsilon = 2n_r + l + \frac{3}{2}$$

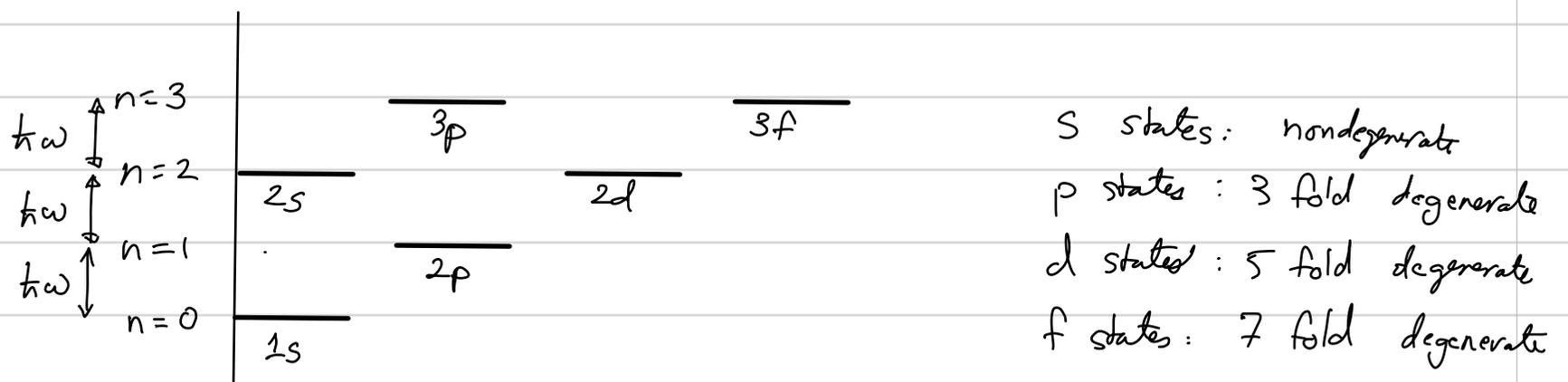
$$\Rightarrow \boxed{E = \hbar \omega \left( 2n_r + l + \frac{3}{2} \right) = \hbar \omega \left( n + \frac{3}{2} \right) \quad \text{where } n = 2n_r + l}$$

$$\boxed{R_{n_r, l}(\bar{r}) = \bar{r}^l e^{-\frac{\bar{r}^2}{2}} L_{n_r}^{l+\frac{1}{2}}(\bar{r}^2)}$$

The energy levels are specified by three quantum numbers,  $n, l, m_l$ ; the energy eigenvalues depend only on  $n$ . The radial quantum number  $n_r = \frac{n-l}{2}$ . Since  $n_r$  is an integer, and  $n_r \geq 0$ , given a value of  $n$ ,  $l$  ranges over

if  $n$  even:  $l = 0, 2, \dots, n$  in steps of 2  
 if  $n$  odd:  $l = 1, 3, \dots, n$  " " " "

We thus have the following energy-level diagram



Note, the states with given  $l$  have parity  $(-1)^l$ . Thus the  $n$  even states are even parity and  $n$  odd are odd parity, as expected.

For each  $l$  there are  $2l+1$  degenerate sublevels. We can thus find the degeneracy  $g_n$

$$n \text{ even} \Rightarrow g_n = \sum_{l=0,2,4}^n (2l+1) = \sum_{k=0}^{n/2} (4k+1) = \left(\frac{n}{2}+1\right) + 4 \sum_{k=0}^{n/2} k$$

$$= \frac{n+2}{2} + 4 \left[ \frac{\frac{n}{2}(\frac{n}{2}+1)}{2} \right] = \frac{n+2 + n(n+2)}{2} = \frac{(n+1)(n+2)}{2}$$

$$n \text{ odd} \Rightarrow g_n = \sum_{l=1,3,5,\dots}^{n-1} (2l+1) = \sum_{k=0}^{\frac{n-1}{2}} (4k+3) = \frac{(n+1)(n+2)}{2}$$



Energy  $E_c = \frac{q_1 q_2}{a_c} = \left( \frac{\mu z_1^2 z_2^2}{m_e} \right) \left( \frac{m_e c^4}{\hbar^2} \right) = \left( \frac{\mu z_1^2 z_2^2}{m_e} \right) 27.2 \text{ eV}$

Time:  $t_c = \frac{\hbar}{E_c} = \left( \frac{m_e}{\mu z_1^2 z_2^2} \right) \frac{\hbar}{E_0} = \left( \frac{m_e}{\mu z_1^2 z_2^2} \right) 2.09 \times 10^{-17} \text{ s}$

