

# QUANTUM MECHANICS I

## PHYS 516

### Solutions to Problem Set # 1

**1. Scaling:** Bohr computed the energy level spectrum of the hydrogen atom using the Old Quantum Theory, Heisenberg did the same using Matrix Mechanics, and so did Schrödinger using Wave Mechanics. They all derived

$$E_N = \frac{E_g}{N^2} \quad E_g = -\frac{1}{2}mc^2\alpha^2/N^2 \quad R_N = Na_B \quad a_B = \hbar^2/me^2 \quad (1)$$

Here  $N = 1, 2, 3, \dots$  is the principal quantum number,  $-e$  is the charge on the electron,  $m$  is the mass of the electron (actually electron-proton reduced mass),  $\alpha = e^2/\hbar c = 1/137.036\dots$  is the fine structure constant, and  $a_B$  is the Bohr radius.  $E_1 = -13.6\text{eV}$  and  $a_B = 0.529 \times 10^{-8}\text{cm}$ .

For each of these pairs compute the binding energy and the size (diameter):

System	Energy	Size
hydrogen atom: $p^+e^-$ (nonrelativistic)	13.6 eV	1.058 Å(diam.)
He <sup>II</sup> :		
mu-mesic atom: $p^+\mu^-$		
pi-mesic atom: $p^+\pi^-$		
positronium: $e^+e^-$		
muonium: $\mu^+\mu^-$		
pionium: $\pi^+\pi^-$		
Muonic atom: $Pb^{82+}\mu^-$		
Si exciton: $\epsilon = 11.9, m_e = 0.8m, m_h = 0.4m$		
GaAs exciton: $\epsilon = 12.5, m_e = 0.07m, m_h = 0.4m$		

El<sup>I</sup> is neutral Element, and El<sup>n+1</sup> is Element without  $n$  of its electrons. For excitons the electron ( $m_e$ ) and hole ( $m_h$ ) effective masses are given as multiples of the free electron mass. Recall that the mass  $m$  used in expressions for the hydrogen atom properties is the proton-electron reduced mass.

**Solution:** A computer code was written. A  $10 \times 8$  array was created. Each row is dedicated to one of the 10 atomic pairs listed.

**Inputs:**

**Col. 1:**  $m_1$

**Col. 2:**  $m_2$

**Col. 3:**  $Z/\epsilon$ . This is the electromagnetic scale factor.

**Outputs:**

**Col. 4:**  $\mu = m_1 m_2 / (m_1 + m_2)$  - This is the mass scaling factor.

**Col. 5:**  $1/(\mu * Z/\epsilon)$  - This is the length scale factor

**Col. 6:**  $\mu * (Z/\epsilon)^2$  - This is the energy scale factor.

**Col. 7:**  $1/(\mu * Z/\epsilon) * a_B$  - Radius of bound state.

**Col. 8:**  $\mu * (Z/\epsilon)^2 * E_B$  - Energy of bound state.

Note that the size of the  $Pb^{82+}\mu^-$  does not appear because of the formatting. It is  $0.0000311 \times 10^{-8}$  cm or  $3.11 \times 10^{-15}$  m. The proton radius is about  $0.86 \times 10^{-15}m$  but the lead nucleus has a radius of  $(208)^{1/3} \times R_p \simeq 5.09 \times 10^{-15}m$ , by scaling arguments. This means that the mu meson spends more of its time inside the lead nucleus than outside. It therefore can be used as a sensitive probe of the nuclear structure of the lead nucleus.

Table 1: Solution of the Coulomb scaling problem. Masses are scaled to the electron mass. Radii are given in terms of the Bohr radius =  $0.529 \times 10^{-8}$  cm and energies expressed in terms of electron volts.

	$m_1$	$m_2$	$Z/\epsilon$	$\mu = \frac{m_1 m_2}{m_1 + m_2}$	$1/(\mu * Z/\epsilon)$	$\mu * (Z/\epsilon)^2$	$a_B / (\mu * Z/\epsilon)$	$E_B \mu * (Z/\epsilon)^2$
1	1836.1500	1.0000	1.0000	.9995	1.0005	.9995	.5293	13.5926
2	7344.6001	1.0000	2.0000	.9999	.5001	3.9995	.2645	54.3926
3	1836.1500	207.0000	1.0000	186.0280	.0054	186.0280	.0028	2529.9805
4	1836.1500	273.0000	1.0000	237.6640	.0042	237.6640	.0022	3232.2300
5	1.0000	1.0000	1.0000	.5000	2.0000	.5000	1.0580	6.8000
6	207.0000	207.0000	1.0000	103.5000	.0097	103.5000	.0051	1407.6000
7	273.0000	273.0000	1.0000	136.5000	.0073	136.5000	.0039	1856.4001
8	381888.0000	207.0000	82.0000	206.8879	.0001	1391113.9554	.0000	18919150.3239
9	.8000	.4000	.0840	.2667	44.6250	.0019	23.6066	.0256
10	.0700	.4000	.0800	.0596	209.8214	.0004	110.9955	.0052

**2. Relativistic Schrodinger Equation:** Schrödinger solved the relativistic problem before he proposed his nonrelativistic equation. You will do that here

a. Write down the relativistic equation for a spinless electron in the presence of a spinless proton.

b. Use separation of variables to “get rid of” the angular dependence.

c. Use the useful transformation  $R(r) = \frac{1}{r}f(r)$  and write down the radial equation in terms of the unknown function  $f(r)$ .

d. Compare this equation with an equation in Table 22.6 from Abramowitz and Stegun. What do you conclude?

e. Show

$$E(n, l, \alpha) = \frac{mc^2}{\sqrt{1 + \frac{\alpha^2}{\left(n + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2}\right)^2 - \alpha^2}\right)^2}}} \quad (2)$$

f. What effect does relativity have on the “Bohr radius” of an electron?

g. Expand the expression for the energy of a relativistic electron without spin in powers of the fine structure constant  $\alpha$  up to and including order six. Compare the first correction to the rest energy with the nonrelativistic spectrum.

