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Problem 2

2 electrons or any 2 1/2 spin particles, 2-body wavefunction for which the sum of the two spins equals 1 does not change its value when exchanged. For the sum 0 we see antisymmetry.

we have, $S_1 = (S_{1x}, S_{1y}, S_{1z})$

$S_2 = (S_{2x}, S_{2y}, S_{2z})$

$$|(S_1+S_2)|^2 = |S_1|^2 + |S_2|^2 + 2(S_1 \cdot S_2)$$

$$= S_1(S_1+1)\hbar^2[I] + S_2(S_2+1)\hbar^2[I] + 2S_1 \cdot S_2$$

$$= \frac{3}{4} + \frac{3}{4} + 2S_1 \cdot S_2 = \frac{1}{2}\left(3 + 4(S_1 \cdot S_2)\right)$$

$$\psi_{2body} = \begin{bmatrix} \psi(\frac{1}{2}, \frac{1}{2}) \\ \psi(\frac{1}{2}, -\frac{1}{2}) \\ \psi(-\frac{1}{2}, \frac{1}{2}) \\ \psi(-\frac{1}{2}, -\frac{1}{2}) \end{bmatrix}$$

We can calculate $[S_1 \cdot S_2]\psi$

where $S_1 \cdot S_2 = S_{1x}S_{2x} + S_{1y}S_{2y} + S_{1z}S_{2z}$

$S_1 \cdot S_2 \psi = [S_{1x}S_{2x} + S_{1y}S_{2y} + S_{1z}S_{2z}]\psi$

we know that $S_x \psi = \frac{\hbar}{2}\sigma_x \psi = \frac{\hbar}{2}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\begin{bmatrix}\phi_1(x)\\ \phi_2(x)\end{bmatrix}$

$$= \frac{\hbar}{2}\begin{bmatrix}\phi_2(x)\\ \phi_1(x)\end{bmatrix}$$

$$S_y \psi = \frac{\hbar}{2}\sigma_y \psi = \frac{\hbar}{2}\begin{bmatrix}-i\phi_2(x)\\ i\phi_1(x)\end{bmatrix}$$

$$S_z \psi = \frac{\hbar}{2}\sigma_z \psi = \frac{\hbar}{2}\begin{bmatrix}\phi_1(x)\\ -\phi_2(x)\end{bmatrix}$$

$$S_{2z}\psi_{2\text{-body}} = \begin{bmatrix}\frac{1}{2}\psi(+\frac{1}{2}, +\frac{1}{2})\\ -\frac{1}{2}\psi(+\frac{1}{2}, -\frac{1}{2})\\ \frac{1}{2}\psi(-\frac{1}{2}, \frac{1}{2})\\ -\frac{1}{2}\psi(-\frac{1}{2}, -\frac{1}{2})\end{bmatrix}$$

$$S_{1z}S_{2z}\psi_{2\text{-body}} = \begin{bmatrix}\frac{1}{4}\psi(\frac{1}{2}, \frac{1}{2})\\ -\frac{1}{4}\psi(\frac{1}{2}, -\frac{1}{2})\\ -\frac{1}{4}\psi(-\frac{1}{2}, \frac{1}{2})\\ \frac{1}{4}\psi(-\frac{1}{2}, -\frac{1}{2})\end{bmatrix}$$

$$S_{2y}\psi_{2\text{-body}} = \begin{bmatrix}-\frac{i}{2}\psi(\frac{1}{2}, -\frac{1}{2})\\ \frac{i}{2}\psi(\frac{1}{2}, +\frac{1}{2})\\ -\frac{i}{2}\psi(-\frac{1}{2}, -\frac{1}{2})\\ \frac{i}{2}\psi(-\frac{1}{2}, +\frac{1}{2})\end{bmatrix}$$

$$S_{1y} S_{2y} \Psi_{2\text{-body}} = \begin{bmatrix} -\frac{1}{4}\Psi\left(\frac{-1}{2}, \frac{-1}{2}\right) \\ \frac{1}{4}\Psi\left(\frac{-1}{2}, \frac{1}{2}\right) \\ \frac{1}{4}\Psi\left(\frac{1}{2}, \frac{-1}{2}\right) \\ -\frac{1}{4}\Psi\left(\frac{1}{2}, \frac{1}{2}\right) \end{bmatrix}$$

