Two spins of *S*=1/2

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Here we discuss the eigenstate for the system formed of two particles (1 and 2) with spin 1/2. The eigenstates are expressed by the superposition of the four states ($\left|+z\right\rangle_1\left|+z\right\rangle_2 = \left|++\right\rangle$, $\left|+z\right\rangle_1\left|-z\right\rangle_2 = \left|+-\right\rangle$, $\left|-z\right\rangle_1\left|+z\right\rangle_2 = \left|-+\right\rangle$, and $\left|-z\right\rangle_1\left|-z\right\rangle_2 = \left|--\right\rangle$. The three eigenstate with the total spin 1 is the symmetric state under the exchange of the particles ($1 \leftrightarrow 2$), forming the triplet state. On the other hand, one eigenstate with the total spin 0 is the antisymmetric under the exchange of the particles ($1 \leftrightarrow 2$), forming the singlet state. This antisymmetric state is one of the four Bell's state. It plays a significant role in the quantum entanglement. The Bells' states are as follows.

$$\left|D_\pm\right\rangle = \frac{1}{\sqrt{2}}(\left|+-\right\rangle \pm \left|-+\right\rangle), \qquad \left|S_\pm\right\rangle = \frac{1}{\sqrt{2}}(\left|++\right\rangle \pm \left|--\right\rangle)$$

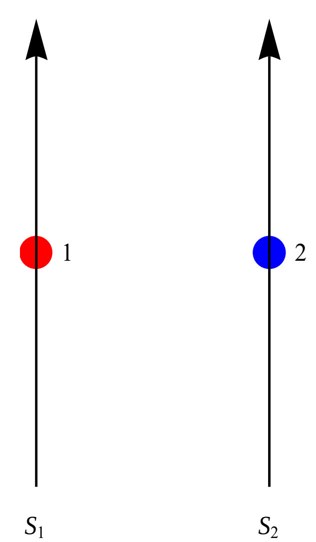
The nature of the symmetry in the state vector for the two particle system under the exchange particles, is closely related to the character of the system whether the system is boson (symmetric) or fermion (antisymmetric).

In order to solve the eigenvalue problem of the two spin system, we introduce the Dirac spin exchange operator, which is equivalent to the swap gate (operator) in the quantum computing.

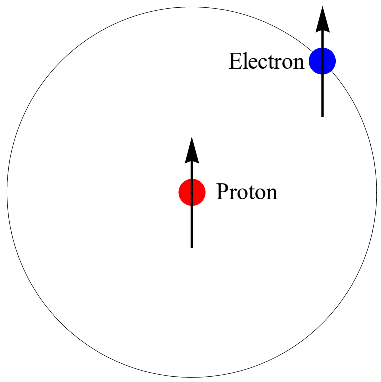
1. Definition

((Hyperfine splitting in hydrogen))

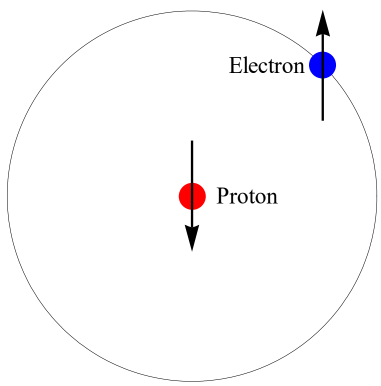
The hydrogen atom consists of an electron sitting in the neighborhood of the proton. There are four states for the ground state of the hydrogen atom.



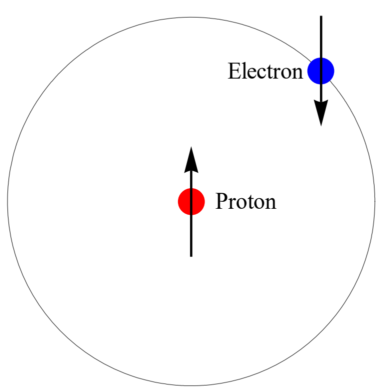
$|++\rangle$: electron up, proton up



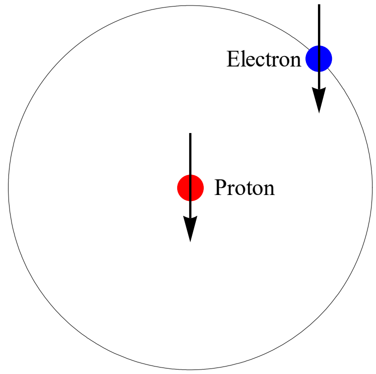
$|+-\rangle$: electron up, proton down



$|-+\rangle$: electron down, proton up



$|--\rangle$: electron down, proton down1



For any state, the state can be described by the linear combination of these four states. We note that these notations are equivalent,

$$\left|+-\right\rangle = \left|+\right\rangle_e \left|-\right\rangle_p = \left|+\right\rangle_e \otimes \left|-\right\rangle_p$$

where $\otimes$ denotes the tensor product (or Kronecker product, or direct product). We use the following formula to set up the eigenkets of two spins with spin $S = \hbar/2$.

$$\hat{\sigma}_z\left|+\right\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \left|+\right\rangle$$

$$\hat{\sigma}_z\left|-\right\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\left|-\right\rangle$$

$$\hat{\sigma}_x\left|+\right\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \left|-\right\rangle$$

$$\hat{\sigma}_x\left|-\right\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \left|+\right\rangle$$

$$\hat{\sigma}_y\left|+\right\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ i \end{pmatrix} = i\left|-\right\rangle$$

$$\hat{\sigma}_y\left|-\right\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -i \\ 0 \end{pmatrix} = -i\left|+\right\rangle$$

We now consider the two spin operators: $\hat{\boldsymbol{\sigma}}_1$ and $\hat{\boldsymbol{\sigma}}_2$ for the particle 1 and particle 2. There are four states:

$$\left|++\right\rangle,\ \left|+-\right\rangle,\ \left|-+\right\rangle,\ \left|--\right\rangle$$

The spin operator $\hat{\boldsymbol{\sigma}}_1$ and $\hat{\boldsymbol{\sigma}}_2$ work on the first spin state and the second spin state, respectively.

