

Physics 521: Problem Set #1 Solutions

Problem 1: Hydrogenic atoms in atomic units

Two oppositely charged particles:

- Charge 1 (negative) $q_1 = -Z_1 e$, mass m_1

- Charge 2 (positive) $q_2 = Z_2 e$, mass m_2

Coulomb interaction: $V(r) = \frac{q_1 q_2}{r} = -Z_1 Z_2 \frac{e^2}{r}$

Relative motion Hamiltonian: $\hat{H} = \frac{p^2}{2\mu} + V(r)$

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \quad (\text{reduced mass})$$

Characteristic Units: scales determined by μ, q_1, q_2, \hbar

Length: a_c , Momentum: $p_c = \frac{\hbar}{a_c}$, Energy: E_c

Relate: $E_c = \frac{p_c^2}{\mu} = \frac{q_1 q_2}{a_c} = \frac{\hbar^2}{a_c^2 \mu}$

\uparrow kinetic energy \uparrow Coulomb energy

Length: $a_c = \frac{\hbar^2}{\mu q_1 q_2} = \frac{m_e}{\mu Z_1 Z_2} \left(\frac{\hbar^2}{m_e e^2} \right) = \frac{m_e}{\mu Z_1 Z_2} (0.53 \text{ \AA})$

Momentum: $p_c = \frac{\hbar}{a_c} = \left(\frac{\mu Z_1 Z_2}{m_e} \right) \frac{\hbar}{0.53 \text{ \AA}} = \frac{\mu Z_1 Z_2}{m_e} 2.10 \frac{\hbar}{\text{\AA}}$

Problem 3: Finite nuclear size effect

(a) In the standard Hamiltonian for atoms the nucleus is treated as a point charge. A more detailed model treats it as a uniformly charged sphere, radius R , so that the charge density

$$\rho(r) = \begin{cases} \left(\frac{3}{4\pi R^3}\right) Ze & r < R \\ 0 & r > R \end{cases}$$

Then by Gauss's law, the electric field created by this charge density is $\oint \mathbf{E} \cdot d\mathbf{a} = 4\pi Q_{enc}(r)$

$$\mathbf{E}(r) = \frac{Q_{enc}(r)}{r^2} = \begin{cases} \frac{r}{R^3} Ze & r < R \\ \frac{Ze}{r^2} & r > R \end{cases}$$

The electrostatic potential, with ground @ ∞

$$\Phi(r) = -\int_{\infty}^r E(r) dr = -\frac{Ze}{r} \quad r > R$$

$$= -\int_R^r \frac{rZe}{R^3} dr + \frac{Ze}{R} \quad r < R$$

$$= -\frac{1}{2} \frac{r^2 Ze}{R^3} + \frac{3Ze}{2R} \quad r < R$$

Potential energy

$$V(r) = -e\Phi(r) = \begin{cases} -\frac{3Ze}{2R} \left(1 - \frac{r^2}{3R^2}\right) & r < R \\ -\frac{Ze^2}{r} & r > R \end{cases}$$

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

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

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

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

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_e/c	E_e	B_c	d_c	m_c
Hydrogen	1	1	1	1	1	1	1	1	1
Sr^{+49}	$\frac{1}{50}$	2500	$\frac{1}{2500}$	50	50	2500	625×10^6	$\frac{1}{2}$	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.

Using appendix eq (A3.2d)

$$\int_0^{\infty} e^{-t} t^{\alpha} U_p(p,s) U_p(p,t) = \underset{\text{integer}}{\alpha!} \frac{(1-s)^{\alpha+1}}{(1-s)^{p+1}} \frac{(1-t)^{\alpha+1}}{(1-t)^{p+1}} \frac{(st)^p}{(1-st)^{\alpha+1}}$$

Using binomial

$$= \frac{(1-s)^{\alpha+1}}{(1-s)^{p+1}} \frac{(1-t)^{\alpha+1}}{(1-t)^{p+1}} \sum_{k=0}^{\infty} \frac{(\alpha+k)!}{k!} (st)^{k+p}$$

