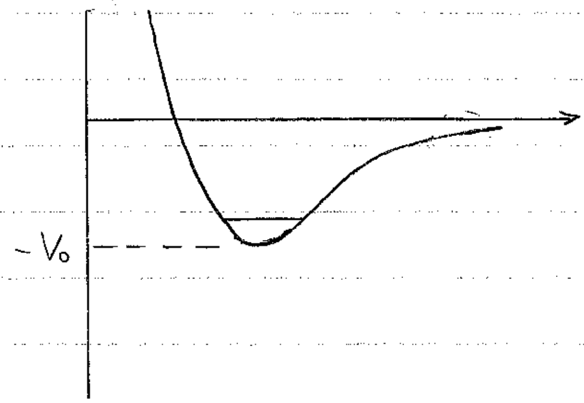
HOMEWORK 6 SOLUTIONS

24) (a) The ground state energy is $\frac{1}{2}\hbar\omega$ above the minimum of the potential so



$$V_0 = \frac{1}{2}\hbar\omega + E_{dis}$$

Here

$$\omega = \sqrt{\frac{k}{\mu}}$$

Hydrogen: $\mu = \frac{m_1 m_2}{m_1 + m_2} = \frac{m_p}{2}$

Deuterium $\mu = \frac{m_d}{2} \simeq m_p \quad \Rightarrow \quad \omega_d = \sqrt{\frac{k}{m_p}} = \frac{1}{\sqrt{2}}\omega_p$

$$V_0 = \frac{1}{2}\hbar\omega_p + 4.477\,eV = \frac{1}{2}\hbar\omega_d + 4.556\,eV$$

$$\frac{1}{2}\hbar(\omega_p - \omega_d) = 0.079\,eV$$

$$\hbar(\omega_p - \omega_d) = \hbar\left(\omega_p - \frac{\omega_p}{\sqrt{2}}\right) = \hbar\omega_p\left(1 - \frac{1}{\sqrt{2}}\right) = 2(.079\,eV)$$

$$\boxed{\hbar\omega_p = 0.539\,eV}$$
$$\boxed{\hbar\omega_d = 0.381\,eV}$$

$$V_0 = \frac{1}{2}\hbar\omega_p + 4.477\,eV$$

$$\boxed{V_0 = 4.747\,eV}$$

(b) For HD

$$\mu = \frac{m_p(2m_p)}{m_p + 2m_p} = \frac{2}{3}m_p \qquad \omega = \sqrt{\frac{k}{\frac{2}{3}m_p}} = \sqrt{\frac{k}{\frac{4}{3}\frac{m_p}{2}}} = \sqrt{\frac{3}{4}}\,\omega_p$$

$$E_{dis} = V_0 - \frac{1}{2}\hbar\omega = 4.747 - \frac{1}{2}\sqrt{\frac{3}{4}}\,\hbar\omega_p = \boxed{4.513\,eV}$$

25) (a) In H_2 the nuclei are fermions so the wave function must be antisymmetric under exchange of the nuclei. In a diatomic molecule exchanging the positions $(\vec{r}_1 \leftrightarrow \vec{r}_2)$ is equivalent to reversing the direction of $\vec{R}$, and our wave functions are proportional to $Y_k^{\lambda}(\theta,\phi)$.

$\therefore$ for even k ψ is symmetric under exchange of the space coordinats. For odd k ψ is antisymmetric.

Parallel spins: spin wave function is symmetric $\Rightarrow$ we need odd k's

For $s=0$ (anti parallel spins) the spin wave function is antisymmetric $\Rightarrow$ we need even k's

(a) $S=1$: $\quad k=1 \rightarrow k=3 \qquad E_{ROT} = \dfrac{k(k+1)\hbar^2}{2\mu R_0^2}$

$$\Delta E = \left[(3)(4)-(1)(2)\right]\frac{\hbar^2}{2\mu R_0^2} = \frac{10\hbar^2}{2\mu R_0^2}$$