$$S_{1x} S_{2x} \Psi_{2\text{-body}} = \begin{bmatrix} \frac{1}{4}\Psi\left(\frac{-1}{2}, \frac{-1}{2}\right) \\ \frac{1}{4}\Psi\left(-\frac{1}{2}, \frac{1}{2}\right) \\ \frac{1}{4}\Psi\left(\frac{1}{2}, \frac{-1}{2}\right) \\ \frac{1}{4}\Psi\left(\frac{1}{2}, \frac{1}{2}\right) \end{bmatrix}$$

$$\therefore [S_1 \cdot S_2] \Psi_{2\text{ body}} = \begin{bmatrix} \frac{1}{4}\Psi\left(\frac{1}{2}, \frac{1}{2}\right) \\ \frac{1}{2}\Psi\left(-\frac{1}{2}, \frac{1}{2}\right) - \frac{1}{4}\Psi\left(\frac{1}{2}, -\frac{1}{2}\right) \\ \frac{1}{2}\Psi\left(\frac{1}{2}, -\frac{1}{2}\right) - \frac{1}{4}\Psi\left(-\frac{1}{2}, \frac{1}{2}\right) \\ \frac{1}{4}\Psi\left(-\frac{1}{2}, -\frac{1}{2}\right) \end{bmatrix}$$

$$|S_1 + S_2|^2 \Psi_{2\text{-body}} = \frac{1}{2}[(3 + 4(S_1 \cdot S_2)]$$

$$= \begin{bmatrix} 2\Psi\left(\frac{1}{2}, \frac{1}{2}\right) \\ \Psi\left(-\frac{1}{2}, \frac{1}{2}\right) + \Psi\left(\frac{1}{2}, -\frac{1}{2}\right) \\ \Psi\left(\frac{1}{2}, -\frac{1}{2}\right) + \Psi\left(-\frac{1}{2}, \frac{1}{2}\right) \\ 2\Psi\left(\frac{-1}{2}, -\frac{1}{2}\right) \end{bmatrix} \rightarrow (1)$$

total spin = 1 (Case 1)

$\Rightarrow |S_1 + S_2|^2 \psi_{2\text{-body}} = 1(1+1)\psi_{2\text{-body}} = 2\psi_{2\text{-body}}$

When total spin = 0 (Case 2)

$\Rightarrow |S_1 + S_2|^2 \psi_{2\text{-body}} = 0$

For case 1:

If we compare the ψ_{2body} matrix with 1,

$\psi(\frac{1}{2}, \frac{-1}{2}) + \psi(\frac{-1}{2}, \frac{1}{2}) = 2\psi(\frac{1}{2}, \frac{-1}{2})$

$\psi(\frac{-1}{2}, \frac{1}{2}) = \psi(\frac{1}{2}, \frac{-1}{2})$

$\therefore \psi(S_{1z}, S_{2z}) = \psi(S_{2z}, S_{1z}) \rightarrow$ 2

In case 2:

$\psi(\frac{1}{2}, \frac{1}{2}) = \psi(\frac{-1}{2}, \frac{-1}{2}) = 0$ is required.

$\psi(\frac{1}{2}, \frac{-1}{2}) = \psi(\frac{-1}{2}, \frac{1}{2}) = 0.$

$\Rightarrow \psi(S_{1z}, S_{2z}) = -\psi(S_{2z}, S_{1z}) \rightarrow$ 3

Hence 2, 3 hence proved

Problem 3

Determine and Derive K_{1s1s}, K_{1s2s}, J_{1s2s}

The ground state wavefunction of H_1, H_2 in $H_0 = H_1 + H_2$ where $H_1 = \frac{|p_1|^2}{2m_0} - \frac{2e^2}{4\pi\varepsilon_0|r_1|}$

$$H_2 = \frac{|p_2|^2}{2m_0} - \frac{2e^2}{4\pi\varepsilon_0|r_2|}$$

is $\phi_{1s}(r) = \frac{1}{\sqrt{\pi a_{He}^3}} e^{-\frac{r}{a_{He}}}$

and $\phi_{2s}(r) = \frac{1}{\sqrt{8\pi a_{He}^3}}\left(1 - \frac{r}{2a_{He}}\right) e^{-\frac{r}{2a_{He}}}$

