E490: Orientation of singlet state

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The problem:

Two electrons occupy the same orbit. Find the polarization vector of each electron.

The solution:

Electrons are physical entities with spin $\frac{1}{2}$. According to the "spin and statistics theorem", particles with half-odd-integer spins (fermions) must be in an antisymmetric state (Pauli Exclusion Principle).

From here we learn that the particles are in one of the following configurations:
1. the position wave functions of the particles are symmetrical and their spins are antisymmetrical.
2. the position wave functions of the particles are antisymmetrical and their spins are symmetrical.

Let us define the position of the first electron as x_1 and the second electron as x_2, and m_{s1}, m_{s2} as the spin-magnetic quantum states.

The eigenfunction is as follows:

$$|\Psi\rangle = |\phi(x_1, x_2)\rangle \otimes |\chi(m_{s1}, m_{s2})\rangle$$

Where ϕ is the spacial part of the wave function and χ is the spin function.
Since we are dealing with two spin $\frac{1}{2}$ we will use the singlet-triplet basis to simplify our calculations.
In order to calculate the polarization vector we will need to use Pauli matrices as our basis.
We expand the Pauli matrices for the spin $\frac{1}{2}$ base. For the first electron we have:

$$\hat{S}_x^{(1)} = \hat{S}_x \otimes \hat{1}_{(2\times2)} = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

And:

$$\hat{S}_y^{(1)} = \hat{S}_y \otimes \hat{1}_{(2\times2)} = \frac{1}{2}\begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}; \quad \hat{S}_z^{(1)} = \hat{S}_z \otimes \hat{1}_{(2\times2)} = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

For the second electron:

$$\hat{S}_x^{(2)} = \hat{1}_{(2\times2)} \otimes \hat{S}_x = \frac{1}{2}\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}; \quad \hat{S}_y^{(2)} = \hat{1}_{(2\times2)} \otimes \hat{S}_y = \frac{1}{2}\begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}$$

$$\hat{S}_z^{(2)} = \hat{1}_{(2\times2)} \otimes \hat{S}_z = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

The Polarization vector is defined as:

$$\overline{M}^{(i)} = (< \hat{S}_x^{(i)} >, < \hat{S}_y^{(i)} >, < \hat{S}_z^{(i)} >)$$

We assume now that the electrons spacial parts of the wave functions is symmetric, hence we are left with the singlet state:

$$|\chi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

$$\langle\chi|\,\hat{S}_x^{(1)}\,|\chi\rangle = \frac{1}{4}\begin{pmatrix} 0 & 1 & -1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} = 0$$

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Giving:

$$\overline{M}^{(1)} = (0, 0, 0)$$

And we recieve the same answer for the second electron:

$$\overline{M}^{(2)} = (0, 0, 0)$$

We see the polarization vectors are not normalized. that is due to the fact the antisymmetric state is entagled.
We now consider other cases where the spacial parts of wave functions are antisymmetrical (without neglecting the fact that both occupy the same orbit).
The remaining states are the triplet states:

i) The triplet first state:

$$|\chi\rangle = |\uparrow\uparrow\rangle$$

$$\langle\chi|\,\hat{S}_x^{(1)}\,|\chi\rangle = 0; \quad \langle\chi|\,\hat{S}_y^{(1)}\,|\chi\rangle = 0; \quad \langle\chi|\,\hat{S}_z^{(1)}\,|\chi\rangle = \frac{1}{2}$$

$$\overline{M}^{(1)} = (0, 0, \frac{1}{2})$$

for the second electron:

$$\overline{M}^{(2)} = (0, 0, \frac{1}{2})$$

ii) The triplet second state:

$$|\chi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

$$\langle\chi|\,\hat{S}_x^{(1)}\,|\chi\rangle = 0; \quad \langle\chi|\,\hat{S}_y^{(1)}\,|\chi\rangle = 0; \quad \langle\chi|\,\hat{S}_z^{(1)}\,|\chi\rangle = 0$$

$$\overline{M}^{(1)} = (0,0,0)$$

the same for the second electron:

$$\overline{M}^{(2)} = (0,0,0)$$

iii) The triplet third state:

$$|\chi\rangle = |\downarrow\downarrow\rangle$$

$$\langle\chi|\,\hat{S}_x^{(1)}\,|\chi\rangle = 0; \quad \langle\chi|\,\hat{S}_y^{(1)}\,|\chi\rangle = 0; \quad \langle\chi|\,\hat{S}_z^{(1)}\,|\chi\rangle = -\frac{1}{2}$$

$$\overline{M}^{(1)} = (0,0,-\frac{1}{2})$$

the same for the second electron:

$$\overline{M}^{(2)} = (0,0,-\frac{1}{2})$$