Homework 11, solutions

problem 1, solution

a) The Schroedinger equation is

$$\Big[\underbrace{\frac{P_{cm}^2}{2M}}_{H_{cm}} + \underbrace{\frac{P_r^2}{2m} + V(r)}_{H_{rel}} \underbrace{- P_B V(r)}_{H_{ex}}\Big] \underbrace{\Phi(\vec{R}_{cm})}_{\text{CM motion}} \underbrace{\Psi(r)}_{\text{relative motion}} \underbrace{\chi(q)}_{\text{spin}} = E\, \Phi(\vec{R}_{cm}) \Psi(r) \chi(q).$$

$H = H_{CM} + H_{rel} + H_{ex}$, $[H_{rel}, H_{ex}] = 0$.

$V_B = -P_B V(r)$. $P_B|++\rangle = |++\rangle$, $P_B|--\rangle = |--\rangle$, $P_B|+-\rangle = |-+\rangle$, $P_B|-+\rangle = |+-\rangle$.

In the basis $\{|++\rangle, |--\rangle, |+-\rangle, |-+\rangle\}$ the matrix of V_B is

$$(V_B) = \begin{array}{c|c} & \begin{array}{cccc} |++\rangle & |--\rangle & |+-\rangle & |-+\rangle \end{array} \\ \begin{array}{c} \langle ++| \\ \langle --| \\ \langle +-| \\ \langle -+| \end{array} & \begin{pmatrix} -V(r) & 0 & 0 & 0 \\ 0 & -V(r) & 0 & 0 \\ 0 & 0 & 0 & -V(r) \\ 0 & 0 & -V(r) & 0 \end{pmatrix} \end{array}.$$

The eigenfunctions are $|++\rangle$, $\frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle)$, $|--\rangle$ with eigenvalue $-V(r)$ and $\frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle)$ with eigenvalue $V(r)$.

The symmetric eigenfunction (triplet state) lie lower in energy.

$\langle V_B\rangle_S = -V(r)$, $\langle V_B\rangle_A = +V(r)$, so the ground state is the triplet state.

b) If both particles had the same T_3 component, the state vector in isospin space would have to be symmetric. (We would have identical particles.) The ground state is symmetric in orbital space, so we need the state vector in spin space to be antisymmetric. This implies higher energy.

problem 2, solution

The two-electron wave function must be antisymmetric with respect to interchange of position and spin variables.

$S=0 \Rightarrow$ symmetric space wavefunction

$S=1 \Rightarrow$ antisymmetric space wave function

$$S=0: \qquad \Psi_S(\vec r_1,\vec r_2) = \frac{\psi_{1s}(\vec r_1)\,\psi_{2s}(\vec r_2) + \psi_{1s}(\vec r_2)\,\psi_{2s}(\vec r_1)}{\sqrt 2}$$

$$S=1: \qquad \Psi_T(\vec r_1,\vec r_2) = \frac{\psi_{1s}(\vec r_1)\,\psi_{2s}(\vec r_2) - \psi_{1s}(\vec r_2)\,\psi_{2s}(\vec r_1)}{\sqrt 2}$$

Let $H = H_0 + \frac{e^2}{|\vec r_1-\vec r_2|}$, and treat $\frac{e^2}{|\vec r_1-\vec r_2|}$ as a perturbation.

The unperturbed energies of Ψ_S and Ψ_T are equal. (ψ_{1s} and ψ_{2s} are eigenfunctions of H_0.) The first order corrections differ by

$$\langle\Psi_S|\frac{e^2}{|\vec r_1-\vec r_2|}|\Psi_S\rangle - \langle\Psi_T|\frac{e^2}{|\vec r_1-\vec r_2|}|\Psi_T\rangle = 2\langle\psi_{1s}(\vec r_1)\,\psi_{2s}(\vec r_2)|\frac{e^2}{|\vec r_1-\vec r_2|}|\psi_{1s}(\vec r_2)\,\psi_{2s}(\vec r_1)\rangle$$

$$= 2\left(\frac{8}{\pi a_0^3}\right)\left(\frac{1}{4\pi a_0^3}\right)e^2\int d^3r_1\,d^3r_2\left(2-\frac{2r_1}{a_0}\right)\left(2-\frac{2r_2}{a_0}\right)\frac{e^{-3(r_1+r_2)/a_0}}{|\vec r_1-\vec r_2|} = \Delta$$

$$\frac{1}{|\vec r_1-\vec r_2|} = \sum_\ell \frac{r_<^\ell}{r_>^{\ell+1}}\,\frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{\ell} Y_{\ell m}(\theta_1\phi_1)\,Y^*_{\ell m}(\theta_2\phi_2).$$

