Hyperfine interaction

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We solve the eigenvalue problem for the exchange interaction between two spins using the KroneckerProduct in Mathematica.

$$\left|+z\right\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \left|-z\right\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

$$\left|\chi_1\right\rangle = \left|+z\right\rangle_1 \otimes \left|+z\right\rangle_2 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \qquad \left|\chi_2\right\rangle = \left|+z\right\rangle_1 \otimes \left|-z\right\rangle_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix},$$

$$\left|\chi_3\right\rangle = \left|-z\right\rangle_1 \otimes \left|+z\right\rangle_2 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \qquad \left|\chi_4\right\rangle = \left|-z\right\rangle_1 \otimes \left|-z\right\rangle_2 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix},$$

The exchange interaction between the electron and the proton (the hyperfine interaction) is given by

$$\hat{J} = \hat{\sigma}_{1x} \otimes \hat{\sigma}_{2x} + \hat{\sigma}_{1y} \otimes \hat{\sigma}_{2y} + \hat{\sigma}_{1z} \otimes \hat{\sigma}_{2z} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

We solve the eigenvalue problem.

Eigensystem[$\hat{J}$]:

Eigenvalues and eigenkets

Triplet state:

E_1=1 $$|\psi_1\rangle = \begin{pmatrix}1\\0\\0\\0\end{pmatrix} = |\chi_1\rangle$$

E_2=1, $$|\psi_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\1\\0\end{pmatrix} = \frac{1}{\sqrt{2}}(|\chi_2\rangle + |\chi_3\rangle)$$

E_3=1 $$|\psi_3\rangle = \begin{pmatrix}0\\0\\0\\1\end{pmatrix} = |\chi_4\rangle$$

Singlet state:

E_4=-3 $$|\psi_4\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix} = \frac{1}{\sqrt{2}}(|\chi_2\rangle - |\chi_3\rangle)$$

The unitary operator:

$$|\psi_i\rangle = \hat{U}|\chi_i\rangle,$$

where

$$\hat{U} = \begin{pmatrix}1 & 0 & 0 & 0\\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}}\\ 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}}\\ 0 & 0 & 1 & 0\end{pmatrix}, \qquad \hat{U}^+ = \begin{pmatrix}1 & 0 & 0 & 0\\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0\\ 0 & 0 & 0 & 1\\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0\end{pmatrix}$$

We also have

$$\hat{U}^{+}\hat{J}\hat{U} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix} \qquad \text{(diagonal matrix)}$$

((**Mathematica**))

```
Clear["Global`*"];
exp_* := exp /. {Complex[re_, im_] :→ Complex[re, -im]}; ψ1 = (1
                                                               0); ψ1 = (1
                                                                          0);
ψ1 = (1
      0); ψ2 = (0
                1); σx = (0 1
                          1 0); σy = (0 -ⅈ
                                      ⅈ  0); σz = (1  0
                                                   0 -1);
I2 = IdentityMatrix[2];

ϕ1 = KroneckerProduct[ψ1, ψ1]; ϕ2 = KroneckerProduct[ψ1, ψ2];
ϕ3 = KroneckerProduct[ψ2, ψ1];
ϕ4 = KroneckerProduct[ψ2, ψ2];

J1 = (KroneckerProduct[σx, σx] + KroneckerProduct[σy, σy]
    + KroneckerProduct[σz, σz]);

J1 // MatrixForm
```

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

```
eq1 = Eigensystem[J1]

{{-3, 1, 1, 1}, {{0, -1, 1, 0}, {0, 0, 0, 1}, {0, 1, 1, 0}, {1, 0, 0, 0}}}

χ1 = Normalize[eq1[[2, 4]]]

{1, 0, 0, 0}

χ2 = Normalize[eq1[[2, 3]]]
```

$$\left\{0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right\}$$

```
χ3 = Normalize[eq1[[2, 2]]]

{0, 0, 0, 1}

χ4 = -Normalize[eq1[[2, 1]]]
```

$$\left\{0, \frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0\right\}$$

```
UT = {χ1, χ2, χ3, χ4}; U = Transpose[UT]; UH = UT*;
U // MatrixForm
```

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

```
UH // MatrixForm
```

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}$$

```
UH.U // Simplify
{{1, 0, 0, 0}, {0, 1, 0, 0}, {0, 0, 1, 0}, {0, 0, 0, 1}}
```

```
eq2 = UH.J1.U // FullSimplify; eq2 // MatrixForm
```

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix}$$

2. Dirac spin exchange operator

$$\hat{J}|\psi_1\rangle = |\psi_1\rangle, \qquad \hat{J}|\chi_1\rangle = |\chi_1\rangle$$

$$\hat{J}|\psi_3\rangle = |\psi_3\rangle, \qquad \hat{J}|\chi_4\rangle = |\chi_4\rangle$$

$$\hat{J}|\psi_2\rangle = |\psi_2\rangle, \qquad \hat{J}(|\chi_2\rangle + |\chi_3\rangle) = |\chi_2\rangle + |\chi_3\rangle$$

$$\hat{J}|\psi_4\rangle = -3|\psi_4\rangle, \qquad \hat{J}(|\chi_2\rangle - |\chi_3\rangle) = -3|\chi_2\rangle + 3|\chi_3\rangle)$$

