Problem Set 1

PY 452

Written by Alan Gabel

Problem 5.1

a) Simple substitution can be used to check that

$$\vec{r}_1 = \vec{R} + \frac{\mu}{m_1}\vec{r}$$

$$\vec{r}_2 = \vec{R} - \frac{\mu}{m_2}\vec{r}$$

To find gradient operator consider equation component wise.

For example:

particle 1, x-component:

$$(\nabla_1)_x = \frac{\partial}{\partial x_1} = \frac{\partial X}{\partial x_1}\cdot\frac{\partial}{\partial X} + \frac{\partial x}{\partial x_1}\frac{\partial}{\partial x}$$

$$= \frac{\mu}{m_2}\frac{\partial}{\partial X} + \frac{\partial}{\partial x}$$

$$= \frac{\mu}{m_2}(\nabla_R)_x + (\nabla_r)_x$$

where I used:

$$\vec{r}_1 = (x_1, y_1, z_1)$$

$$\vec{r} = (x, y, z)$$

$$\vec{R} = (X, Y, Z)$$

b) Use $H\Psi = \left(-\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 + V(\vec{r}_1 - \vec{r}_2)\right)\Psi = E\Psi$

and insert substitution from part (a)

c) Substitute $\Psi(\vec{R},\vec{r}) = \Psi_R(\vec{R})\,\Psi_r(\vec{r})$ and divide

The equation by $\Psi(\vec{R},\vec{r})$ to get

$$\left[\frac{-\hbar^2}{2(m_1+m_2)} \frac{\nabla_R^2 \Psi_R(\vec{R})}{\Psi_R(\vec{R})}\right] + \left[-\frac{\hbar^2}{2\mu} \frac{\nabla_r^2 \Psi_r(\vec{r})}{\Psi_r(\vec{r})} + V(\vec{r})\right] = E$$

The 1st term depends only on $\vec{R}$ and the second on $\vec{r}$ so

They must be constants. Call these constants E_R and E_r, respectively.

Problem 5.2

a) We found that $E \propto m_e$, so percent error is given by

$$\frac{\Delta E}{E} = \frac{m_e - \mu}{\mu}.$$

Using $\mu = \frac{m_e + m_p}{m_e m_p}$ where m_e is electron mass, m_p is proton mass

$$\boxed{\text{Percent error} = \frac{\Delta E}{E} = 5.44 \times 10^{-4}}$$

b) Wavelength of transition is given by

$$\frac{1}{\lambda} = R\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) \quad \text{where} \quad R = \frac{m}{4\pi c \hbar^3}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2 = 1.097 \times 10^7\ m^{-1}$$

for $m = m_e$

using $n_f = 2$

$n_i = 3$

$m = \mu_{hydrogen} = \frac{m_e m_p}{m_e + m_p}$ or $m = \mu_{deuterium} = \frac{m_e \cdot 2m_p}{m_e + 2m_p}$

we get

$$\boxed{\lambda_{deuterium} - \lambda_{hydrogen} = 1.79 \times 10^{-10}\ m}$$

c) For positronium, $\mu = \dfrac{m_e m_e}{m_e + m_e} = \dfrac{m_e}{2}$

So $\boxed{E_{positronium} = \dfrac{E_{hydrogen}}{2} = \dfrac{13.6\text{ eV}}{2} = 6.8\text{ eV}}$

d) Again use $\dfrac{1}{\lambda} = R\left(\dfrac{1}{n_f} - \dfrac{1}{n_i}\right)$; $R = \dfrac{\mu}{4\pi c\hbar^3}\left(\dfrac{e^2}{4\pi\epsilon_0}\right)^2$

with $\mu = \dfrac{(206.77 m_e) m_p}{206.77 m_e + m_p}$

$n_f = 1$

$n_i = 2$

Then, $\boxed{\lambda = 6.54 \times 10^{-10}\text{ m}}$

Problem 5.5

a) Hamiltonian is given by $H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2}$