$a_{He} = \frac{a_0}{2}$ $a_0 = 0.529 A^\circ$

~~K_{1s2s}~~ $K_{1s1s} = \int dr_1 \int dr_2 \left[\frac{e|\phi_{1s}(r_1)|^2 e|\phi_{1s}(r_2)|^2}{4\pi\varepsilon_0|r_{21}|}\right]$

$$K_{1s1s} = \int dr_1 \int dr_2 \, e\frac{|\phi_{1s}(r_1)|^2 \cdot e|\phi_{1s}(r_2)|^2}{4\pi\varepsilon_0|r_1 - r_2|} \quad (1)$$

$$\frac{1}{r_{12}} = \frac{1}{2\pi^2}\int dk \, \frac{e^{ik\cdot(\bar{r}_1 - \bar{r}_2)}}{k^2} \quad \text{(fourier transform)} \quad (2)$$

Putting (2) in (1), we get

$$K_{1s1s} = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{2\pi^2}\int \frac{dk}{k^2}\left(\int dr_1\, e^{ik\cdot r_1}\,|\phi_{1s}(r_1)|^2\right)\left(\int d\bar{r}_2\, e^{-ik\cdot r_2}\,|\phi_{1s}(r_2)|^2\right).$$

$$= \frac{1}{4\pi\varepsilon_0}\frac{e^2}{2\pi^2}\int \frac{dk}{k^2}\, g(k)\, g^*(k)$$

we can conside.

$$g(k) = \int dr\, e^{ikr}\,|\phi_{1s}(r)|^2.$$

$$g(k) = \int dr\, e^{ikr}\left|\frac{1}{\sqrt{\pi a_{He}^3}}\, e^{-\frac{r}{a_{He}}}\right|^2.$$

$|\phi_{1s}(r)|^2$ depends only on magnitude of r, we can select the vector to lie in the direction of a certain z-axis

$$g(k) = \int_0^{\infty} dr\, r^2\, 2\pi \int_0^{\pi} d\theta\, \sin\theta\, e^{ikr\cos\theta}\,|\phi_{1s}(r)|^2.$$

Using ~~mat~~ online integrator, the above can be simplified to yield

$$g(k) = \frac{16}{\left(4 + a_{He}^2 k^2\right)^2}$$

$\cancel{k_e = \frac{1}{4\pi\epsilon_0}}$

$$K_{1s1s} = \frac{1}{4\pi\epsilon_0}\frac{e^2}{2\pi^2}\int\frac{dk}{k^2}\left(\frac{16}{(4+a^2_{He}k^2)^2}\right)^2$$

ousoug yields

$$\frac{5e^2}{32\pi\epsilon_0 a_0}.$$

$$\phi_{2s}(r) = \frac{1}{\sqrt{8\pi a^3_{He}}}\left(1-\frac{r}{2a_{He}}\right)e^{-\frac{r}{2a_{He}}}$$

$$K_{1s2s} = \frac{1}{4\pi\epsilon_0}\frac{e^2}{2\pi^2}\int\frac{d\bar{k}}{k^2}\int dr_1 e^{ikr_1}|\phi_{1s}(r_1)|^2)$$

$$\times \int dr_2 e^{-ikr_2}|\phi_{2s}(r_2)|^2).$$

$$K_{1s2s} = \frac{1}{4\pi\epsilon_0}\frac{e^2}{2\pi^2}\int\frac{dk}{k^2}g_1(k)g_2(k)$$

~~to~~ simplify $g_1(k) = \int dr e^{ikr}|\phi_{1s}(r)|^2.$

$$g_1(k) = \int dr\, e^{ikr}|\phi_{1s}(r)|^2$$

$$= \int_0^\infty dr\, r^2 2\pi\int_0^\pi d\theta\sin\theta\, e^{ikr\cos\theta}|\phi_{1s}(r)|^2$$

$$= \frac{16}{(4+a_0^2k^2)^2}$$

$$g_2(k) = \int dr\, e^{-ikr} |\phi_{2s}(r)|^2$$

$$= \int_0^\infty dr\, r^2 2\pi \int_0^\pi d\theta \sin\theta\, e^{ikr\cos\theta} |\phi_{2s}(r)|^2$$