Then we have

$$\left(\frac{\hat{J}+\hat{1}}{2}\right)|\chi_1\rangle = |\chi_1\rangle, \qquad \left(\frac{\hat{J}+\hat{1}}{2}\right)|\chi_4\rangle = |\chi_4\rangle$$

$$\left(\frac{\hat{J}+\hat{1}}{2}\right)|\chi_3\rangle = |\chi_2\rangle, \qquad \left(\frac{\hat{J}+\hat{1}}{2}\right)|\chi_2\rangle = |\chi_3\rangle$$

In other words, we can define the Dirac spin exchange operator

$$\hat{P}_{12} = \frac{1}{2}(\hat{1}+\hat{J}) = \frac{1}{2}(\hat{1}+\hat{\boldsymbol{\sigma}}_1\cdot\hat{\boldsymbol{\sigma}}_2)$$

where for example,

$$\hat{P}_{12}|+z\rangle_1 \otimes |-z\rangle_2 = |+z\rangle_1 \otimes |-z\rangle_2$$

3. Spin angular momentum

The total spin angular momentum:

$$\hat{\boldsymbol{S}} = \hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2 = \frac{\hbar}{2}(\hat{\boldsymbol{\sigma}}_1 + \hat{\boldsymbol{\sigma}}_2)$$

Then we have

$$\begin{aligned}\hat{\boldsymbol{S}}^2 &= \frac{\hbar^2}{4}(\hat{\boldsymbol{\sigma}}_1 + \hat{\boldsymbol{\sigma}}_2)^2 \\ &= \frac{\hbar^2}{4}(\hat{\boldsymbol{\sigma}}_1{}^2 + \hat{\boldsymbol{\sigma}}_2{}^2 + 2\hat{\boldsymbol{\sigma}}_1\cdot\hat{\boldsymbol{\sigma}}_1) \\ &= \frac{3\hbar^2}{2}\hat{1} + \frac{\hbar^2}{2}\hat{J}\end{aligned}$$

and

$$\hat{S}_z = \frac{\hbar}{2}(\hat{\sigma}_{1z} + \hat{\sigma}_{2z}) = \frac{\hbar}{2}(\hat{\sigma}_{1z}\otimes\hat{1}_2 + \hat{1}_1\otimes\hat{\sigma}_{2z})$$

$$\hat{S}_x = \frac{\hbar}{2}(\hat{\sigma}_{1x} + \hat{\sigma}_{2x}) = \frac{\hbar}{2}(\hat{\sigma}_{1x}\otimes\hat{1}_2 + \hat{1}_1\otimes\hat{\sigma}_{2x})$$

$$\hat{S}_y = \frac{\hbar}{2}(\hat{\sigma}_{1y} + \hat{\sigma}_{2y}) = \frac{\hbar}{2}(\hat{\sigma}_{1y}\otimes\hat{1}_2 + \hat{1}_1\otimes\hat{\sigma}_{2y})$$

We get

$$\hat{\boldsymbol{S}}^2 = \hbar^2 \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}, \qquad \hat{S}_z = \hbar \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$\hat{S}_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}, \qquad \hat{S}_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i & -i & 0 \\ i & 0 & 0 & -i \\ i & 0 & 0 & -i \\ 0 & i & i & 0 \end{pmatrix}$$

and the commutation relation

$$[\hat{\boldsymbol{S}}^2, \hat{S}_z] = 0$$

In summary

$$|\psi_1\rangle = |l=1, m=1\rangle, \quad |\psi_2\rangle = |l=1, m=0\rangle, \quad |\psi_3\rangle = |l=1, m=-1\rangle$$

$$|\psi_4\rangle = |l=0, m=0\rangle$$

We also note that the spins of electron and proton are expressed by

$$\hat{S}_{ez} = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \qquad \hat{S}_{pz} = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

respectively.

((**Mathematica-2**))

Simultaneous eigenkets of $\hat{\boldsymbol{S}}^2$ and $\hat{S}_z$. The Mathematica program-2 is the sequence of the Mmathematica program-1.

```
Sz = ℏ/2 (KroneckerProduct[σz, I2] + KroneckerProduct[I2, σz]);
ST = 3 ℏ^2/2 KroneckerProduct[I2, I2] + ℏ^2/2 J1;
Sz // MatrixForm
```

$$\begin{pmatrix} \hbar & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\hbar \end{pmatrix}$$

```
ST // MatrixForm
```

$$\begin{pmatrix} 2\hbar^2 & 0 & 0 & 0 \\ 0 & \hbar^2 & \hbar^2 & 0 \\ 0 & \hbar^2 & \hbar^2 & 0 \\ 0 & 0 & 0 & 2\hbar^2 \end{pmatrix}$$

```
Sz.ST - ST.Sz // Simplify
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

Sz.χ1 - ħ χ1
{0, 0, 0, 0}

Sz.χ2
{0, 0, 0, 0}

Sz.χ3 + ħ χ3
{0, 0, 0, 0}

Sz.χ4
{0, 0, 0, 0}

ST.χ1 - 2 ħ^2 χ1
{0, 0, 0, 0}
ST.χ2 - 2 ħ^2 χ2
{0, 0, 0, 0}

ST.χ3 - 2 ħ^2 χ3
{0, 0, 0, 0}

ST.χ4
{0, 0, 0, 0}
```

