OtherAtoms

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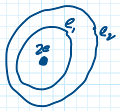
Other Atoms

⟹ The Ground State of Helium

⟹ many electron system



⟹ Indistinguishability in QM.

Quantum Particles ar indistinguishable

what this means.

- Say on has N indistinguishable Particle described by quantum State of

$$|\psi(1,2,3,4,\cdots i,j \cdots N\rangle$$

- They are indistinguishable if their Hamiltonian H commuts with P_{ij} – permutation operator

$$[H, P_{ij}] = 0$$

- Therefore both Should have same eigenstates

Find the eigenstates:

- Consider $P_{ij}|\psi(1,2,3\ldots i,j\cdots N\rangle = |\psi(1,2\ldots j,i\cdots N)$

apply again

$$P_{ij}P_{ij}|\psi(1,2\cdots i,j\cdots N\rangle = P_{ij}|\psi(1,2\cdots j,i\cdots N\rangle$$

$$= |\psi(1,2\cdots i,j\cdots N\rangle$$

- Therefore $P_{ij}^2|\psi(1,2\cdots i,j\cdots N\rangle = \lambda^2|\psi(1,2\cdots i,j\cdots N\rangle$

where $\lambda^2 = 1$

- if one have eigenstate of Permutation Operator $\hat{P}_{ij}$, they should have two eigenvalues + and –

$$P_{ij}|\psi_+(1,2\cdots i,j\cdots N\rangle = |\psi_+(1,2\cdots i,j\cdots N)$$

$$\Downarrow \qquad \Downarrow$$

$$\psi_+(1,2\cdots j,i\cdots N\rangle = |\psi_+(1,2\cdots i,j\cdots N\rangle$$

Symmetric vs i j

$$P_{ij}|\psi_-(1,2\cdots i,j\cdots N)\rangle = -1|\psi_-(1,2\cdots i,j\cdots N)\rangle$$

$$\Downarrow$$

$$|\psi_-(1,2\cdots j,i\cdots N)\rangle = -|\psi_-(1,2\cdots i,j\cdots N)\rangle$$

antisymmetric vs $i \rightleftarrows j$

$+ \longrightarrow$ Bosons

$- \longrightarrow$ Fermions

$\Rightarrow$ Consider Two Electron Case

$$P_{ij}\,\psi_-|q_1,q_2\rangle = \psi|q_2 q_1\rangle = -\psi(q_1 q_2)$$

Follows the Pauli Principle that two Fermions can not be in the same quantum state

$$P_{ij}\,\psi(q_1 q_2) = |\psi(q_2 q_1)\rangle = -\psi(q_1 q_2)\rangle$$

if $q_1 = q_2$

$$|\psi(q q)\rangle = -|\psi(q q)\rangle = 0$$

– Hamiltonian of 2-electron Atom

$$H_0 = \frac{P_1^2}{2m} - \frac{Z\alpha}{r_1} + \frac{P_2^2}{2m} - \frac{Z\alpha}{r_2} + \frac{\alpha}{|r_1 - r_2|}$$

– Eigenstate

$$|\psi\rangle|n_1 \ell_1 m_1\, \overset{\frac{1}{2}}{s_1} m_{s_1};\ n_2 \ell_2 m_2\, \overset{\frac{1}{2}}{s_2} m_{s_2}\rangle$$

antisymmetric $n_1 \ell_1 m_1 m_{s_1} \rightleftarrows n_2 \ell_2 m_2 m_{s_2}$

– Wave Function – Consider the Ground State

$$\Phi_{J M_J n_1 n_2} = \sum C^{J M_J}_{j_1 j_2} |\psi\rangle_{n_1 \ell_1 m_1 m_{s_1} n_2 \ell_2 m_2 m_{s_2}}$$

$$J = J_1 + J_2 \qquad J_1 = L_1 + S_1 \quad J_2 = L_2 + S_2$$

G.S $\ell_1 = 0 \quad \ell_2 = 0$

$$\Phi_{J, M_J\, 1 1} = C^{J M_J}_{S_1 m_{s_1} S_2 m_{s_2}} |\psi_{100, m_{s_1}, 100\, m_{s_2}}\rangle$$

antisymmetric $m_{s_1} \rightleftarrows m_{s_2}$

$$J = S_1 + S_2, \qquad \begin{array}{l} J = 1 \\ J = 0 \end{array}$$

$J = 1 \qquad |\Phi_{11}\rangle = |\chi_{\frac{1}{2}}\rangle|\chi_{\frac{1}{2}}\rangle = |\chi_{m_{s_1}}\rangle|\chi_{m_{s_2}}\rangle$

$$|\Phi_{10}\rangle = \frac{1}{\sqrt{2}}\left(|\chi^1_{\frac{1}{2}}\rangle|\chi^2_{-\frac{1}{2}}\rangle + |\chi_{-\frac{1}{2}}\rangle|\chi_{\frac{1}{2}}\rangle\right)$$