$e^{-3(r_1+r_2)/a_0}$ is invariant under separate rotations of $\vec r_1$ and $\vec r_2$. Therefore only $\ell=0$ term survives the angular integration. We have

$$\Delta = 2(4\pi)^2\left(\frac{8}{\pi a_0^3}\right)\left(\frac{1}{4\pi a_0^3}\right)e^2\int_{r_1=0}^{\infty} r_1^2\,dr_1\left(2-\frac{2r_1}{a_0}\right)e^{-3r_1/a_0}\int_{r_2=0}^{\infty} r_2^2\,dr_2\left(2-\frac{2r_2}{a_0}\right)\frac{e^{-3r_2/a_0}}{r_>}$$

$$= \frac{64e^2}{a_0^6}\,2\int_{r_1=0}^{\infty} r_1^2\,dr_1\left(2-\frac{2r_1}{a_0}\right)e^{-3r_1/a_0}\int_{r_2=r_1}^{\infty} r_2^2\,dr_2\left(2-\frac{2r_2}{a_0}\right)\frac{e^{-3r_2/a_0}}{r_2} = \frac{64}{729}\,\frac{e^2}{a_0} = 2.39\,\text{eV}$$

(All integrals are in the table.)

problem 3, solution.......

$$H = \frac{P_1^2}{2m} + \frac{P_2^2}{2m} + \frac{1}{2}Cx_1^2 + \frac{1}{2}Cx_2^2 + \frac{1}{2}K(x_1 - x_2)^2.$$

a) Let $R = \frac{1}{2}(x_1 + x_2)$, $r = (x_2 - x_1)$, $x_1 = R - \frac{1}{2}r$, $x_2 = R + \frac{1}{2}r$.

$L = T - V = \frac{1}{2}m(\dot{x}_1^2 + \dot{x}_2^2) - V = \frac{1}{2}(M\dot{R}^2 + \mu\dot{r}^2) - V$ where $M = 2m$ and $\mu = \frac{m}{2}$.

$P_R = \frac{\partial L}{\partial \dot{R}} = M\dot{R}$, $P_r = \frac{\partial L}{\partial \dot{r}} = \mu\dot{r}$, $H = \frac{P_R^2}{2M} + \frac{P_r^2}{2\mu} + V.$

We want $V = \frac{1}{2}Cx_1^2 + \frac{1}{2}Cx_2^2 + \frac{1}{2}Kx_1^2 + \frac{1}{2}Kx_2^2 - Kx_1x_2 = \frac{1}{2}AR^2 + \frac{1}{2}Br^2$

$$= \frac{1}{2}A\left(\frac{1}{4}x_1^2 + \frac{1}{4}x_2^2 + \frac{1}{2}x_1x_2\right) + \frac{1}{2}B(x_1^2 + x_2^2 - 2x_1x_2).$$

Therefore $\frac{1}{2}(C + K) = \frac{1}{2}\left(\frac{A}{4} + B\right)$, $-K = \frac{1}{4}A - B$, or $A = 2C$, $B = \frac{C}{2} + K$.

$$H = \frac{P_R^2}{2M} + \frac{1}{2}AR^2 + \frac{P_r^2}{2\mu} + \frac{1}{2}Br^2.$$

To make the transition to Quantum Mechanics let P_R, P_r, R, and r become operators.

b) Let $\psi(R,r) = \chi(R)\,\phi(r)$. Then

$$-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial R^2}\chi(R) + \frac{1}{2}AR^2\chi(R) = E_1\chi(R), \quad -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2}\phi(r) + \frac{1}{2}Br^2\phi(r) = E_2\phi(r).$$

$E = E_1 + E_2$. $E_1 = (n_1 + \frac{1}{2})\hbar\omega_1$, $E_2 = (n_2 + \frac{1}{2})\hbar\omega_2$. $\omega_1^2 = \frac{A}{M}$, $\omega_2^2 = \frac{B}{\mu}$.

$n_1 = 0, 1, 2, \cdots$, $n_2 = 0, 1, 2, \cdots$.

c) For indistinguishable bosons the total wavefunction must be symmetric under interchange of the two particles, for indistinguishable fermions it must be antisymmetric.

Under interchange $R \to R$, $r \to -r$. $\phi_{n_2}(r)$ has even parity if n_2 is even and odd parity if n_2 is odd.

To get an even space function we need n_2 even, to get an odd space function we need n_2 odd.

If the spin function is symmetric then we have $E = E_{n_1} + E_{n_2}$, n_2 = even for bosons and $E = E_{n_1} + E_{n_2}$, n_2 = odd for fermions.

d) $\phi_{n_2}(0) = 0$ if n_2 = odd, $r = 0 \Rightarrow x_1 = x_2$, $\phi_{n_2 = \text{odd}}(x_1 = x_2) = 0$.