$\sim 10$  attoseconds

Internal Electric field @ particle 1  $E_c = \frac{q_2}{a_c^2} = \left( \frac{\mu z_1 z_2}{m_e} \right)^2 \frac{z_2 e}{a_0^2} \approx \left( \frac{\mu z_1^2 z_2^3}{m_e^2} \right) 5 \times 10^9 \frac{\text{V}}{\text{cm}}$

Electric dipole moment  $d_c = \left( \frac{q_1 - q_2}{2} \right) a_c = \left( \frac{z_1 + z_2}{2} \right) \left( \frac{m_e}{\mu} \right) \left( \frac{1}{z_1 z_2} \right) e a_0$

Aside  $e a_0 = 8.5 \times 10^{-30} \text{ C-m} = 2.54 \text{ Debye}$   
 $1 \text{ debye} = 10^{-18} \text{ esu} \cdot \text{\AA}$

Speed (ratio of c)  $\frac{v_c}{c} = \frac{a_c}{c t_c} = \frac{q_c}{c \frac{\hbar}{E_c}} = \frac{q_1 q_2}{\hbar c} = \left( \frac{z_1 z_2}{2} \right) \frac{e^2}{\hbar c}$

$= (z_1 z_2) \alpha$  fine structure constant

Internal B-field @ particle 1  $B_c = \frac{v_c}{c} E_c = (z_1 z_2) (\alpha E_c) = \left( \frac{\mu^2 z_1^3 z_2^4}{m_e^2} \right) \left[ \frac{e}{a_0^2} \alpha \right]$

$\sim 10^5 \text{ Gauss}$

Magnetic dipole moment  $\mu_c = \text{Current} \times \text{Area} = \frac{q_1 q_2}{t_c c} a_c^2$

$2 \times \mu_B = \text{Bohr magneton}$

$$\Rightarrow \mu_c = \left( \frac{a_c}{t_c c} \right) (q_1 a_c) = \alpha d_c = \left( \frac{Z_1 + Z_2}{2} \right) \left( \frac{m_e}{\mu} \right) \left( \frac{e \hbar}{m c} \right)$$

Now for each case given:

(i) Hydrogen defines "atomic units":

-  $a_c = a_0 = 0.53 \text{ \AA}$  Bohr radius

-  $E_c = E_0 = 27.2 \text{ eV}$  Hartree

-  $t_c = 2.4 \times 10^{-17} \text{ s}$

-  $E_c = 5 \times 10^9 \frac{\text{V}}{\text{cm}} = 1.7 \times 10^7 \frac{\text{statV}}{\text{cm}}$

-  $B_c = \alpha E_c = 1.2 \times 10^5 \text{ Gauss}$  (Not standard atomic unit)

-  $d_c = 2.5 \times 10^{-18} \text{ cgs} = 2.5 \text{ debye}$

-  $\mu_c = 2\mu_B = \alpha d_c = 1.8 \text{ ergs/Gauss} = 1.8 \times 10^{-24} \frac{\text{Joule}}{\text{Tesla}}$

(ii) Heavy ion:  $Z_1 = 1, Z_2 = 50, \mu \approx m_e$

(iii) Muonium:  $m_1 \approx 200 m_e, m_2 = m_p \approx 2000 m_p, \mu \approx 180 m_e$

(iv) Positronium:  $Z_1 = Z_2 = 1, m_1 = m_2 = m_e, \mu = \frac{m_e}{2}$

Summary table: Characteristic Units in a.u.

	$a_c$	$E_c$	$t_c$	$p_c$	$v_c/c$	$E_c$	$B_c$	$d_c$	$m_c$
Hydrogen	1	1	1	1	1	1	1	1	1
$\text{Sn}^{+49}$	$\frac{1}{50}$	2500	$\frac{1}{2500}$	50	50	$6.25 \times 10^6$	$6.25 \times 10^6$	$\frac{1}{2}$	25
Muonium	$\frac{1}{180}$	180	$\frac{1}{180}$	180	1	32400	32400	$\frac{1}{180}$	$\frac{1}{180}$
Positronium	2	$\frac{1}{2}$	2	$\frac{1}{2}$	1	$\frac{1}{4}$	$\frac{1}{4}$	2	2

From these results we see that

- for heavy elements the electron can be highly relativistic and magnetic effects grow
- Muonium sees huge field because the muon is so close to the nucleus.

Other useful relations

Given constants  $e, m_e, \hbar, c$  we have additional series

• rest energy:  $E_{\text{rest}} = m_e c^2$

$$\Rightarrow \frac{E_0}{m_e c^2} = \frac{m_e \hbar^4}{\hbar^2 m_e c^2} = \frac{e^4}{(\hbar c)^2} = \alpha^2$$

$$\Rightarrow E_0 = \alpha^2 m_e c^2$$

• Compton wavelength:  $\lambda_c = \frac{\hbar}{m_e c} = \alpha a_0$

• Classical electron radius:  $r_{\text{class}} = \frac{m_e c^2}{e^2} = \frac{\lambda_c}{\alpha}$