$$= \frac{1 - 3a_{He}^2 k^2 + 2a_{He}^4 k^4}{(1 + 2a_{He}^4 k^4)^2}$$

$$\therefore K_{1s2s} = \frac{1}{4\pi\varepsilon_0} \frac{e^2}{2\pi^2} \int \frac{dk}{k^2} \left(\frac{16}{(4 + a_0^2 k^2)^2}\right) \left(\frac{1 - 3a_{He}^2 k^2 + 2a_{He}^4 k^4}{(1 + 2a_{He}^4 k^4)^2}\right)$$

$$= \frac{17e^2}{162 a_0} \pi \varepsilon_0$$

Now to calculate exchange engy, J_{1s2s}

$$J_{1s2s} = \frac{1}{4\pi\varepsilon_0} \frac{e^2}{2\pi^2} \int \frac{dk}{k^2} \int dr_1\, e^{ikr} \phi_{1s}(r_1) \phi_{2s}^*(r_1) \int dr_2\, e^{-ikr_2} \phi_{2s}(r_2) \phi_{1s}^*(r_2))$$

$$g_{12}(k) = \int dr\, e^{ikr} \phi_{1s}(r) \phi_{2s}^*(r)$$ if we consider

$$= \frac{256\sqrt{2} a_{He}^2 k^2}{(9 + 4a_{He}^2 k^2)^3}$$

$$\Rightarrow J_{1s2s} = \frac{8e^2}{729 a_0 \pi \varepsilon_0}$$

HW#8

Problem 1

Derive the four spinorial parts in a 2-ē system and apply the operators S^2 and S_z on them.

$$S = S_1 + S_2 = \frac{\hbar}{2}\sigma_1 + \frac{\hbar}{2}\sigma_2$$

$$\sigma = (\sigma_x, \sigma_y, \sigma_z)$$

$$S^2 = S.S = \frac{\hbar^2}{4}(\sigma_1^2 + \sigma_2^2 + 2\sigma_1.\sigma_2) = \frac{\hbar^2}{2}(3I + \sigma_1.\sigma_2)$$

$$\sigma_1.\sigma_2 = \sigma_{1x}\sigma_{2x} + \sigma_{1y}\sigma_{2y} + \sigma_{1z}\sigma_{2z}$$

$\sigma_x|0\rangle = |1\rangle$; $\sigma_y|0\rangle = i|1\rangle$; $\sigma_z|0\rangle = |0\rangle$; $\sigma_x|1\rangle = |0\rangle$

$\sigma_y|1\rangle = -i|0\rangle$; $\sigma_z|1\rangle = -|1\rangle$.

$$\sigma_1.\sigma_2|0\rangle_1|0\rangle_2 = |0\rangle_1|0\rangle_2$$

$$S^2|0\rangle_1|0\rangle_2 = \frac{\hbar^2}{2}(3I + \sigma_1.\sigma_2)|0\rangle_1|0\rangle_2$$

$$= 2\hbar^2|0\rangle_1|0\rangle_2$$

$$S_z|0\rangle_1|0\rangle_2 = \frac{\hbar}{2}[\sigma_{1z}|0\rangle_1|0\rangle_2 + \sigma_{2z}|0\rangle_1|0\rangle_2] = \hbar$$

Similarly for $\Xi_S(S_1,S_2) = \frac{1}{\sqrt{2}}[|0\rangle_1|1\rangle_2 + |0\rangle_2|1\rangle_1]$

$$S^2\,\Xi_S(S_1,S_2) = \frac{\hbar^2}{2}(3I + \sigma_1.\sigma_2)\left(\frac{1}{\sqrt{2}}|0\rangle_1|1\rangle_2 + |0\rangle_2|1\rangle_1\right]$$

$$\cancel{= \frac{\hbar^2}{2}(3I + \sigma_1.\sigma_2)}$$

$$\sigma_1.\sigma_2(\Xi_S(S_1,S_2)) = \frac{1}{\sqrt{2}}\big(\sigma_{1x}|0\rangle_1\sigma_{2x}|1\rangle + \sigma_{1y}|0\rangle\sigma_{2y}|1\rangle + \sigma_{1z}|0\rangle\sigma_{2z}|1\rangle$$

$$+ \sigma_{1x}|1\rangle\sigma_{2x}|0\rangle + \sigma_{1y}|1\rangle\sigma_{2y}|0\rangle + \sigma_{1z}|1\rangle\sigma_{2z}|0\rangle\big]$$