$$\hat{\sigma}_{1y}\left|-+\right\rangle = -i\left|++\right\rangle$$

$$\hat{\sigma}_{1y}\left|++\right\rangle = i\left|-+\right\rangle$$

$$\hat{\sigma}_{1y}\left|+-\right\rangle = i\left|--\right\rangle$$

$$\hat{\sigma}_{1y}\left|--\right\rangle = -i\left|+-\right\rangle$$

and

$$\hat{\sigma}_{2x}\left|-+\right\rangle = \left|--\right\rangle$$

$$\hat{\sigma}_{2x}\left|++\right\rangle = \left|+-\right\rangle$$

$$\hat{\sigma}_{2x}\left|+-\right\rangle = \left|++\right\rangle$$

$$\hat{\sigma}_{2x}\left|--\right\rangle = \left|-+\right\rangle$$

In the most general case we could have more complex things.

$$\hat{\sigma}_{1x}\hat{\sigma}_{2z}\left|++\right\rangle = \hat{\sigma}_{1x}(\hat{\sigma}_{2z}\left|++\right\rangle) = \hat{\sigma}_{1x}\left|++\right\rangle = \left|-+\right\rangle$$

$$\hat{\sigma}_{1x}\hat{\sigma}_{2z}\left|+-\right\rangle = \hat{\sigma}_{1x}(\hat{\sigma}_{2z}\left|+-\right\rangle) = -\hat{\sigma}_{1x}\left|+-\right\rangle = -\left|--\right\rangle$$

$$\hat{\sigma}_{1x}\hat{\sigma}_{2z}\left|-+\right\rangle = \hat{\sigma}_{1x}(\hat{\sigma}_{2z}\left|-+\right\rangle) = \hat{\sigma}_{1x}\left|-+\right\rangle = \left|++\right\rangle$$

$$\hat{\sigma}_{1x}\hat{\sigma}_{2z}\left|--\right\rangle = \hat{\sigma}_{1x}(\hat{\sigma}_{2z}\left|--\right\rangle) = -\hat{\sigma}_{1x}\left|--\right\rangle = -\left|+-\right\rangle$$

2. Dirac spin exchange operator (I)

We introduce the Dirac spin exchange operator as follows.

$$\hat{A} = \hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2 = \hat{\sigma}_{1x} \cdot \hat{\sigma}_{2x} + \hat{\sigma}_{1y} \cdot \hat{\sigma}_{2y} + \hat{\sigma}_{1z} \cdot \hat{\sigma}_{2z}$$

(a)

$$\hat{\sigma}_{1x}\cdot\hat{\sigma}_{2x}\left|++\right\rangle = \left|--\right\rangle$$

$$\hat{\sigma}_{1y}\cdot\hat{\sigma}_{2y}\left|++\right\rangle = -\left|--\right\rangle$$

$$\hat{\sigma}_{1z}\cdot\hat{\sigma}_{2z}\left|++\right\rangle = \left|++\right\rangle$$

Then

$$\hat{A}\left|++\right\rangle = \left|++\right\rangle = 2\left|++\right\rangle - \left|++\right\rangle$$

$$\frac{(\hat{A}+\hat{1})}{2}\left|++\right\rangle = \left|++\right\rangle$$

(b)

$$\hat{\sigma}_{1x}\cdot\hat{\sigma}_{2x}\left|+-\right\rangle = \left|-+\right\rangle$$

$$\hat{\sigma}_{1y}\cdot\hat{\sigma}_{2y}\left|+-\right\rangle = \left|-+\right\rangle$$

$$\hat{\sigma}_{1z}\cdot\hat{\sigma}_{2z}\left|+-\right\rangle = -\left|+-\right\rangle$$

Then

$$\hat{A}\left|+-\right\rangle = 2\left|-+\right\rangle - \left|+-\right\rangle$$

$$\frac{(\hat{A}+\hat{1})}{2}\left|-+\right\rangle = \left|+-\right\rangle$$

(c)

$$\hat{\sigma}_{1x}\cdot\hat{\sigma}_{2x}\left|-+\right\rangle = \left|+-\right\rangle$$

$$\hat{\sigma}_{1y}\cdot\hat{\sigma}_{2y}\left|-+\right\rangle = \left|+-\right\rangle$$

$$\hat{\sigma}_{1z}\cdot\hat{\sigma}_{2z}\left|-+\right\rangle = -\left|-+\right\rangle$$

Then

$$\hat{A}\left|-+\right\rangle = 2\left|+-\right\rangle - \left|-+\right\rangle$$

$$\frac{(\hat{A}+\hat{1})}{2}|-+\rangle = |+-\rangle$$

(d)

$$\hat{\sigma}_{1x}\cdot\hat{\sigma}_{2x}|--\rangle = |++\rangle$$

$$\hat{\sigma}_{1y}\cdot\hat{\sigma}_{2y}|--\rangle = -|++\rangle$$

$$\hat{\sigma}_{1z}\cdot\hat{\sigma}_{2z}|--\rangle = |--\rangle$$

Then

$$\hat{A}|--\rangle = |--\rangle = 2|--\rangle - |--\rangle$$

or

$$\frac{(\hat{A}+\hat{1})}{2}|--\rangle = |--\rangle$$

((**Dirac exchange operator**))

Now we introduce a new operator $\hat{P}_{12}$, which has the following properties. $\hat{P}_{12}$ is called the Dirac spin exchange operator. When $\hat{P}_{12}$ operates on the state $|\psi\rangle = |\alpha\rangle_1|\beta\rangle_2$, we have

$$\hat{P}_{12}|\psi\rangle = \hat{P}_{12}|\alpha\rangle_1|\beta\rangle_2 = |\alpha\rangle_2|\beta\rangle_1 = |\beta\rangle_1|\alpha\rangle_2$$

From the definition, we get

$$\hat{P}_{12}|++\rangle = |++\rangle$$

$$\hat{P}_{12}|+-\rangle = |-+\rangle$$

$$\hat{P}_{12}|-+\rangle = |+-\rangle$$

$$\hat{P}_{12}|--\rangle = |--\rangle$$

The matrix of $\hat{P}_{12}$ under the basis of $\{|++\rangle, |+-\rangle, |-+\rangle, |--\rangle\}$ is given by

$$\hat{P}_{12} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

We find that $\hat{P}_{12}$ is related to $\hat{A}$ as,

$$\hat{A} = 2\hat{P}_{12} - \hat{1}$$

or

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

From the relations,

$$\hat{P}_{12}\left|++\right\rangle = \left|++\right\rangle, \qquad \hat{P}_{12}\left|--\right\rangle = \left|--\right\rangle$$

$\left|++\right\rangle$ is the eigenstate of $\hat{P}_{12}$ with the eigenvalue +1.