4. Zeeman energy

We consider the Hamiltonian consists of the exchange interaction and the Zeeman energy is given by

$$\begin{aligned}\hat{H} &= J\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2 - \mu_1 B\hat{\sigma}_{1z} - \mu_1 B\hat{\sigma}_{2z} \\ &= J(\hat{\sigma}_{1x} \otimes \hat{\sigma}_{2x} + \hat{\sigma}_{1y} \otimes \hat{\sigma}_{2y} + \hat{\sigma}_{1z} \otimes \hat{\sigma}_{2z}) - \mu_1 B(\hat{\sigma}_{1z} \otimes \hat{1}_2) - \mu_2 B(\hat{1}_1 \otimes \hat{\sigma}_{2z})\end{aligned}$$

This Hamiltonian can be described by the 4x4 matrix given by

$$\hat{H} = \begin{pmatrix} J - \mu_1 B - \mu_2 B & 0 & 0 & 0 \\ 0 & -J - \mu_1 B + \mu_2 B & 2J & 0 \\ 0 & 2J & -J + \mu_1 B - \mu_2 B & 0 \\ 0 & 0 & 0 & J + \mu_1 B + \mu_2 B \end{pmatrix}$$

So we can solve the eigenvalue problems

Energy eigenvalue	Eigenket
$J - (\mu_1 + \mu_2)B$	$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$
$-J + \sqrt{4J^2 + B^2(\mu_1 - \mu_2)^2}$	$\begin{pmatrix} 0 \\ [\sqrt{4J^2 + B^2(\mu_1 - \mu_2)^2} - (\mu_1 - \mu_2)B]/2J \\ 1 \\ 0 \end{pmatrix}$

which corresponds to the state $\frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}$ $\quad (= |j = 1, m = 0\rangle)$

Energy eigenvalue	Eigenket
$J + (\mu_1 + \mu_2)B$	$\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$
$-J - \sqrt{4J^2 + B^2(\mu_1 - \mu_2)^2}$	$\begin{pmatrix} 0 \\ [\sqrt{4J^2 + B^2(\mu_1 - \mu_2)^2} + (\mu_1 - \mu_2)B]/2J \\ -1 \\ 0 \end{pmatrix}$

which corresponds to the state $\frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}$ $\quad (= |j = 0, m = 0\rangle)$

Note that the eigenkets are not normalized.

((Mthaemtica))

```
Clear["Global`*"];
exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]}; ψ1 = (1
0); ψ1 = (1
0);
ψ1 = (1
0); ψ2 = (0
1); σx = (0 1
1 0); σy = (0 -ⅈ
ⅈ 0); σz = (1 0
0 -1);
I2 = IdentityMatrix[2];

ϕ1 = KroneckerProduct[ψ1, ψ1]; ϕ2 = KroneckerProduct[ψ1, ψ2];
ϕ3 = KroneckerProduct[ψ2, ψ1];
ϕ4 = KroneckerProduct[ψ2, ψ2];

K1 = J (KroneckerProduct[σx, σx] + KroneckerProduct[σy, σy]
    + KroneckerProduct[σz, σz]);
K2 = -μ1 B KroneckerProduct[σz, I2] - μ2 B KroneckerProduct[I2, σz];
H1 = K1 + K2; H1 // MatrixForm
```

$$\begin{pmatrix} J - B\mu1 - B\mu2 & 0 & 0 & 0 \\ 0 & -J - B\mu1 + B\mu2 & 2J & 0 \\ 0 & 2J & -J + B\mu1 - B\mu2 & 0 \\ 0 & 0 & 0 & J + B\mu1 + B\mu2 \end{pmatrix}$$

```
eq1 = Eigensystem[H1] // Simplify
```

$$\Big\{\Big\{J - B(\mu1+\mu2),\ J + B(\mu1+\mu2),\ -J - \sqrt{4J^2 + B^2(\mu1-\mu2)^2},\ -J + \sqrt{4J^2 + B^2(\mu1-\mu2)^2}\Big\},$$
$$\Big\{\{1,0,0,0\},\ \{0,0,0,1\},\ \Big\{0,\ \frac{-\sqrt{4J^2 + B^2(\mu1-\mu2)^2} + B(-\mu1+\mu2)}{2J},\ 1,\ 0\Big\},$$
$$\Big\{0,\ \frac{\sqrt{4J^2 + B^2(\mu1-\mu2)^2} + B(-\mu1+\mu2)}{2J},\ 1,\ 0\Big\}\Big\}\Big\}$$

REFERENCES

John S. Townsend , *A Modern Approach to Quantum Mechanics*, second edition (University Science Books, 2012).