$$\boxed{H = -\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x_2}}$$

Define the n^{th} excited state single particle wavefunction:

$$\psi_n(x) = \sqrt{\frac{2}{a}}\,\sin\left(\frac{n\pi}{a}x\right) \qquad 0 \le x \le a$$

with energy $E_n = n^2 K$, $\quad K \equiv \frac{\pi^2\hbar^2}{2ma^2}$

so Fermion Ground state is

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}}\psi_1(x_1)\psi_2(x_2) - \frac{1}{\sqrt{2}}\psi_2(x_1)\psi_1(x_2)$$

with energy $E = E_1 + E_2 = 5K$

b)

b) Higher excited states are... ...

Distinguishable:

	Wavefunction	Energy
Ground:	$\psi_1(x_1)\,\psi_1(x_2)$	$E_1+E_1 = 2K$
1st excited:	$\psi_1(x_1)\,\psi_2(x_2)$ OR $\psi_2(x_1)\,\psi_1(x_2)$	$E_2+E_1 = 5K$
2nd Excited:	$\psi_2(x_1)\,\psi_2(x_2)$	$E_2+E_2 = 8K$
3rd Excited:	$\psi_1(x_1)\,\psi_3(x_2)$ OR $\psi_3(x_1)\,\psi_1(x_2)$	$E_1+E_3 = 10K$

Bosons

	Wavefunction	Energy
Ground:	$\psi_1(x_1)\psi_2(x_1)$	$E_1+E_1 = 2K$
1st excited	$\frac{1}{\sqrt{2}}\psi_2(x_1)\psi_1(x_2) + \frac{1}{\sqrt{2}}\psi_1(x_1)\psi_2(x_2)$	$E_1+E_2 = 5K$
2nd excited:	$\psi_2(x_1)\psi_2(x_2)$	$E_2+E_2 = 8K$
3rd excited:	$\frac{1}{\sqrt{2}}\psi_3(x_1)\psi_1(x_2) + \frac{1}{\sqrt{2}}\psi_1(x_1)\psi_3(x_2)$	$E_3+E_1 = 10K$

Fermions

	Wave Function	Energy
Ground:	$\frac{1}{\sqrt{2}}\psi_2(x_1)\psi_1(x_2) - \frac{1}{\sqrt{2}}\psi_1(x_1)\psi_2(x_2)$	$E_1 + E_2 = 5K$
1st excited:	$\frac{1}{\sqrt{2}}\psi_3(x_1)\psi_1(x_2) - \frac{1}{\sqrt{2}}\psi_1(x_1)\psi_3(x_2)$	$E_1 + E_3 = 10K$
2nd excited	$\frac{1}{\sqrt{2}}\psi_3(x_1)\psi_2(x_2) - \frac{1}{\sqrt{2}}\psi_2(x_1)\psi_3(x_2)$	$E_2 + E_3 = 13K$

- Notice that for fermions, the two particles can not have the same energy (thus can't be in the same state).

Problem 5.7

- Each state will be the sum of terms of the form

$$\psi_\alpha(x_1)\,\psi_\beta(x_2)\,\psi_\gamma(x_3)$$

where $\alpha \neq \beta \neq \gamma$ and $\alpha, \beta, \gamma \in \{a, b, c\}$

- For <u>Distinguishable</u> particles this is straightforward.

$$\boxed{\psi_{Dist.}(x_1, x_2, x_3) = \psi_a(x_1)\,\psi_b(x_2)\,\psi_c(x_3)}$$

- For Indistinguishable Bosons there will be a term for every permutation of the 3 particles in 3 possible states, so 6 terms all together. They must each have the same coefficient, which for normalization purposes is $\frac{1}{\sqrt{6}}$. So

$$\psi_{Boson}(x_1, x_2, x_3) = \frac{1}{\sqrt{6}}\Big\{ \psi_a(x_1)\,\psi_b(x_2)\,\psi_c(x_3)$$

$$+\psi_a(x_1)\,\psi_c(x_2)\,\psi_b(x_3)$$

$$+\psi_b(x_1)\,\psi_a(x_2)\,\psi_c(x_3)$$

$$\ldots \text{etc.} \Big\}$$

8

- If the particles are fermions, All the same terms are present but not all are positive. The overall sign doesn't matter so just choose one as positive. For the other terms, multiply by -1 for each switch of indicies. (For example

