More interesting Hamiltonian to work on the VQE algorithm

Let us find out the matrix representation of a Hamiltonian system of two spin1/2 particles, an example of this system is the hydrogen atom, has a spin1/2 proton in the nucleus and a spin1/2 electron located around. What interesting about this Hamiltonian, is that he describes the spin-spin interaction.

Along the z-axis this system forms basis states, which contains 4 states:

$$|\uparrow\uparrow\rangle = |\uparrow\rangle_1|\uparrow\rangle_2\,,\ |\uparrow\downarrow\rangle = |\uparrow\rangle_1|\downarrow\rangle_2\,,\ |\downarrow\uparrow\rangle = |\downarrow\rangle_1|\uparrow\rangle_2\,,\ |\downarrow\downarrow\rangle = |\downarrow\rangle_1|\downarrow\rangle_2\,,$$

Where: $|\quad\rangle_1 : state\ fot\ the\ particle\ 1 \quad and \quad |\quad\rangle_2 : state\ for\ the\ particle\ 2$

Some requirements:

- ✓ $\hat{\vec{S}} = \hat{\vec{S}}_x + \hat{\vec{S}}_y + \hat{\vec{S}}_z$
- ✓ $S_+ = S_x + iS_y\,, \quad S_- = S_x - iS_y$
- ✓ $S_z|\pm Z\rangle = \pm\frac{\hbar}{2}|\pm Z\rangle\,,\ S_+|\downarrow\rangle = \hbar|\uparrow\rangle\,,\ S_-|\uparrow\rangle = \hbar|\downarrow\rangle\,,\ S_+|\uparrow\rangle = 0\,,\ S_-|\downarrow\rangle = 0$

We define the Hamiltonian that describes this interaction as:

$$\hat{H} = \frac{2A}{\hbar^2}\hat{\vec{S}}_1.\hat{\vec{S}}_2$$

Where he is proportional to the spin operator for the particles 1 and 2($\hat{\vec{S}}_1\ and\ \hat{\vec{S}}_2$).

The $\frac{2A}{\hbar^2}$ is a normalization factor, where A is the measure of the strength of this interaction and has unit energy.

Now let us go ahead and find the matrix:

$$\hat{H} = \frac{2A}{\hbar^2}\hat{\vec{S}}_1.\hat{\vec{S}}_2 = \frac{2A}{\hbar^2}\left(\hat{\vec{S}}_{1x}\hat{\vec{S}}_{2x} + \hat{\vec{S}}_{1y}\hat{\vec{S}}_{2y} + \hat{\vec{S}}_{1z}\hat{\vec{S}}_{2z}\right) = \frac{A}{\hbar^2}(\hat{\vec{S}}_{1+}\hat{\vec{S}}_{2-} + \hat{\vec{S}}_{1-}\hat{\vec{S}}_{2+} + 2\,\hat{\vec{S}}_{1z}\hat{\vec{S}}_{2z})$$

What are the components of this Hamiltonian matrix? To know that, we need to compute all combinations of the following expression:

$$\langle\quad|\hat{H}|\quad\rangle$$

Given that: $\langle\quad|$ and $|\quad\rangle$ are between the basis states cited above.

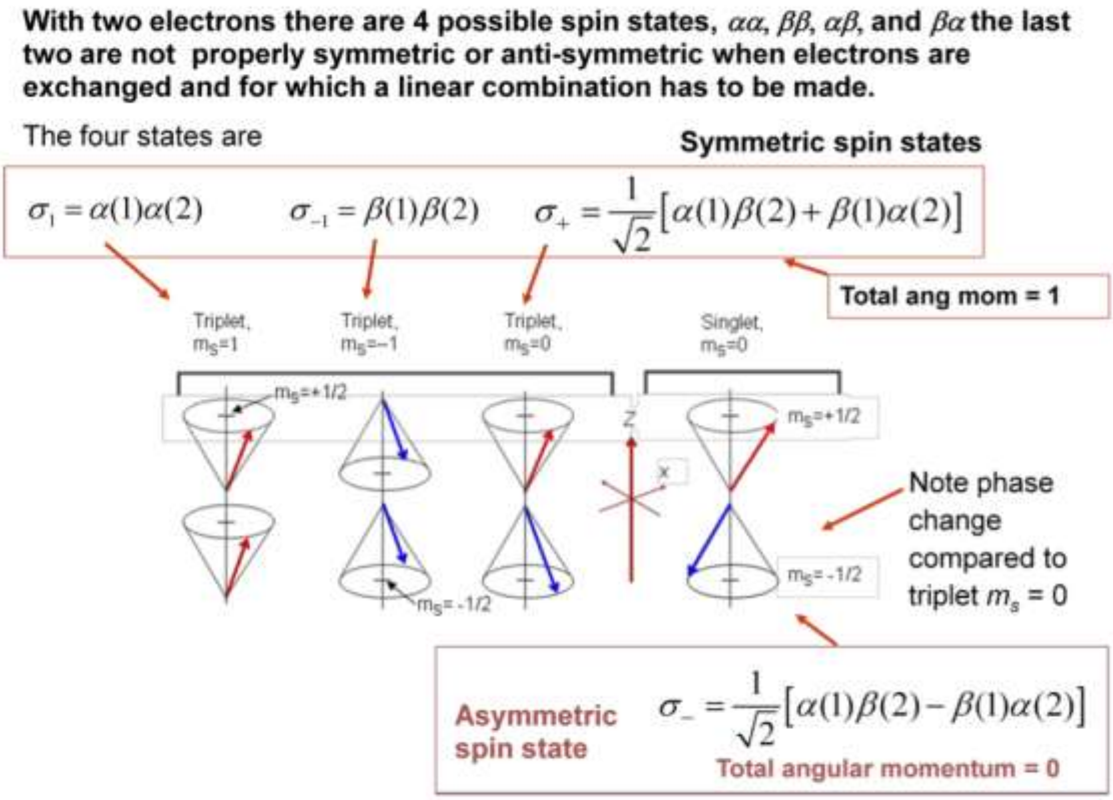
Using the requirements, to conclude the elements of the matrix (it's an exercise to do), we end up with:

$$\hat{H} = A\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 1 & 0 \\ 0 & 1 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$$

Obviously two eigenvalues come up for free, looking at the matrix: $\frac{A}{2}$ and $\frac{A}{2}$

And the two other come from the middle 2 by 2 submatrix: $\frac{A}{2}$ $and -\frac{3A}{2}$

The states of the eigenvalue $\frac{A}{2}$ form a spin 1 system, the state of the ground state energy$-\frac{3A}{2}$, form a spin 0 system. The following figure makes it easy to understand:



(https://i.stack.imgur.com/Rh9xf.png)