Modern Homework 30 — William Jardee — 11/12

1. +4

a)

$$1 = C_A^2 \int |\psi_A(r_1)\psi_B(r_2) - \psi_A(r_2)\psi_B(r_1)| \, d\tau$$

$$= C_A^2 \left[\int (\psi_A^*(r_1)\psi_B^*(r_2) - \psi_A^*(r_2)\psi_B^*(r_1))(\psi_A(r_1)\psi_B(r_2) - \psi_A(r_2)\psi_B(r_1)) \, d\tau \right]$$

There should be a $d\tau$ for both r variables, as they are independent variables.

$$= C_A^2 \Big[\int |\psi_A(r_1)|^2 |\psi_B(r_2)|^2 d\tau + \int |\psi_A(r_2)|^2 |\psi_B(r_1)|^2 d\tau$$
$$- \int [\psi_A^*(r_1)\psi_B^*(r_2)\psi_A(r_2)\psi_B(r_1) + \psi_A^*(r_2)\psi_B^*(r_1)\psi_B(r_2)\psi_A(r_1)] \, d\tau \Big]$$

by change of variables $d\tau_1 \to d\tau_2$

$$= C_A^2 \left[2 - 2\int \psi_A^*(r_1)\psi_B^*(r_2)\psi_A(r_2)\psi_B(r_1) \, d\tau \right] = C_A^2 \left[2 - 2\int \psi_A(r_1)\psi_B^*(r_1)\right]\left[\int \psi_A(r_1)\psi_B(r_1)\right]$$

$$= C_A \left[2 - 2\left|\int \psi_A(r_1)\psi_B^*(r_1)\, d\tau_1\right|\right]^{-1/2}$$

~~this is as simple as we were able to make it.~~

~~I know it's wrong, but the best I got~~

$$\boxed{\text{so } C_A = \left[2 - 2\left|\int \psi_A(r_1)\psi_B^*(r_1)\, d\tau_1\right|\right]^{-1/2}}$$

b) i.)

$$C_A = \frac{1}{\sqrt{2}}\left[1 - \int \psi_A^*(r_1)\psi_B^*(r_2)\psi_A(r_2)\psi_B(r_1)\, d\tau\right]^{-1/2}$$

$$C_A = \frac{1}{\sqrt{2}}\left[1 - \int |\psi_{n_1}^*(r_1)|\,|\psi_{n_2}^*(r_2)|\,|\psi_{n_1}(r_2)|\,|\psi_{n_2}(r_1)|\, d\tau\right]^{-1/2}$$

$$= \frac{1}{\sqrt{2}}\left[1 - \underbrace{\int \sin\left(\frac{n_1\pi r_1}{L}\right)\sin\left(\frac{n_2\pi r_1}{L}\right)\sin\left(\frac{n_1\pi r_2}{L}\right)\sin\left(\frac{n_2\pi r_2}{L}\right) d\tau}_{\text{zero over period}}\right]^{-1/2}$$

$$= \frac{1}{\sqrt{2}}[1]^{-1/2} = \frac{1}{\sqrt{2}}$$

$$\psi = \sqrt{\frac{1}{2}}\left[\sin\left(\frac{n_1\pi r_1}{L}\right)\sin\left(\frac{n_2\pi r_2}{L}\right) - \sin\left(\frac{n_1\pi r_2}{L}\right)\sin\left(\frac{n_2\pi r_1}{L}\right)\right]$$

ii)

$$E\psi = -\frac{\hbar^2}{2m}\left[\nabla_1^2\psi + \nabla_2^2\psi\right]$$

$$= -\frac{\hbar^2}{2m}\Big[-\left(\frac{n_1\pi}{L}\right)^2 \sin\left(\frac{n_1\pi r_1}{L}\right)\sin\left(\frac{n_2\pi r_2}{L}\right) + \left(\frac{n_2\pi}{L}\right)^2 \sin\left(\frac{n_1\pi r_2}{L}\right)\sin\left(\frac{n_2\pi r_1}{L}\right)$$
$$- \left(\frac{n_2\pi}{L}\right)^2 \sin\left(\frac{n_1\pi r_1}{L}\right)\sin\left(\frac{n_2\pi r_2}{L}\right) + \left(\frac{n_1\pi}{L}\right)^2 \sin\left(\frac{n_1\pi r_2}{L}\right)\sin\left(\frac{n_2\pi r_1}{L}\right)\Big]$$

$$= +\frac{\hbar^2}{2m}\left[\left(\frac{n_1\pi}{L}\right)^2 + \left(\frac{n_2\pi}{L}\right)^2\right]\psi$$

$$E = \frac{\hbar^2\pi^2}{2mL^2}\left[n_1^2 + n_2^2\right]$$

2. +3 a) We can extrapolate our result from 1 & say

$$E = \frac{\hbar^2 \pi^2}{2mL^2}\left[1^2+2^2+3^2+\cancel{4^2}+5^2\right] = 55\frac{\hbar^2\pi^2}{8mL^2} = 55\frac{(hc)^2}{8mc^2L^2}$$

$$\boxed{E = \cancel{20}.7\,eV}$$

Electrons in a PiB still have spin, so there will be spin pairing.

b) Bosons don't have to fit the Pauli exclusion principle, as they allow the symmetric wave function.

$$E = \frac{\hbar^2\pi^2}{2mL^2}\left[1^2+1^2+1^2+1^2+1^2\right] = 5\frac{(hc)^2}{8mc^2L^2}$$

$$E = 0.00712\,eV$$

3. +4 The splitting comes from a B field. If $L=0$, there is no movement and resulting current to induce a B-field. So, the only shell void of spin-orbit ~~also~~ a splitting is the s shell. So, I sort of s is the only open shell.

Sees Split:	Doesn't See split:
· B $2s^2 2p^1$	· Li $[He]2s^1$
· Al $3s^2 3p^1$	· Na $[Ne]3s^1$
· Ga $3d^{10} 4s^2 4p^1$	· K $[Ar]4s^1$
· U $5f^3 6d\ 7s^2$	· Cu $3d^{10} 4s^1$
	· Ag $4d^{10} 5s^1$
	· Cs $[Xe]6s^1$
	· Au $[Xe, 4f^{14} 5d^{10}]6s^1$