From the relations,

$$\hat{P}_{12}\left|+-\right\rangle = \left|-+\right\rangle$$

$$\hat{P}_{12}\left|-+\right\rangle = \left|+-\right\rangle$$

we can easily show that

$$\hat{P}_{12}\left(\frac{\left|+-\right\rangle + \left|-+\right\rangle}{\sqrt{2}}\right) = \left(\frac{\left|+-\right\rangle + \left|-+\right\rangle}{\sqrt{2}}\right)$$

and

$$\hat{P}_{12}\left(\frac{\left|+-\right\rangle - \left|-+\right\rangle}{\sqrt{2}}\right) = -\left(\frac{\left|+-\right\rangle - \left|-+\right\rangle}{\sqrt{2}}\right)$$

which means that

$\dfrac{\left|+-\right\rangle + \left|-+\right\rangle}{\sqrt{2}}$ is the eigenstate of $\hat{P}_{12}$ with the eigenvalue +1.

$\frac{|+-\rangle - |-+\rangle}{\sqrt{2}}$ is the eigenstate of $\hat{P}_{12}$ with the eigenvalue +1.

((**Note**)) Quantum computing

The Dirac spin exchange operator is equivalent to the swap (exchange operator) in quantum computing.

We consider two qubits (quantum bit), $|0\rangle$ and $|1\rangle$, instead of $|+z\rangle = |+\rangle$ and $|-z\rangle = |-\rangle$.

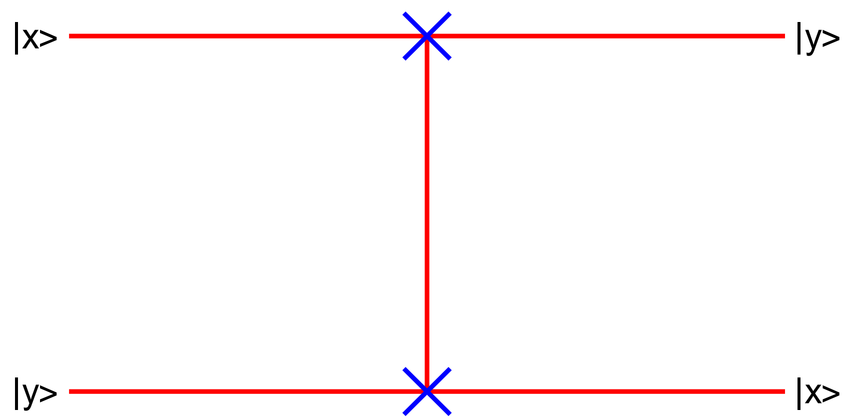


Fig. SWAP gate which is one of the quantum gates.

In this gate;

$$|00\rangle \rightarrow |00\rangle,$$
$$|01\rangle \rightarrow |10\rangle,$$
$$|10\rangle \rightarrow |01\rangle,$$
$$|11\rangle \rightarrow |11\rangle$$

Using the unitary operator for the swapping, these can be rewritten as

$$\hat{U}_{SW}|00\rangle = |00\rangle$$
$$\hat{U}_{SW}|01\rangle = |10\rangle$$
$$\hat{U}_{SW}|10\rangle = |01\rangle$$
$$\hat{U}_{SW}|11\rangle = |11\rangle$$

with

$$\hat{U}_{SW} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

3. Eigenvalue problem for the Dirac exchange operator

We solve the eigenvalue problem of the Dirac's spin exchange operator. The results are as follows.

$\hat{P}_{12}|\psi_1\rangle = |\psi_1\rangle$, (eigenvalue; 1)

$\hat{P}_{12}|\psi_2\rangle = |\psi_2\rangle$, (eigenvalue; 1)

$\hat{P}_{12}|\psi_3\rangle = |\psi_3\rangle$, (eigenvalue; 1)

$\hat{P}_{12}|\psi_4\rangle = -|\psi_4\rangle$ (eigenvalue; -1)

where

$$|\psi_1\rangle = |++\rangle$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}[|+-\rangle + |-+\rangle]$$

$$|\psi_3\rangle = |--\rangle$$

$$|\psi_4\rangle = \frac{1}{\sqrt{2}}[|+-\rangle - |-+\rangle]$$

((**Mathematica**))

```
Clear["Global`*"]; P1 = (1 0 0 0
                         0 0 1 0
                         0 1 0 0
                         0 0 0 1);

eq1 = Eigensystem[P1]

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

χ1 = eq1[[2, 4]]; χ2 = eq1[[2, 3]]; χ3 = eq1[[2, 2]];
χ4 = eq1[[2, 1]];

eq2 = Orthogonalize[{χ1, χ2, χ3, χ4}]; ψ1 = eq2[[1]];
ψ2 = eq2[[2]]; ψ3 = eq2[[3]];
ψ4 = -eq2[[4]];

ψ1

{1, 0, 0, 0}

ψ2
```

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

ψ3

{0, 0, 0, 1}

ψ4

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

P1.ψ1 – ψ1

{0, 0, 0, 0}

P1.ψ2 – ψ2

{0, 0, 0, 0}

P1.ψ3 – ψ3

{0, 0, 0, 0}

P1.ψ4 + ψ4

{0, 0, 0, 0}

4. Dirac spin exchange operator (II)

It is noted that

$$\hat{J}_+ \left| j,m \right\rangle = \hbar\sqrt{(j-m)(j+m+1)} \left| j,m+1 \right\rangle$$

$$\hat{J}_- \left| j,m \right\rangle = \hbar\sqrt{(j+m)(j-m+1)} \left| j,m-1 \right\rangle$$

Using these relations, we get

$$\hat{\sigma}_+ \left| -z \right\rangle = 2\left| +z \right\rangle, \qquad \hat{\sigma}_- \left| +z \right\rangle = 2\left| -z \right\rangle$$