$$S^2 E_S(s_1,s_2) = \frac{\hbar^2}{2}(3I+\sigma_1.\sigma_2)\left(\frac{1}{\sqrt2}|0\rangle_1|1\rangle_2 + |0\rangle_2|1\rangle_1\right)$$
$$= 2\hbar^2.$$

$$S_2\left(\frac{1}{\sqrt2}|0\rangle_1|1\rangle_2 + |0\rangle_2|1\rangle_1\right) = \frac{1}{\sqrt2}\frac{\hbar}{2}\Big[\sigma_{12}|0\rangle_1|1\rangle_2 + \sigma_{22}|0\rangle_1|1\rangle_2$$
$$+ \sigma_{12}|0\rangle_2|1\rangle + \sigma_{22}|0\rangle_2|1\rangle_1\Big)$$
$$= 0$$

Now for $E_S(s_1,s_2) = |1\rangle_1|1\rangle_2$

$$S^2 E_S(s_1,s_2) = \frac{\hbar^2}{2}(3I+\sigma_1.\sigma_2)(|1\rangle_1|1\rangle_2)$$

$$\sigma_1.\sigma_2(|1\rangle_1|1\rangle_2) = \sigma_{1x}|1\rangle_1\sigma_{2x}|1\rangle_2 + \sigma_{1y}|1\rangle_1\sigma_{2y}|1\rangle_2$$
$$+ \sigma_{1z}|1\rangle_1\sigma_{2z}|1\rangle_2$$
$$= |0\rangle|0\rangle + \ -|0\rangle|0\rangle \ + |1\rangle|1\rangle.$$

$$S^2 E_S(s_1,s_2) = \frac{\hbar^2}{2}(3I+\sigma_1.\sigma_2)(|1\rangle_1|1\rangle_2)$$
$$= \frac{\hbar^2}{2}(3I(|1\rangle_1|1\rangle_1 + |1\rangle_1|1\rangle_1)$$
$$= 2\hbar^2$$

$$S_2(|1\rangle_1|1\rangle_2) = \frac{\hbar}{2}[\sigma_{1z}|1\rangle|1\rangle_1 + \sigma_{2z}|1\rangle|1\rangle_2)$$

$$= \frac{\hbar}{2}[-|1\rangle_1|1\rangle_2 - |1\rangle_1|1\rangle]$$

$$= -\hbar.$$

For $\Xi_A(s_1, s_2) = \frac{1}{\sqrt{2}}[|0\rangle_1|1\rangle_2 - |0\rangle_2|1\rangle_1]$,

$$S^2 E_A(s_1,s_2) = \frac{\hbar}{2}^2(3I + \sigma_1 \cdot \sigma_2)\left[\frac{1}{\sqrt{2}}|0\rangle_1|1\rangle_2 - |0\rangle_2|1\rangle_1\right]$$

$$= \frac{\hbar}{2}^2 \, \sigma_1 \cdot \sigma_2 \left[\frac{1}{\sqrt{2}}|0\rangle_1|1\rangle_2 - |0\rangle_2|1\rangle_1\right]$$

$$= \frac{1}{\sqrt{2}}\Big[\sigma_{1x}|0\rangle_1\sigma_{2x}|1\rangle_2 + \sigma_{1y}|0\rangle_1\sigma_{2y}|1\rangle_2 + \sigma_{1z}|0\rangle_1\sigma_{2z}|1\rangle_2$$
$$- \sigma_{1x}|0\rangle_1\sigma_{2x}|0\rangle_2 - \sigma_{2y}|0\rangle\sigma_{1y}|1\rangle_1 + \sigma_{1z}|1\rangle\sigma_{2z}|0\rangle_2\Big]$$

$$S^2 E_A(s_1,s_2) = 0.$$

$$S_2 E_A(s_1,s_2) = \frac{\hbar}{2}\frac{1}{\sqrt{2}}\Big[\sigma_{1z}(|0\rangle_1|1\rangle_2 - |0\rangle_2|1\rangle_1)$$
$$+ \sigma_{2z}(|0\rangle_1|1\rangle_2 - |0\rangle_2|1\rangle_1)\Big)$$

$$= \underline{\underline{0}}$$