**Solution:**

a.  $\left\{ \left(E + \frac{e^2}{r}\right)^2 + (\hbar c)^2 \nabla^2 - (mc^2)^2 \right\} \psi = 0$

b. c. Make the substitution  $\psi(r, \theta, \phi) = \frac{1}{r}R(r)Y_m^l(\theta, \phi)$  and obtain

$$\left\{ \frac{E^2 - (mc^2)^2}{(\hbar c)^2} + \frac{2E e^2}{(\hbar c)^2 r} + \left(\frac{d}{dr}\right)^2 - \frac{l(l+1)}{r^2} + \frac{(e^2)^2}{(\hbar c)^2 r^2} \right\} R(r) = 0$$

d. Scale the radial coordinate  $r = \gamma z$  and obtain

$$\left\{ \frac{E^2 - (mc^2)^2}{(\hbar c)^2} \gamma^2 + \frac{2E e^2}{(\hbar c)^2 z} \gamma + \left(\frac{d}{dz}\right)^2 - \frac{l(l+1) - \alpha^2}{z^2} \right\} R(z) = 0$$

e. Compare with **22.6.17** in Abramowitz and Stegun:

Physics	Mathematics
$\frac{E^2 - (mc^2)^2}{(\hbar c)^2} \gamma^2$	$-\frac{1}{4}$
$\frac{2Ee^2}{(\hbar c)^2} \gamma$	$\frac{2n + \beta + 1}{2}$
$-l(l + 1) + \alpha^2$	$\frac{1 - \beta^2}{4}$

Here  $\alpha = e^2/\hbar c$  is the fine structure constant and  $\beta$  is a parameter associated with the associated Laguerre polynomials  $L_n^{(\beta)}(z)$ .

We attack the last equation first:  $-l(l + 1) + \alpha^2 = \frac{1-\beta^2}{4}$ , which unwinds to  $\beta/2 = \sqrt{(l + \frac{1}{2})^2 - \alpha^2}$ . This is placed into the right hand side of the middle equation, giving  $n + \frac{1}{2} + \sqrt{(l + \frac{1}{2})^2 - \alpha^2} = N(\alpha)$ . If  $\alpha = 0$ ,  $N(0) = n + \frac{1}{2} + (l + \frac{1}{2}) = n + l + 1 = N$ , where  $N$  is Bohr's Principal Quantum Number. So

$$N(\alpha) - N = \sqrt{(l + \frac{1}{2})^2 - \alpha^2} - (l + \frac{1}{2}) = -\frac{\alpha^2}{2l + 1} - \frac{\alpha^4}{(2l + 1)^3} - \frac{2\alpha^6}{(2l + 1)^5} - \dots$$

For the ground state with  $N = 1$  (Princial quantum number),  $n = 0$  (radial quantum number) and  $l = 0$  (angular quantum number), so  $1(\alpha) = 1 - \alpha^2 - \alpha^4 - 2\alpha^6 \dots$ . We continue by taking the ratio of the first equation to the square of the second (to rid ourselves of the scale factor  $\gamma$ ):

$$\frac{E^2 - (mc^2)^2}{(2E\alpha)^2} = -\frac{1}{4N(\alpha)^2}$$

$$\frac{E^2 - (mc^2)^2}{E^2} = -\frac{\alpha^2}{N(\alpha)^2}$$

One last piece of algebra gives the result

$$\frac{E}{mc^2} = \frac{1}{\sqrt{1 + \left(\frac{\alpha}{N(\alpha)}\right)^2}}$$

**e.** Now go back and find the scale factor  $\gamma$ , which determines the size of the Bohr radius.

$$\frac{2E}{(\hbar c)^2} e^2 \gamma = N(\alpha) \Rightarrow \gamma = \frac{a_B}{2} N(\alpha) \sqrt{1 + \left(\frac{\alpha}{N(\alpha)}\right)^2}$$

In the ground state we use  $1(\alpha)$  as given above to find

$$a_B \rightarrow a_B \sqrt{(1 - \alpha^2 - \alpha^4 - 2\alpha^6)^2 + \alpha^2} \xrightarrow{\text{Maple}^{\text{©}}} a_B \left(1 - \frac{1}{2}\alpha^2 - \frac{5}{8}\alpha^4 - \frac{21}{16}\alpha^6 - \dots\right)$$

The Bohr orbit radius decreases. The decrease may be interpreted as a relativistic contraction in the transverse direction due to its speed  $v \simeq \alpha c$ .

Finally, we expand the expression for the energy in ascending powers of  $\alpha$  using Maple(!) or some other sanity-preserving software:

$$E \simeq mc^2 \left\{ 1 - \frac{1}{2N^2}\alpha^2 + \left( \frac{3}{8N^4} - \frac{1}{N^3(2l+1)} \right) \alpha^4 + \alpha^6 \left( -\frac{5}{16N^6} + \frac{3}{5N^5(2l+1)} - \frac{2N+3(2l+1)}{2N^4(2l+1)^3} \right) \right\}$$