Since

$$\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2 = \hat{\sigma}_{1x}\hat{\sigma}_{2x} + \hat{\sigma}_{1y}\hat{\sigma}_{2y} + \hat{\sigma}_{1z}\hat{\sigma}_{2z} = \frac{1}{2}(\hat{\sigma}_{1+}\hat{\sigma}_{2-} + \hat{\sigma}_{1-}\hat{\sigma}_{2+}) + \hat{\sigma}_{1z}\hat{\sigma}_{2z}$$

we calculate

$$\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2 \left| ++ \right\rangle = [\frac{1}{2}(\hat{\sigma}_{1+}\hat{\sigma}_{2-} + \hat{\sigma}_{1-}\hat{\sigma}_{2+}) + \hat{\sigma}_{1z}\hat{\sigma}_{2z}]\left| ++ \right\rangle$$
$$= \hat{\sigma}_{1z}\hat{\sigma}_{2z}\left| ++ \right\rangle = \left| ++ \right\rangle$$

$$\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2 \left| -- \right\rangle = [\frac{1}{2}(\hat{\sigma}_{1+}\hat{\sigma}_{2-} + \hat{\sigma}_{1-}\hat{\sigma}_{2+}) + \hat{\sigma}_{1z}\hat{\sigma}_{2z}]\left| -- \right\rangle$$
$$= \hat{\sigma}_{1z}\hat{\sigma}_{2z}\left| -- \right\rangle = \left| -- \right\rangle$$

$$\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2 \left| +- \right\rangle = [\frac{1}{2}(\hat{\sigma}_{1+}\hat{\sigma}_{2-} + \hat{\sigma}_{1-}\hat{\sigma}_{2+}) + \hat{\sigma}_{1z}\hat{\sigma}_{2z}]\left| +- \right\rangle$$
$$= (\frac{1}{2}\hat{\sigma}_{1-}\hat{\sigma}_{2+} + \hat{\sigma}_{1z}\hat{\sigma}_{2z})\left| +- \right\rangle$$
$$= 2\left| -+ \right\rangle - \left| +- \right\rangle$$

$$\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2 \left| -+ \right\rangle = [\frac{1}{2}(\hat{\sigma}_{1+}\hat{\sigma}_{2-} + \hat{\sigma}_{1-}\hat{\sigma}_{2+}) + \hat{\sigma}_{1z}\hat{\sigma}_{2z}]\left| -+ \right\rangle$$
$$= (\frac{1}{2}\hat{\sigma}_{1+}\hat{\sigma}_{2-} + \hat{\sigma}_{1z}\hat{\sigma}_{2z})\left| -+ \right\rangle$$
$$= 2\left| +- \right\rangle - \left| -+ \right\rangle$$

Then we have

$$(\frac{\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2 + \hat{1}}{2})\left| -- \right\rangle = \left| -- \right\rangle$$

$$(\frac{\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2 + \hat{1}}{2})\left| -- \right\rangle = \left| -- \right\rangle$$

$$(\frac{\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2 + \hat{1}}{2})\left| +- \right\rangle = \left| -+ \right\rangle$$

$$(\frac{\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2 + \hat{1}}{2})\left| -+ \right\rangle = \left| +- \right\rangle$$

Thus the Dirac exchange operator can be defined as

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

4. Total spin angular momentum

Suppose that $\hat{\mathbf{S}}_1$ and $\hat{\mathbf{S}}_2$ are commute. We define the total spin angular momentum as

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

and

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

Then we get

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

Note that

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

Then we have

$$\hat{\boldsymbol{S}}^2 = \frac{\hbar^2}{2}(3\hat{1} + \hat{\boldsymbol{\sigma}}_1\cdot\hat{\boldsymbol{\sigma}}_2) = \frac{\hbar^2}{2}(2\hat{1} + \hat{1} + \hat{\boldsymbol{\sigma}}_1\cdot\hat{\boldsymbol{\sigma}}_2) = \hbar^2(\hat{1} + \hat{P}_{12})$$

We also see that

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

((**Proof**))

$$[\hat{\sigma}_i, \hat{\sigma}_j] = 2i\varepsilon_{ijk}\hat{\sigma}_k$$

$$
\begin{aligned}
[\hat{\boldsymbol{S}}^2, \hat{S}_z] &= \frac{\hbar^3}{4}[3\hat{1} + \hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2, \hat{\sigma}_{1z} + \hat{\sigma}_{2z}] \\
&= \frac{\hbar^3}{4}[\hat{\sigma}_{1x}\hat{\sigma}_{2x} + \hat{\sigma}_{1y}\hat{\sigma}_{2y} + \hat{\sigma}_{1z}\hat{\sigma}_{2z}, \hat{\sigma}_{1z} + \hat{\sigma}_{2z}] \\
&= \frac{\hbar^3}{4}[\hat{\sigma}_{1x}\hat{\sigma}_{2x} + \hat{\sigma}_{1y}\hat{\sigma}_{2y}, \hat{\sigma}_{1z} + \hat{\sigma}_{2z}] \\
&= \frac{\hbar^3}{4}\{-[\hat{\sigma}_{1z}, \hat{\sigma}_{1x}]\hat{\sigma}_{2x} + [\hat{\sigma}_{1y}, \hat{\sigma}_{1z}]\hat{\sigma}_{2y} - \hat{\sigma}_{1x}[\hat{\sigma}_{2z}, \hat{\sigma}_{2x}] + \hat{\sigma}_{1y}[\hat{\sigma}_{2y}, \hat{\sigma}_{2z}]\} \\
&= \frac{\hbar^3}{4}(-2i\hat{\sigma}_{1y}\hat{\sigma}_{2x} + 2i\hat{\sigma}_{1x}\hat{\sigma}_{2y} - 2i\hat{\sigma}_{1x}\hat{\sigma}_{2y} + 2i\hat{\sigma}_{1y}\hat{\sigma}_{2x}) \\
&= 0
\end{aligned}
$$

This means that there are simultaneous eigenkets of $\hat{\mathbf{S}}^2$ and $\hat{S}_z$. Here we use the basis of

$$
\begin{aligned}
&|1\rangle = |++\rangle, \\
&|2\rangle = |+-\rangle, \\
&|3\rangle = |-+\rangle \\
&|4\rangle = |--\rangle,
\end{aligned}
$$

$$
\hat{\boldsymbol{S}}^2|++\rangle = \hbar^2(\hat{1} + \hat{P}_{12})|++\rangle = 2\hbar^2|++\rangle
$$

$$
\hat{S}_z|++\rangle = \frac{\hbar}{2}(\hat{\sigma}_{1z} + \hat{\sigma}_{2z})|++\rangle = \hbar|++\rangle
$$

which corresponds to the state $|\, j = 1, m = 1\rangle$

$$
\hat{\boldsymbol{S}}^2|--\rangle = \hbar^2(\hat{1} + \hat{P}_{12})|--\rangle = 2\hbar^2|--\rangle
$$

$$
\hat{S}_z|--\rangle = \frac{\hbar}{2}(\hat{\sigma}_{1z} + \hat{\sigma}_{2z})|--\rangle = -\hbar|--\rangle
$$

which corresponds to the state $|\, j = 1, m = -1\rangle$

$$
\hat{\boldsymbol{S}}^2|+-\rangle = \hbar^2(\hat{1} + \hat{P}_{12})|+-\rangle = \hbar^2(|+-\rangle + |-+\rangle)
$$

$$
\hat{S}_z|+-\rangle = \frac{\hbar}{2}(\hat{\sigma}_{1z} + \hat{\sigma}_{2z})|+-\rangle = 0
$$

$$\hat{\boldsymbol{S}}^2 |-+\rangle = \hbar^2 (\hat{1} + \hat{P}_{12}) |-+\rangle = \hbar^2 (|-+\rangle + |+-\rangle)$$

$$\hat{S}_z |-+\rangle = \frac{\hbar}{2} (\hat{\sigma}_{1z} + \hat{\sigma}_{2z}) |-+\rangle = 0$$