Plug in $\alpha = p+2$

$$\rightarrow = (1-s)^2 (1-t)^2 \sum_{k=0}^{\infty} \frac{(p+2+k)!}{k!} (st)^{k+p}$$

$$= (1+s^2-2s)(1+t^2-2t) \sum_{q=p}^{\infty} \frac{(q+2)!}{(q-p)!} (st)^q$$

$$= \sum_{q=p}^{\infty} \sum_{q'=p}^{\infty} \frac{I_{pq, pq'}^{\alpha=p+2}}{q! q'!} s^q t^{q'}$$

Equating the coefficients where $q = q'$

$$\Rightarrow I_{pq, pq}^{\alpha=p+2} = (q!)^2 \left[\frac{(q+2)!}{(q-p)!} + \frac{4(q+1)!}{(q-p-1)!} + \frac{q!}{(q-2-p)!} \right]$$

$$= \frac{(q!)^3}{(q-p)!} \left[(q+2)(q+1) + 4(q+1)(q-p) + (q-p)(q-p) \right]$$

Now, according to the appendix 3 A3.25
with $p=2l+1$, $q=n+l \Rightarrow N_{ne} = \frac{(q-p)!}{(q!)^3 (2q-p+1)}$

Putting it all together

$$\langle r \rangle_{nl} = \frac{n a_0}{2z} \left[\frac{(q+2)(q+1) + 4(q+1)(q-p) + (q-p)(q-p-1)}{2q-p+1} \right]$$

Plug in $p=2l+1$ $q=n+l$

$$\Rightarrow \langle r \rangle_{nl} = \frac{n a_0}{2z} \left[3n - \frac{l(l+1)}{n} \right]$$

$$\boxed{\langle r \rangle_{nl} = \frac{n^2 a_0}{z} \left[1 + \frac{1}{2} \left(1 - \frac{l(l+1)}{n^2} \right) \right]}$$

phew! What a mess

(b) For circular states \Rightarrow max angular momentum
(no radial kinetic energy) $\Rightarrow l=n-1$

$$\Rightarrow \langle r \rangle_{nl} = \frac{n^2 a_0}{z} \left[1 + \frac{1}{2} \left[1 - \frac{n(n-1)}{n^2} \right] \right] \xrightarrow{n \rightarrow \infty} 0$$

$$\Rightarrow \langle r \rangle_{nl} = n^2 \frac{a_0}{z}$$

the Bohr result.

(c) Feynman-Hellman

Consider expectation value as function of parameters

$$\langle n_r, \xi | \hat{H}(\xi) | n_r, \xi \rangle = E_{n_r}(\xi)$$

Take partial w.r.t. some ξ

$$\begin{aligned} \Rightarrow \left(\frac{\partial}{\partial \xi} \langle n_r, \xi | \right) \hat{H}(\xi) | n_r, \xi \rangle + \langle n_r, \xi | \hat{H} \left(\frac{\partial}{\partial \xi} | n_r, \xi \rangle \right) \\ + \langle n_r, \xi | \frac{\partial \hat{H}(\xi)}{\partial \xi} | n_r, \xi \rangle = \frac{\partial E_{n_r}(\xi)}{\partial \xi} \end{aligned}$$

But $\hat{H}(\xi) | n_r, \xi \rangle = E_{n_r}(\xi) | n_r, \xi \rangle$ and adjoint

$$\rightarrow \text{First two term} = E_{n_r} \frac{\partial}{\partial \xi} (\langle n_r, \xi | n_r, \xi \rangle) = 0$$

same normalization

$$\boxed{\langle n_r, \xi | \frac{\partial \hat{H}(\xi)}{\partial \xi} | n_r, \xi \rangle = \frac{\partial E_{n_r}(\xi)}{\partial \xi}}$$