Here

$$\mu = \frac{m_p}{2} = \frac{1}{2}\left(938\ \mathrm{MeV}/c^2\right) = \frac{1}{2}\left(9.38\times10^{8}\ \mathrm{eV}/c^2\right)$$

$$\Delta E = 10\,\frac{(197.3\,\mathrm{eV\cdot nm})^2}{(2)(\frac{1}{2})(9.38\times10^{8}\,\mathrm{eV})(0.074\,\mathrm{nm})^2} = \boxed{0.0758\,\mathrm{eV}}$$

(b) $S=0$: Even k's $\Rightarrow$ $k=0 \rightarrow k=2 \qquad \Delta E = \left[6-0\right]\dfrac{\hbar^2}{2\mu R_0^2}$

$$= \boxed{0.0455\,\mathrm{eV}}$$

(c) For deuterium we want a symmetric wave function $\Rightarrow$ symmetric spin wave functions go with symmetric space functions $\Rightarrow$ even k. Here $\mu = m_p$ instead of $m_p/2$ so

$k=0 \rightarrow k=2$ gives $\boxed{\Delta E = 0.0227\,\mathrm{eV}}$

26) (a) We have $\frac{k(k+1)\hbar^2}{2\mu R_0^2} = \frac{(1)(2)\hbar^2}{2\mu R_0^2} = 0.002588\,eV$

$$\mu = \frac{(1)(35)}{(1)+(35)}\,u = \frac{35}{36}\,u$$

$$1u \cdot c^2 = (1.66\times10^{-27}\,kg)(3\times10^{8}\,m/s)^2 = 1.494\times10^{-10}\,J$$
$$= 932.6\ MeV.$$

$$\Rightarrow R_0^2 = \frac{(\hbar c)^2}{\frac{35}{36}(9.326\times10^8 eV)(0.002588eV)} = 0.0166\ nm^2$$

$$\boxed{R_0 = 0.12880\ nm}$$

(b) $\hbar\omega = \hbar\sqrt{\frac{k}{\mu}} = 0.357860\ eV$

$$k = \left(\frac{\mu}{\hbar^2}\right)\cdot(\hbar\omega)^2 = \frac{\frac{35}{36}(9.326\times10^8 eV)(0.357860 eV)^2}{(197.3 eV\cdot nm)^2}$$

$$\boxed{k = 2983\ eV/nm^2}$$

(c) So we have
$$V(R) = -V_0 + \frac{1}{2}k(R-R_0)^2 + \frac{k(k+1)\hbar^2}{2\mu R^2}$$

Find the minimum of the full potential

$$\frac{dV}{dR} = k(R-R_0) - 2\frac{k(k+1)\hbar^2}{2\mu R^3} = 0$$

$\Rightarrow$
$$k(R-R_0) = \frac{k(k+1)\hbar^2}{\mu R^3}$$

Technically this is a 4^{th} order polynomial with 4 roots. But the root we want is probably an R just slightly greater than R_0. So try

$$R - R_0 = \frac{1}{k_s}\frac{k(k+1)\hbar^2}{\mu R_0^3} = \frac{1}{2983\,eV/nm^3}\,\frac{(7)(8)(197.3eV\cdot nm)^2}{\frac{35}{36}(9.326\times10^8 eV)(0.1288)^3}$$

$$\boxed{R = R_0 + 3.77\times10^{-4}\,nm}$$

R is very close to R_0, so the approximation of using $R \simeq R_0$ on the R.H.S. is reasonable.

(d) Using $E_7 = 0.072292$ we get

$$\frac{k(k+1)\hbar^2}{2\mu R_0^2} = E_7 \qquad R_0 = \left(\frac{7(8)\hbar^2}{2\mu E_7}\right)^{\frac{1}{2}} = 0.12895\,\text{nm}$$

So the actual stretching is more like 1.5×10^{-4} nm.

27) The wave functions consist of a spin part and a space part

$$\psi = \psi_{n\ell m} = \psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{\frac{3}{2}} e^{-r/a_0}$$

For the spin wave functions use $\chi_s^{m_s}$ where $s=0,1$ and $m_s = -s, \cdots, s$.