We now consider the matrix elements of $\hat{S}^2$ under the subspace of $|+-\rangle$ and $|-+\rangle$.

$$\hat{\boldsymbol{S}}^2 = \hbar^2 \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

((**Mathematica**))

```
Clear["Global`*"]; A = (1 1
                        1 1);

eq1 = Eigensystem[A]
```

{{2, 0}, {{1, 1}, {-1, 1}}}

```
ψ2 = Normalize[eq1[[2, 1]]]
```

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

```
ψ0 = -Normalize[eq1[[2, 2]]]
```

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

```
UT = {ψ2, ψ0}
```

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

```
U = Transpose[UT]
```

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

```
UH = UT
```

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

```
UH.A.U
```

{{2, 0}, {0, 0}}

$$\hat{S}^2 \left|\psi_S\right\rangle = 2\hbar^2 \left|\psi_S\right\rangle$$

$$\hat{S}^2 \left|\psi_A\right\rangle = 0$$

where

$$\left|\psi_S\right\rangle = \frac{1}{\sqrt{2}}(\left|+-\right\rangle + \left|-+\right\rangle)$$

$$\left|\psi_A\right\rangle = \frac{1}{\sqrt{2}}(\left|+-\right\rangle - \left|-+\right\rangle)$$

Note that

$$\hat{S}_z\left|\psi_S\right\rangle = 0, \qquad \hat{S}_z\left|\psi_A\right\rangle = 0$$

Thus

$\left|\psi_S\right\rangle$ is the eigenket of $\hat{\mathbf{S}}^2$ with $2\hbar^2$ and of $\hat{S}_z$ with $\hbar$.

$\left|\psi_A\right\rangle$ is the eigenket of $\hat{\mathbf{S}}^2$ with 0 and of $\hat{S}_z$ with 0.

The above results are summarized as follows.

((**Triplet**))

$\left|++\right\rangle$ (j=1, m = 1)

$\left|\psi_s\right\rangle = \frac{1}{\sqrt{2}}(\left|+-\right\rangle + \left|-+\right\rangle)$ (j = 1, m = 0)

$\left|--\right\rangle$ (j = 1, m = -1)

((**Singlet**))

$\left|\psi_A\right\rangle = \frac{1}{\sqrt{2}}(\left|+-\right\rangle - \left|-+\right\rangle)$ (j = 0, m = 0)

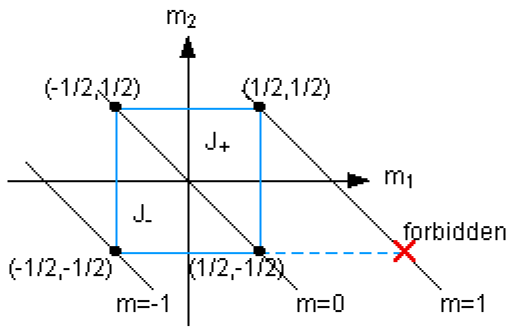
((**Note**))

$D_{1/2} x D_{1/2} = D_1 + D_0$

Clebsch-Gordan coefficient

(i) ***j* = 1**

$m = m_1 + m_2$



$$\left|\frac{1}{2},\frac{1}{2}\right\rangle\left|\frac{1}{2},\frac{1}{2}\right\rangle \qquad (m=1)$$

$$\frac{\left|\frac{1}{2},\frac{1}{2}\right\rangle\left|\frac{1}{2},-\frac{1}{2}\right\rangle+\left|\frac{1}{2},-\frac{1}{2}\right\rangle\left|\frac{1}{2},\frac{1}{2}\right\rangle}{\sqrt{2}} \qquad (m=0)$$

$$\left|\frac{1}{2},-\frac{1}{2}\right\rangle\left|\frac{1}{2},-\frac{1}{2}\right\rangle \qquad (m=-1)$$

(ii) $\boldsymbol{j=0}$ **(**$m=0$**)**

$$\frac{\left|\frac{1}{2},\frac{1}{2}\right\rangle\left|\frac{1}{2},-\frac{1}{2}\right\rangle-\left|\frac{1}{2},-\frac{1}{2}\right\rangle\left|\frac{1}{2},\frac{1}{2}\right\rangle}{\sqrt{2}} \qquad (m=0)$$

((**Mathematica**))

- **j1=1/2 and j2=1/2, J = 1.**

```
Clear["Global`*"]; CCGG[{j1_, m1_}, {j2_, m2_}, {j_, m_}] :=
 Module[{s1},
  s1 = If[Abs[m1] ≤ j1 && Abs[m2] ≤ j2 && Abs[m] ≤ j,
    ClebschGordan[{j1, m1}, {j2, m2}, {j, m}], 0]]

CG[j2_, m2_, j1_, L_] := Sum[CCGG[{j1, m1}, {L, m2 - m1},
    {j2, m2}] a[j1 , m1] b[L, m2 - m1], {m1, -j1, j1}]

CG[1, 1, 1/2, 1/2]
```

$a\left[\frac{1}{2}, \frac{1}{2}\right] b\left[\frac{1}{2}, \frac{1}{2}\right]$

```
CG[1, 0, 1/2, 1/2]
```

$$\frac{a[\frac{1}{2}, \frac{1}{2}]\, b[\frac{1}{2}, -\frac{1}{2}]}{\sqrt{2}} + \frac{a[\frac{1}{2}, -\frac{1}{2}]\, b[\frac{1}{2}, \frac{1}{2}]}{\sqrt{2}}$$

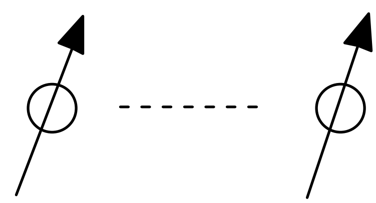
```
CG[1, -1, 1/2, 1/2]
```

$$a[\frac{1}{2}, -\frac{1}{2}]\, b[\frac{1}{2}, -\frac{1}{2}]$$

```
CG[0, 0, 1/2, 1/2]
```

$$\frac{a[\frac{1}{2}, \frac{1}{2}]\, b[\frac{1}{2}, -\frac{1}{2}]}{\sqrt{2}} - \frac{a[\frac{1}{2}, -\frac{1}{2}]\, b[\frac{1}{2}, \frac{1}{2}]}{\sqrt{2}}$$