(d) Now we can use the clever trick

$$\bullet \text{ Let } \xi = e^2 \Rightarrow \frac{\partial \hat{H}}{\partial e^2} = -\frac{Z}{r} \quad \frac{\partial E_{n_r}}{\partial e^2} = \frac{2}{e^2} E$$

$$\Rightarrow -Z \langle n_r, \xi | \frac{1}{r} | n_r, \xi \rangle = \frac{2}{e^2} E_{n_r}(\xi) = \frac{2}{e^2} \left(-\frac{Z^2 e^2}{2 a_0 n^2} \right)$$

$$\rightarrow \boxed{\langle \frac{1}{r} \rangle_{n\ell} = \frac{Z}{a_0 n^2}} \quad \checkmark$$

• Let $\xi = l \Rightarrow \frac{\partial \hat{H}}{\partial l} = \frac{(2l+1)\hbar^2}{2m_e r^2} \quad \frac{\partial E}{\partial l} = -\frac{2}{n} E_n$

$$\Rightarrow (l + \frac{1}{2}) \frac{\hbar^2}{m_e} \langle \frac{1}{r^2} \rangle_{nl} = -\frac{2}{n} \frac{Z^2}{-2n^2} \left(\frac{e^2}{a_0} \right)$$

$$\Rightarrow \langle \frac{1}{r^2} \rangle_{nl} = \frac{Z^2}{n^3(l + \frac{1}{2})} \frac{m_e e^2}{\hbar a_0} \quad \left[= \left(\frac{Z}{a_0} \right)^2 \frac{1}{n^3(l + \frac{1}{2})} \right]$$

• Consider $\langle [\frac{\partial}{\partial r}, \hat{H}] \rangle_{nlm} = \langle nlm | \frac{\partial \hat{H}}{\partial r} - \hat{H} \frac{\partial}{\partial r} | nlm \rangle$
 $= 0$ since $\hat{H} | nlm \rangle = E_n | nlm \rangle$
 $\langle nlm | \hat{H} = \langle nlm | E_n$

Now $\langle [\frac{\partial}{\partial r}, \hat{H}] \rangle = \frac{\hbar^2 l(l+1)}{2m} \langle [\frac{\partial}{\partial r}, \frac{1}{r^2}] \rangle - Ze^2 \langle [\frac{\partial}{\partial r}, \frac{1}{r}] \rangle$

Now $[\frac{\partial}{\partial r}, \frac{1}{r^2}] f = \frac{\partial}{\partial r} \left(\frac{f}{r^2} \right) - \frac{1}{r^2} \frac{\partial f}{\partial r} = -\frac{2f}{r^3}$

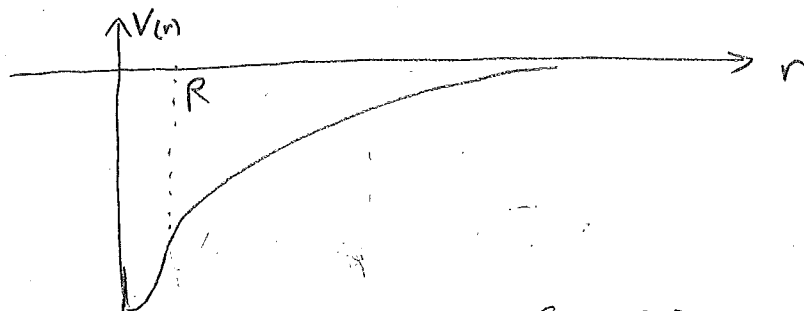
$[\frac{\partial}{\partial r}, \frac{1}{r}] f = \frac{\partial}{\partial r} \left(\frac{f}{r} \right) - \frac{1}{r} \frac{\partial f}{\partial r} = -\frac{f}{r^2}$

$$\Rightarrow \langle [\frac{\partial}{\partial r}, \hat{H}] \rangle = -\frac{\hbar^2 l(l+1)}{m_e} \langle \frac{1}{r^3} \rangle + Ze^2 \langle \frac{1}{r^2} \rangle = 0$$

$$\Rightarrow \langle \frac{1}{r^3} \rangle_{nl} = \frac{Ze^2 m_e}{l(l+1)\hbar^2} \langle \frac{1}{r^2} \rangle = \frac{Z}{a_0} \frac{1}{l(l+1)} \langle \frac{1}{r^2} \rangle_{nl}$$