$ABC \rightarrow +1$

$ACB \rightarrow (-1)$

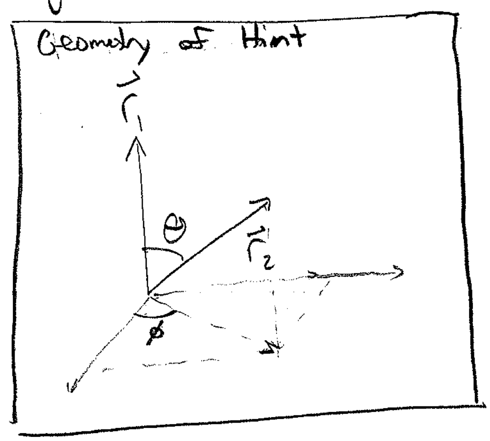
$CAB \rightarrow (-1)(-1) = +1$

so

$$\psi_{\text{fermion}}(x_1, x_2, x_3) = \frac{1}{\sqrt{6}} \Big\{ \psi_a(x_1)\,\psi_b(x_2)\,\psi_c(x_3) - \psi_a(x_1)\,\psi_c(x_2)\,\psi_b(x_3) - \psi_b(x_1)\,\psi_a(x_2)\,\psi_c(x_3) \ \ldots \text{etc.} \Big\}$$

Problem 5.11

a) The expecation value is found from the integral:



$$\left\langle \frac{1}{|\vec{r}_1 - \vec{r}_2|} \right\rangle = \int d^3\vec{r}_1\, d^3\vec{r}_3\, \frac{|\Psi_0(\vec{r}_1, \vec{r}_2)|^2}{|\vec{r}_1 - \vec{r}_2|}$$

$$= \int d^3\vec{r}_1\, d^3\vec{r}_2\, \frac{\left(\frac{8}{\pi a^3}\right)^2 e^{-\frac{4(r_1+r_2)}{a}}}{|\vec{r}_1 - \vec{r}_2|}$$

This can be made into a dimensionless integral by letting

$$\vec{r}_1{}' = \frac{\vec{r}_1}{a}, \quad \vec{r}_2{}' = \frac{\vec{r}_2}{a} \quad \text{and} \quad d^3\vec{r}_1 = a^3 d\vec{r}_1{}', \quad d^3\vec{r}_2 = a^3 d\vec{r}_2{}'$$

so

$$\left\langle \frac{1}{|\vec{r}_1 - \vec{r}_2|} \right\rangle = \frac{1}{a} \cdot \left(\frac{8}{\pi}\right)^2 \int d^3\vec{r}_1{}'\, d^3\vec{r}_2{}'\, \frac{e^{-4(r_1' + r_2')}}{|\vec{r}_1{}' - \vec{r}_2{}'|} \quad \propto \frac{1}{a}$$

Performing the integral gives the correct coefficient as

$$\boxed{\left\langle \frac{1}{|\vec{r}_1 - \vec{r}_2|} \right\rangle = \frac{5}{4a}}$$

b) The electron interaction can be estimated as

$$V_{interaction} \approx \left\langle \frac{e^2}{4\pi\epsilon_0 |\vec{r}_1 - \vec{r}_2|} \right\rangle = \frac{e^2}{4\pi\epsilon_0} \cdot \frac{5}{4a} = 34 \text{ eV}$$

Naive Ground state energy estimation from the book is

$$E_0 = -109 \text{ eV}.$$

So the naive guess plus interaction correction is

$$\boxed{E_{corrected} = E_0 + V_{interaction} = -75 \text{ eV}}$$

- The experimentally measured result is -79 eV (not to bad)