5. Exchange interaction



$\mu_e\sigma_e$ $(\mu_e < 0)$ $\mu_p\sigma_p$ $(\mu_p < 0)$

We now consider the spin Hamiltonian

$$\hat{H} = E_0\hat{1} + J\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2 = E_0 + J(2\hat{P}_{12} - \hat{1})$$

(for convenience we assume $E_0 = 0$).

$$\hat{H}|++\rangle = J|++\rangle$$

$|++\rangle$ is the eigenstate of $\hat{H}$ with the eigenvalue J.

$$\hat{H}|--\rangle = J|--\rangle$$

$|--\rangle$ is the eigenstate of $\hat{H}$ with the eigenvalue J.

$$\hat{H}|+-\rangle = J(2|-+\rangle - |+-\rangle)$$

$$\hat{H}|-+\rangle = J(2|+-\rangle - |-+\rangle)$$

$$\hat{H} = \begin{pmatrix} -J & 2J \\ 2J & -J \end{pmatrix} = J\begin{pmatrix} -1 & 2 \\ 2 & -1 \end{pmatrix}$$

Eigensystem[$\hat{H}$] in the subspace of { $|+-\rangle$ and $|-+\rangle$ }.

(a) Eigenvalue problem-I

$$\hat{H} = -J\begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix} + 2J\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = -J\hat{1} + 2J\hat{\sigma}_x$$

$$\hat{H}|+x\rangle = (-J\hat{1} + 2J\hat{\sigma}_x)|+x\rangle = J|+x\rangle$$

and

$$\hat{H}|-x\rangle = (-J\hat{1} + 2J\hat{\sigma}_x)|-x\rangle = -3J|-x\rangle$$

where

$$|+x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}[|+-\rangle + |-+\rangle],$$

$$|-x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}}[|+-\rangle - |-+\rangle].$$

Thus

$|+x\rangle$ is the eigenket of $\hat{H}$ with the energy (J).

$|-x\rangle$ is the eigenket of $\hat{H}$ with the energy (-3J).

(b) Eigenvalue problem II (Alternative method)

We solve the eigenvalue problem using a conventional method.

For E = -3J

$$|\psi_S\rangle = \hat{U}|+-\rangle = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

For $E = J$

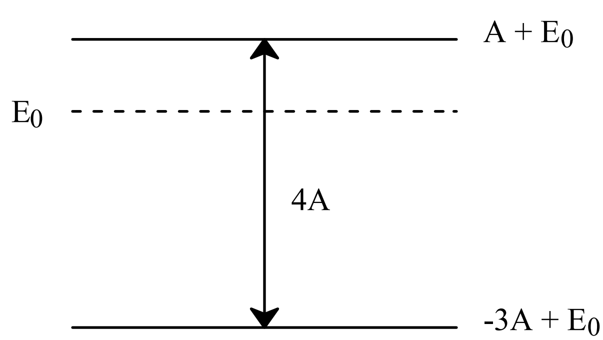
$$|\psi_A\rangle = \hat{U}|-+\rangle = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} U_{12} \\ U_{22} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}$$

The Unitary operator is given by

$$\hat{U} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}.$$

Therefore we have the triplet state and singlet state.

Eigenket	Energy eigenvalue
((Triplet))	
$\|++\rangle$	J
$\|\psi_S\rangle = \frac{1}{\sqrt{2}}(\|+-\rangle + \|-+\rangle)$	J
$\|--\rangle$	J
((Singlet))	
$\|\psi_A\rangle = \frac{1}{\sqrt{2}}(\|+-\rangle - \|-+\rangle)$	-3J



6. Zeeman splitting

The Hamiltonian is given by

$$\hat{H} = J\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2 - \mu_1 \hat{\boldsymbol{\sigma}}_1 \cdot \boldsymbol{B} - \mu_2 \hat{\boldsymbol{\sigma}}_2 \cdot \boldsymbol{B}$$

The magnetic moment of electron: $\frac{2\mu_1}{\hbar}\hat{\boldsymbol{S}}_1 = \mu_1 \hat{\boldsymbol{\sigma}}_1$ (μ_1<0)

The magnetic moment of proton: $\frac{2\mu_2}{\hbar}\hat{\boldsymbol{S}}_2 = \mu_2 \hat{\boldsymbol{\sigma}}_2$ (μ_2>0)

When the magnetic field $\boldsymbol{B}$ is applied along the z axis,

$$\hat{H} = \hat{H}_0 + \hat{H}_1$$

with

$$\hat{H}_0 = J\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2 = J(2\hat{P}_{12} - 1)$$

$$\hat{H}_1 = -(\mu_1 \hat{\sigma}_{1z} + \mu_2 \hat{\sigma}_{2z})B$$

$$\hat{H}_1 \left| ++ \right\rangle = -(\mu_1 \hat{\sigma}_{1z} + \mu_2 \hat{\sigma}_{2z})B\left| ++ \right\rangle = -(\mu_1 + \mu_2)B\left| ++ \right\rangle$$

$$\hat{H}_1 \left| -- \right\rangle = -(\mu_1 \hat{\sigma}_{1z} + \mu_2 \hat{\sigma}_{2z})B\left| -- \right\rangle = (\mu_1 + \mu_2)B\left| -- \right\rangle$$

$$\hat{H}_1 \left| +- \right\rangle = -(\mu_1 \hat{\sigma}_{1z} + \mu_2 \hat{\sigma}_{2z})B\left| +- \right\rangle = -(\mu_1 - \mu_2)B\left| +- \right\rangle$$

$$\hat{H}_1 \left| -+ \right\rangle = -(\mu_1 \hat{\sigma}_{1z} + \mu_2 \hat{\sigma}_{2z})B\left| -+ \right\rangle = (\mu_1 - \mu_2)B\left| -+ \right\rangle$$

$$\hat{H}_0 \left| ++ \right\rangle = J\left| ++ \right\rangle$$

$$\hat{H}_0 \left| -- \right\rangle = J\left| -- \right\rangle$$

$$\hat{H}_0 \left| +- \right\rangle = J(2\left| -+ \right\rangle - \left| +- \right\rangle)$$

$$\hat{H}_0 \left| -+ \right\rangle = J(2\left| +- \right\rangle - \left| -+ \right\rangle)$$

Thus

$$\hat{H}\left| ++ \right\rangle = [J - (\mu_1 + \mu_2)B]\left| ++ \right\rangle$$

$|++\rangle$ is the eigenket of $\hat{H}$ with the energy eigenvalue $[J-(\mu_1+\mu_2)B]$

$$\hat{H}|--\rangle = [J+(\mu_1+\mu_2)B]|--\rangle$$

$|--\rangle$ is the eigenket of $\hat{H}$ with the energy eigenvalue $[J+(\mu_1+\mu_2)B]$.