For a one dimensional atom with nucleus of charge Ze and radius R , the potential is

$$V(r) = \begin{cases} -\frac{3}{2} \frac{Ze^2}{R} \left(1 - \frac{r^2}{3R^2}\right) & r < R \\ -\frac{Ze^2}{r} & r > R \end{cases}$$



$$(a) H_1 = H_{\text{finite}} - H_{\text{point}} = \begin{cases} -\frac{3}{2} \frac{Ze^2}{R} \left(1 - \frac{r^2}{3R^2} - \frac{2}{3} \frac{R}{r}\right) & r < R \\ 0 & r > R \end{cases}$$

$$E_0^{(1)} = \langle 1s | H_1 | 1s \rangle = -\frac{3}{2} \frac{Ze^2}{R} \int_0^R u_{10}^* \left(1 - \frac{r^2}{3R^2} - \frac{2}{3} \frac{R}{r}\right) u_{10} dr$$

Scaling to the appropriate atomic units of length and energy

$$r \Rightarrow \left(\frac{a_0}{Z}\right) r \quad E \Rightarrow \left(\frac{Ze^2}{a_0}\right) E$$

$$U(r) = 2re^{-r} \text{ (in these "atomic" units)}$$

$$E_0^{(1)} = -\frac{6}{R} \int_0^R \left(r^2 e^{-2r} - \frac{r^4}{3R^2} e^{-2r} - \frac{2}{3} R r e^{-2r}\right) dr$$

$$= -\frac{6}{R} \left[-\frac{e^{-2r}}{2} \left(r^2 + r + \frac{1}{2}\right) \Big|_0^R + \frac{e^{-2r}}{6R^2} \left(r^4 + r^3 + 3r^2 + 3r + \frac{3}{2}\right) \Big|_0^R - \frac{2R}{3} \left(-\frac{e^{-2r}}{2} (r + \frac{1}{2})\right) \Big|_0^R \right]$$

$$= -\frac{6}{R} \left[e^{-2R} \left(-\frac{1}{2}R^2 - \frac{1}{2}R - \frac{1}{4} + \frac{1}{6}R^2 + \frac{1}{3}R + \frac{1}{2} + \frac{1}{2R} + \frac{1}{4R^2} + \frac{1}{3}R^2 + \frac{1}{6}R \right) + \frac{1}{4} - \frac{R}{6} - \frac{1}{4R^2} \right]$$

$$\Rightarrow E_0^{(1)} = -\frac{6}{R} \left[\frac{e^{-2R}}{4R^2} [R^2 + 2R + 1] + \frac{1}{4R^2} \left[R^2 - \frac{2R^3}{3} - 1 \right] \right]$$

$$E_0^{(1)} = -\frac{3}{2R^3} \left[e^{-2R} (R+1)^2 + R^2 - \frac{2}{3}R^3 - 1 \right]$$

or in usual CGS units $R \rightarrow R \left(\frac{Z}{a_0} \right)$
 $E_0^{(1)} \rightarrow E_0^{(1)} \cdot \frac{Z^2 e^2}{a_0}$

Equation (a)

(b) For Pb $Z=82$ $R = 8 \times 10^{-3} \text{ cm}$ (Electronic state:)

$$R = R \left(\frac{Z}{a_0} \right) = 1.24 \times 10^{-2} \quad E_0^{(0)} = \frac{Z^2 e^2}{2a_0} = 90.77 \text{ keV}$$

$$\Rightarrow \frac{E_0^{(1)}}{E_0^{(0)}} = 2 \times \text{Equation (a)} = 1.12 \times 10^{-4}$$

$$\frac{\langle r^{(1)} \rangle}{R} = \left(\frac{a_0}{Z} \right) \frac{1}{R} = 80.64$$