$|\phi_{1-1}\rangle = |\chi_{-\frac{1}{2}}\rangle|\chi_{-\frac{1}{2}}\rangle$

This is not antisymmetric

$J=0 \quad |\overset{spin}{\phi_{00}}\rangle = \frac{1}{\sqrt{2}}\left(\overset{u_1}{|\chi_{+\frac{1}{2}}\rangle}\overset{d_2}{|\chi_{-\frac{1}{2}}\rangle} - \overset{d_1}{|\chi_{-\frac{1}{2}}\rangle}\overset{u_2}{|\chi_{\frac{1}{2}}\rangle}\right)$

$\underset{J\ m_J}{\phi_{00}^{100;100}} = |\psi_{100}\rangle|\psi_{100}\rangle \cdot \frac{1}{\sqrt{2}}(u_1 d_2 - d_1 u_2)$

Wave Function

$$\boxed{\psi(r_1 r_2) = R_{10}(r_1)Y_0(\hat{r}_1)R_{10}(r_2)Y_0(\hat{r}_2)\frac{1}{\sqrt{2}}(u_1 d_2 - d_1 u_2)}$$

$\Rightarrow$ if interaction between electrons are neglected

$$H = H_0 = \frac{P_1^2}{2m} - \frac{Z\alpha}{r_1} + \frac{P_2^2}{2m} - \frac{Z\alpha}{r_2}$$

$$E_{n_1 n_2} = -\frac{Z^2\alpha^2 m}{2n_1^2} - \frac{Z^2\alpha^2 m}{2n_2^2}$$

This is 0'th order

	Zero Order	Experiment
H^-	-27.21	-14.35
He	-108.85	-78.93
Li^+	-244.90	-198.1

1'st order $H' = \frac{\alpha}{|r_1 - r_2|}$

$$\Delta' = \langle \psi_{\substack{100,m_{s_1}\\100,m_{s_2}}} | \frac{\alpha}{|r_1-r_2|} | \psi_{\substack{100,m_{s_1}\\100,m_{s_2}}} \rangle =$$

$$= \int \psi_{100}^{+}(r_1)Y_0(\hat{r}_1)\psi_{100}^{+}(r_2)Y_0(\hat{r}_2)\frac{\alpha}{|r_1-r_2|}\psi_{100}(r_1)Y_0(\hat{r}_1)\psi_{100}(r_2)Y_0(\hat{r}_2)\, d^3r_1\, d^3r_2$$

$$\psi_{100} = \sqrt{\frac{Z^3}{\pi a^3}}\, e^{-\frac{Zr}{a}} \qquad E_1^0 = -\frac{\alpha^2 m}{2}$$

$$a = \frac{1}{m\alpha}$$

$$\Delta' = \frac{\alpha [illegible]}{\pi^2 a^6}\iint \frac{e^{[illegible]}e^{[illegible]}}{|r_1-r_2|}\, dr_1\, dr_2$$

For evaluation of this Integral use

$$\frac{1}{r} = \frac{4\pi}{(2\pi)^3}\int \frac{1}{k^2} e^{i\vec{k}\vec{r}} d^3k$$

$$\Delta^{(1)} = \frac{\cancel{e} z^6}{a^6 2\pi^4}\int \frac{1}{k^2}\left(\int e^{-\frac{2zr}{a}} e^{i\vec{k}\vec{r}} d^3r\right)^2 d^3k$$

$$\Delta' = \frac{128\alpha}{\pi^2}\left(\frac{z}{a}\right)^8 \int \frac{1}{k^2\left\{\left(\frac{2z}{a}\right)^2 + k^2\right\}^4} d^3k = -\frac{5}{4} z E_0$$

$$\Delta^{(1)} = -\frac{5}{4} z E_0$$

$$E_G = 2E_0 - \frac{5}{4} z E_0 = \left(2 - \frac{5}{4} z\right) E_0$$

System is bound if $E_G^{2z} < E^{z}$

	First Order	Experiment	Single E	
H^-	-10.20	-14.35	-13.61	Will decay to $H + e$
He	-74.83	-78.85	-54.43	
Li^+	-193.28	-198.1	-122.45	