We now consider a matrix of the subspace of $|+-\rangle$ and $|-+\rangle$;

$$\hat{H}|+-\rangle = J(2|-+\rangle - |+-\rangle) - (\mu_1-\mu_2)B|+-\rangle$$

$$\hat{H}|-+\rangle = J(2|+-\rangle - |-+\rangle) + (\mu_1-\mu_2)B|+-\rangle$$

or

$$\hat{H} = \begin{pmatrix} -J-(\mu_1-\mu_2)B & 2J \\ 2J & -J+(\mu_1-\mu_2)B \end{pmatrix}$$
$$= -J\hat{1} - (\mu_1-\mu_2)B\hat{\sigma}_z + 2J\hat{\sigma}_x$$

The eigenvalue problem can be solved as follows.

$$\hat{H} = -J\hat{1} + \sqrt{4J^2+(\mu_1-\mu_2)^2B^2}\left[\frac{-(\mu_1-\mu_2)B}{\sqrt{4J^2+(\mu_1-\mu_2)^2B^2}}\hat{\sigma}_z + \frac{2J}{\sqrt{4J^2+(\mu_1-\mu_2)^2B^2}}\hat{\sigma}_x\right]$$
$$= -J\hat{1} + \sqrt{4J^2+(\mu_1-\mu_2)^2B^2}\,\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n}$$

where

$$\boldsymbol{n} = (\sin\theta, 0, \cos\theta)$$

with

$$\cos\theta = \frac{-(\mu_1-\mu_2)B}{\sqrt{4J^2+(\mu_1-\mu_2)^2B^2}}, \qquad \sin\theta = \frac{2J}{\sqrt{4J^2+(\mu_1-\mu_2)^2B^2}},$$

Eigenvalue problem:

$$\hat{H}|\pm\boldsymbol{n}\rangle = [-J\hat{1} + \sqrt{4J^2+(\mu_1-\mu_2)^2B^2}\,\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n}]|\pm\boldsymbol{n}\rangle$$
$$= [-J \pm \sqrt{4J^2+(\mu_1-\mu_2)^2B^2}\,]|\pm\boldsymbol{n}\rangle$$

$|+\boldsymbol{n}\rangle$ is the eigenket of $\hat{H}$ with the eigenvalue E_1;

$$|+\boldsymbol{n}\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix}, \qquad E_1 = -J + \sqrt{4J^2 + (\mu_1 - \mu_2)^2 B^2}$$

$|-\boldsymbol{n}\rangle$ is the eigenket of $\hat{H}$ with the eigenvalue E_2;

$$|+\boldsymbol{n}\rangle = \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \end{pmatrix}, \qquad E_2 = -J - \sqrt{4J^2 + (\mu_1 - \mu_2)^2 B^2}$$

((Mathematica))

```
Clear["Global`*"]; H = ( -J - (μ1 - μ2) B        2 J
                           2 J          -J + (μ1 - μ2) B );

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

$$\left\{\left\{-J-\sqrt{4 J^2+B^2 (\mu 1-\mu 2)^2}, -J+\sqrt{4 J^2+B^2 (\mu 1-\mu 2)^2}\right\},\right.$$
$$\left\{\left\{\frac{-\sqrt{4 J^2+B^2 (\mu 1-\mu 2)^2}+B(-\mu 1+\mu 2)}{2 J}, 1\right\},\right.$$
$$\left.\left.\left\{\frac{\sqrt{4 J^2+B^2 (\mu 1-\mu 2)^2}+B(-\mu 1+\mu 2)}{2 J}, 1\right\}\right\}\right\}$$

```
E1 = eq1[[1, 1]]; E2 = eq1[[1, 2]]; E3 = J - B (μ1 + μ2); E4 = J + B (μ1 + μ2);
rule1 = {μ2 → -1000 μ1, J → 1, B → 10^4 B1, μ1 → 10^-7};

E11 = E1 //. rule1 // Simplify; E22 = E2 //. rule1 // Simplify;
E33 = E3 //. rule1 // Simplify; E44 = E4 //. rule1 // Simplify;
tab1 = {E11, E22, E33, E44};
```