First take the matrix elements of W_{dd} where the only part that matters is the second term. Write

$$\vec{S} = \vec{S}_e + \vec{S}_p \quad \Rightarrow \quad S^2 = S_e^2 + S_p^2 + 2\vec{S}_e\cdot\vec{S}_p \quad \Rightarrow$$

$$\vec{S}_e\cdot\vec{S}_p = \frac{1}{2}\left[S^2 - S_e^2 - S_p^2\right]$$

so

$$\langle\chi_s^{m_s}|\vec{S}_e\cdot\vec{S}_p|\chi_s^{m_s}\rangle = \frac{\hbar^2}{2}\left[s(s+1) - \frac{1}{2}\left(\frac{3}{2}\right) - \frac{1}{2}\left(\frac{3}{2}\right)\right] = \left(\frac{s(s+1)}{2} - \frac{3}{4}\right)\hbar^2$$

$$= \begin{cases} -\frac{3}{4}\hbar^2 & s=0 \\ +\frac{1}{4}\hbar^2 & s=1 \end{cases}$$

The spin wave functions $\chi_s^{m_s}$ are eigenfunctions of S^2, S_e^2 and S_p^2 so we get no off-diagonal terms. For the spatial integral we get

$$\langle\psi|\delta^3(\vec{r})|\psi\rangle = \int_{\substack{\text{all}\\\text{space}}} \delta^3(\vec{r})\,|\psi(\vec{r})|^2\,d^3r = |\psi(0)|^2 = \frac{1}{\pi a_0^3}$$

Combining all the parts we have

$$\boxed{\langle \psi_s^{m_s} | W_{dd} | \psi_s^{m_s} \rangle = \frac{\mu_0}{4\pi} e^2 \left(\frac{g_e}{2m_e}\right)\left(\frac{g_p}{2m_p}\right)\left(\frac{2\pi}{3}\right) \times \frac{\hbar^2}{\pi a_0^3} \times \begin{cases} -\frac{3}{4} & s=0 \\ +\frac{1}{4} & s=1 \end{cases}}$$

Next do

$$H = g_e \frac{e}{2m_e} \vec{S}_e \cdot \vec{B} = g_e \frac{eB}{2m_e} S_{e,z} \qquad \text{for } \vec{B} \text{ along } \hat{z}.$$

Now we need explicit spin wave functions

$$X_1^1 = \chi_e^+ \chi_p^+ \qquad X_1^{-1} = \chi_e^- \chi_p^- \qquad X_1^0 = \frac{1}{\sqrt{2}}\left[\chi_e^+ \chi_p^- + \chi_e^- \chi_p^+\right]$$

$$X_0^0 = \frac{1}{\sqrt{2}}\left[\chi_e^+ \chi_p^- - \chi_e^- \chi_p^+\right]$$

Now

$$S_{e,z} \chi_e^\pm = \pm \frac{\hbar}{2} \chi_e^\pm$$

$\Rightarrow$

$$S_{e,z} X_1^1 = \frac{\hbar}{2} \chi_e^+ \chi_p^+ = \frac{\hbar}{2} X_1^1$$

$$S_{e,z} X_1^{-1} = -\frac{\hbar}{2} \chi_e^- \chi_p^- = -\frac{\hbar}{2} X_1^{-1}$$

$$S_{ez} X_1^0 = \frac{1}{\sqrt{2}}\left[\frac{\hbar}{2} \chi_e^+ \chi_p^- + \left(-\frac{\hbar}{2}\right) \chi_e^- \chi_p^+\right] = \frac{\hbar}{2} X_0^0$$

$$S_{ez} X_0^0 = \frac{1}{\sqrt{2}}\left[\frac{\hbar}{2} \chi_e^+ \chi_p^- - \left(-\frac{\hbar}{2}\right) \chi_e^- \chi_p^+\right] = \frac{\hbar}{2} X_1^0$$

From this we can read off all the matrix elements.