• For the muon bound by the Lead Nucleus:

First we must rescale the Bohr radius and the Rydberg to the reduced mass of the two bodied system.

$$m_{\text{red}} = m_{\mu} = 206.77 m_e$$

$$a_0 \Rightarrow a_0 \left(\frac{m_e}{m_{\text{red}}} \right)^{1/2} = \frac{a_0}{206.77}$$

thus the dimensionless Radius we have defined

$$\bar{R} = R \left(\frac{206.77}{a_0} \right) Z = 2.56 \quad (R > \langle r \rangle)$$

(Next page)

The ground state of the "unperturbed" system

$$E_0^{(0)} = \frac{1}{2} \frac{Z^2 e^2}{a_0} (206.77) = 18.9 \text{ MeV}$$

$$\Rightarrow \frac{E_0^{(1)}}{E_0^{(0)}} = 2 \times \text{Equation (a)} (\bar{R})$$

Again since the energy we found was in units of $\frac{Z^2 e^2}{a_0^*}$ and the ground state energy = $\frac{1}{2} \frac{Z e^2}{a_0^*}$ where a_0^* is the rescaled Bohr radius

$$= +3 \frac{1}{(2.56)^3} \left[e^{-2(2.56)} (2.56+1)^2 + (2.56)^2 - \frac{2}{3} (2.56)^3 - 1 \right]$$

$$\frac{E_0^{(1)}}{E_0^{(0)}} = 0.9945$$

$$\frac{\langle r^{(0)} \rangle}{R} = \frac{a_0}{(206.7)Z} \frac{1}{R} = 0.39$$

(c) To summarize what we calculated in part (b)

- For the bound electron the mean radius is 80 times larger than the radius of the nucleus, and thus, the electron spends "little time" inside the nucleus (or equivalently $\psi(x) \ll 1$ for $r \leq R$). Thus, the corrections for finite nucleus radius is very small ($\sim 0.01\%$)

- For the bound muon, the mean radius of the unperturbed state is smaller than the nuclear radius, and thus the muon spends little time outside the nucleus. Therefore the correction for finite potential is not a perturbation, but the dominant effect. Thus, our result in part (b) is unreliable as is reflected in the fact (over)

that the first order correction were on the order of the zeroth order energy

A more accurate model can be formulated by noting that inside the nucleus the potential is parabolic.

Thus we can model the muonic atom as being a muon bound in an isotropic harmonic oscillator potential. (Note: this was the Thompson model of the atom - "plumb pudding")

$$\text{Thus } V_{\text{eff}} = -\frac{3}{2} \frac{Ze^2}{R} + \frac{1}{2} \left(\frac{Ze^2}{R^3} \right) r^2$$

$$= V_0 + \frac{1}{2} k r^2 \quad \text{where } V_0 = -\frac{3}{2} \frac{Ze^2}{R}$$
$$k = \frac{Ze^2}{R^3}$$

The Ground State energy is thus

$$E_{\text{ground}} - V_0 = \frac{3}{2} \hbar \omega_0 = \frac{3}{2} \hbar \sqrt{\frac{k}{M_\mu}} = \frac{3}{2} \hbar \sqrt{\frac{Ze^2}{M_\mu R^3}} = 13.843 \text{ MeV}$$

$$E_{\text{ground}} = -8.3 \text{ MeV}$$

Also the mean radius for an isotropic harmonic oscillator:

$$\langle r \rangle = 3 \sqrt{\langle x^2 \rangle} = \frac{3}{2} \sqrt{\frac{\hbar}{2m\omega_0}} = 6.71 \times 10^{-13} \text{ cm}$$

$$\Rightarrow \frac{\langle r \rangle}{R} = 0.839$$

Thus $\langle r \rangle < R$ as expected, but not as small as predicted by a Bohr model.