Lets order the states as follows

$$\phi_1 = \psi(\vec{r})\, X_1^1$$
$$\phi_2 = \psi(\vec{r})\, X_1^{-1}$$
$$\phi_3 = \psi(\vec{r})\, X_1^0$$
$$\phi_4 = \psi(\vec{r})\, X_0^0$$

$\Rightarrow$

$$H_{11} = \langle \phi_1 | H | \phi_1 \rangle = g_e \left(\frac{eB}{2m_e}\right) \cdot \frac{\hbar}{2} \qquad H_{22} = -g_e \left(\frac{eB}{2m_e}\right) \cdot \frac{\hbar}{2}$$

$$H_{34} = H_{43} = +g_e\left(\frac{eB}{2m_e}\right)\frac{\hbar}{2}$$

Let $\boxed{a = \frac{g_e}{2}\left(\frac{e\hbar}{2m_e}\right)B}$ $\Rightarrow H = \begin{bmatrix} a & 0 & 0 & 0 \\ 0 & -a & 0 & 0 \\ 0 & 0 & 0 & a \\ 0 & 0 & a & 0 \end{bmatrix}$

And for W_{dd} we had

$$W = \begin{bmatrix} b & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & b & 0 \\ 0 & 0 & 0 & -3b \end{bmatrix}$$

where $\boxed{b = \left(\frac{\mu_0}{4\pi}\right) g_e g_p \left(\frac{e\hbar}{2m_e}\right)\left(\frac{e\hbar}{2m_p}\right)\left(\frac{2\pi}{3}\right)\left(\frac{1}{\pi a_0^3}\right)\cdot\left(\frac{1}{4}\right)}$

So overall the perturbation matrix is this.

$$\begin{bmatrix} b+a & 0 & 0 & 0 \\ 0 & b-a & 0 & 0 \\ 0 & 0 & b & a \\ 0 & 0 & a & -3b \end{bmatrix}$$

$\Rightarrow$ to find the eigenvalues.

$$\mathrm{Det}\begin{bmatrix} b+a-E & 0 & 0 & 0 \\ 0 & b-a-E & 0 & 0 \\ 0 & 0 & b-E & a \\ 0 & 0 & a & -3b-E \end{bmatrix} = (b+a-E)(b-a-E)(b-E)(-3b-E) - (b+a-E)(b-a-E)a^2$$

$$= (b+a-E)(b-a-E)\left[(b-E)(-3b-E) - a^2\right]$$

$$= \quad '' \qquad '' \quad \left[E^2 + 2bE - 3b^2 - a^2\right]$$

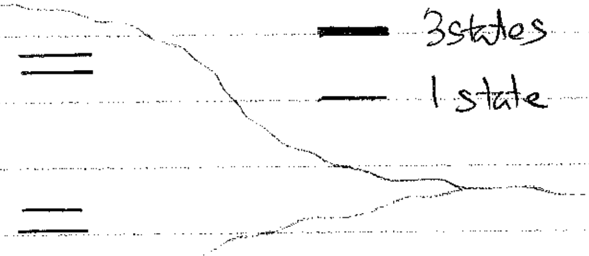
so the roots are

$\boxed{E_1 = b+a \quad E_2 = b-a}$ and $E = \dfrac{-2b \pm \left[4b^2 + 4(3b^2 + a^2)\right]^{\frac{1}{2}}}{2}$

$$E = -b \pm \left[b^2 + 3b^2 + a^2\right]^{\frac{1}{2}} = -b \pm \left[4b^2 + a^2\right]^{\frac{1}{2}}$$

$$\boxed{E_3 = -b + \left[4b^2 + a^2\right]^{\frac{1}{2}}} \quad \boxed{E_4 = -b - \left[4b^2 + a^2\right]^{\frac{1}{2}}}$$

In zero field $a = 0 \Rightarrow E_1 = E_2 = E_3 = b$; $E_4 = -3b$.



In strong field $a >> b \Rightarrow$

$E_1 = a + b \qquad E_2 = -a + b$

$E_3 \simeq a - b \qquad E_4 = -a - b$

For the eigenstates we have $\boxed{\psi_1 = \phi_1}$ $\boxed{\psi_2 = \phi_2}$ and ψ_3 and ψ_4 are linear combinations of ϕ_3 and ϕ_4

$$\begin{bmatrix} b & a \\ a & -3b \end{bmatrix}\begin{bmatrix} \alpha_3 \\ \alpha_4 \end{bmatrix} = \begin{bmatrix} b\alpha_3 + a\alpha_4 \\ a\alpha_3 - 3b\alpha_4 \end{bmatrix} = E\begin{bmatrix} \alpha_3 \\ \alpha_4 \end{bmatrix}$$

<u>State 3</u>

$$b\alpha_3 + a\alpha_4 = \left(-b + \left[4b^2 + a^2\right]^{\frac{1}{2}}\right)\alpha_3 \Rightarrow \underline{2b\alpha_3 + a\alpha_4 = [\cdots]^{\frac{1}{2}}\alpha_3}$$

$$a\alpha_3 - 3b\alpha_4 = \left(-b + \left[4b^2 + a^2\right]^{\frac{1}{2}}\right)\alpha_4 \Rightarrow \underline{a\alpha_3 - 2b\alpha_4 = [\cdots]\,\alpha_4}$$

The second equation gives

$$a\alpha_3 = \left(\left[4b^2 + a^2\right]^{\frac{1}{2}} + 2b\right)\alpha_4$$

and to normalize we need $\alpha_3^2 + \alpha_4^2 = 1 \Rightarrow$

$$\alpha_4^2 + \left[\frac{(4b^2 + a^2)^{\frac{1}{2}} + 2b}{a}\right]^2 \alpha_4^2 = 1$$

$$\alpha_4^2 \left[\frac{a^2 + \left(2b + \sqrt{4b^2 + a^2}\right)^2}{a^2}\right] = 1$$

$$\alpha_4^2 = \frac{a^2}{a^2 + 4b^2 + (4b^2 + a^2) + 4b\sqrt{4b^2 + a^2}}$$

$$\alpha_4 = \frac{a}{\left[8b^2+2a^2+4b\sqrt{4b^2+a^2}\right]^{\frac{1}{2}}}$$

$\Rightarrow$

$$\alpha_3 = \sqrt{1-\alpha_4^2} = \frac{2b+\sqrt{4b^2+a^2}}{\left[8b^2+2a^2+4b\sqrt{4b^2+a^2}\right]^{\frac{1}{2}}}$$

LIMITS

$B \to 0 \Rightarrow a \to 0 \quad \alpha_3 \to 1 \quad \psi_3$ has $S=1, m_s=0$

$B \to$ large $\Rightarrow a >> b \quad \alpha_3 \to \frac{1}{\sqrt{2}} \quad \alpha_4 \to \frac{1}{\sqrt{2}} \quad \psi_4 \to \chi_e^+ \chi_p^-$

State 4:

$$b\alpha_3 + a\alpha_4 = \left(-b - \left[4b^2+a^2\right]^{\frac{1}{2}}\right)\alpha_3$$

$$a\alpha_3 - 3b\alpha_4 = \left(\quad '' \quad \right)\alpha_4$$

From the 1st equation

$$a\alpha_4 = -\left(2b + \left[4b^2+a^2\right]^{\frac{1}{2}}\right)\alpha_3$$

By the same algebra

$$\alpha_4 = \frac{2b+\sqrt{4b^2+a^2}}{\left[8b^2+2a^2+4b\sqrt{4b^2+a^2}\right]^{\frac{1}{2}}}$$

and

$$\alpha_3 = \frac{-a}{\left[8b^2+2a^2+4b\sqrt{4b^2+a^2}\right]^{\frac{1}{2}}}$$

$B \to 0 \Rightarrow \quad \alpha_4 \to 1 \quad \psi_4 \simeq \phi_4 \Rightarrow S=0, m_s=0$

$B \to$ large $\Rightarrow \quad \alpha_4 \to \frac{1}{\sqrt{2}} \quad \alpha_3 \to -\frac{1}{\sqrt{2}} \quad \psi_4 \to -\chi_e^- \chi_p^+$