```
Plot[Evaluate[tab1], {B1, 0, 5},
 PlotStyle → Table[{Hue[0.08 i], Thick}, {i, 0, 4}],
 AxesLabel → {"B(T)", "E"}]
```

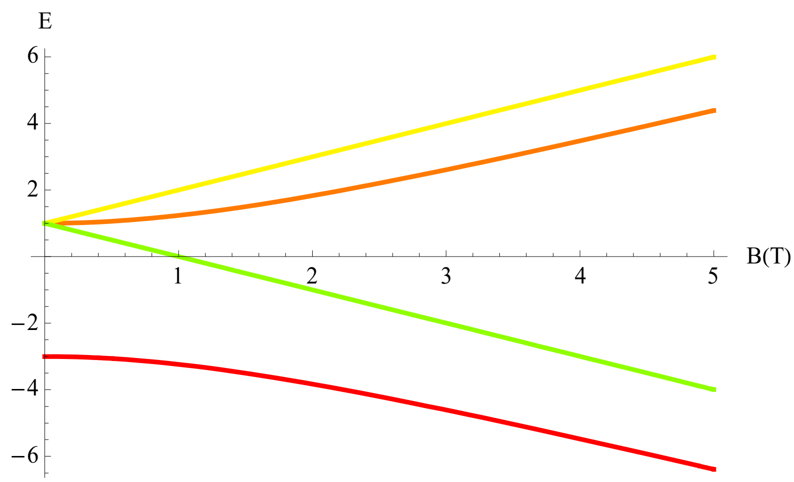


Fig. Zeeman splitting of the ground state of hydrogen. $B \neq 0$:the levels are denoted as E_I, E_{III}, E_{II}, and E_{IV} from the top to the bottom. $B = 0$: there are two levels. One level is E_{IV}, and another level is degenerate (E_I, E_{III}, E_{II}).

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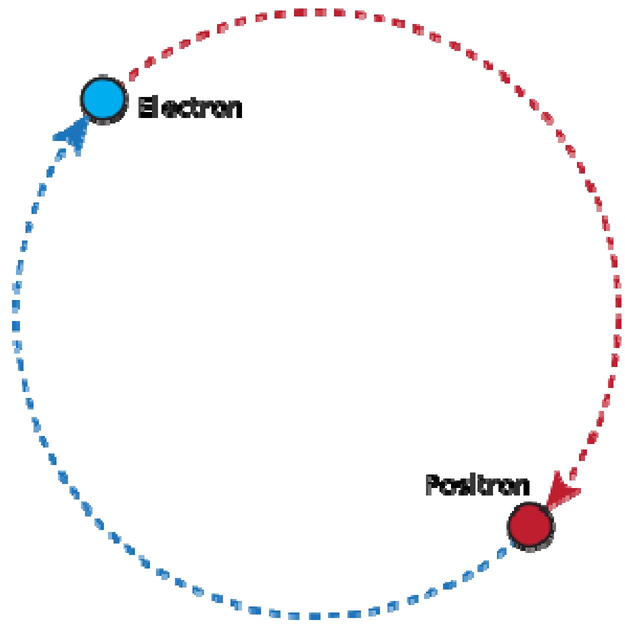
7. Positronium in the presence of a magnetic field



Positronium (**Ps**) is a system consisting of an electron and its anti-particle, a positron, bound together into an "exotic atom". The system is unstable: the two particles annihilate each other to produce two gamma ray photons after an average lifetime of 125 picoseconds or three gamma ray photons after 142 nanoseconds in vacuum, depending on the relative spin states of the positron and electron. The orbit of the two particles and the set of energy levels is similar to that of the hydrogen atom (electron and proton).

Consider the p**ositronium** consisting of positron and electron. In the presence of a uniform and static magnetic field B along the z-axis, the Hamiltonian is given by

$$\hat{H} = A\hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2 + \frac{eB}{mc}(\hat{S}_{1z} - \hat{S}_{2z})$$

Obtain the energy eigenvalues and eigenkets of the Hamiltonian $\hat{H}$.

((**Solution**))

$$\hat{H} = \frac{2A}{\hbar^2}\hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2 + \omega_0(\hat{S}_{1z} - \hat{S}_{2z})$$

where

$$\hat{\boldsymbol{S}}_1 = \frac{\hbar}{2}\hat{\boldsymbol{\sigma}}_1, \qquad \hat{\boldsymbol{S}}_2 = \frac{\hbar}{2}\hat{\boldsymbol{\sigma}}_2.$$

The Hamiltonian can be rewritten as

$$\hat{H} = \frac{A}{2}\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_1 + \frac{\hbar\omega_0}{2}(\hat{\sigma}_{1z} - \hat{\sigma}_{2z})$$

Here note that

$$\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2 = 2\hat{P}_{12} - 1$$

where $\hat{P}_{12}$ is the spin exchange operatpr. Then the Hamiltonian $\hat{H}$ can be rewritten as

$$\hat{H} = A(\hat{P}_{12} - \frac{1}{2}\hat{1}) + \frac{1}{2}\hbar\omega_0(\hat{\sigma}_{1z} - \hat{\sigma}_{2z})$$

There are four kinds of two-spin states;

$$|++\rangle, \qquad |+-\rangle, \qquad |-+\rangle, \qquad |--\rangle$$

So we get

$$\hat{H}|++\rangle = \frac{A}{2}|++\rangle$$

$$\hat{H}|+-\rangle = A|-+\rangle - \frac{A}{2}|+-\rangle + \hbar\omega_0|+-\rangle$$
$$= (-\frac{A}{2} + \hbar\omega_0)|+-\rangle + A|-+\rangle$$

$$\hat{H}|-+\rangle = A|+-\rangle - \frac{A}{2}|-+\rangle - \hbar\omega_0|-+\rangle$$
$$= -(\frac{A}{2} + \hbar\omega_0)|-+\rangle + A|+-\rangle$$

$$\hat{H}|--\rangle = \frac{A}{2}|--\rangle$$

Then $|++\rangle$ is the eigenket of $\hat{H}$ with eigenvalue *A*/2. $|--\rangle$ is the eigenket of $\hat{H}$ with eigenvalue *A*/2. We now consider the eigenvalue problems (subgroup) using the basis of $\{|+-\rangle, |-+\rangle\}$.

$$\hat{H}_{sub} = \begin{pmatrix} \langle +-|\hat{H}|+-\rangle & \langle +-|\hat{H}|-+\rangle \\ \langle -+|\hat{H}|+-\rangle & \langle -+|\hat{H}|-+\rangle \end{pmatrix}$$
$$= \begin{pmatrix} (-\frac{A}{2} + \hbar\omega_0) & A \\ A & -(\frac{A}{2} + \hbar\omega_0) \end{pmatrix}$$

This Hamiltonian can be described by using the Pauli matrices as

$$\hat{H}_{sub} = \begin{pmatrix} \langle +-|\hat{H}|+-\rangle & \langle +-|\hat{H}|-+\rangle \\ \langle -+|\hat{H}|+-\rangle & \langle -+|\hat{H}|-+\rangle \end{pmatrix}$$
$$= \begin{pmatrix} (-\frac{A}{2} + \hbar\omega_0) & A \\ A & -(\frac{A}{2} + \hbar\omega_0) \end{pmatrix}$$
$$= -\frac{A}{2}\hat{1} + \hbar\omega_0\hat{\sigma}_z + A\hat{\sigma}_x$$

This can be rewritten as

$$\hat{H}_{sub} = -\frac{A}{2}\hat{1} + \sqrt{A^2 + (\hbar\omega_0)^2}[\frac{\hbar\omega_0}{\sqrt{A^2 + (\hbar\omega_0)^2}}\hat{\sigma}_z + \frac{A}{\sqrt{A^2 + (\hbar\omega_0)^2}}\hat{\sigma}_x]$$
$$= -\frac{A}{2}\hat{1} + \sqrt{A^2 + (\hbar\omega_0)^2}(\cos\theta\hat{\sigma}_z + \sin\theta\hat{\sigma}_x)$$
$$= -\frac{A}{2}\hat{1} + \sqrt{A^2 + (\hbar\omega_0)^2}\,\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n}$$

where $\hat{\boldsymbol{\sigma}}$ is the matrix under the basis of $\{|1\rangle = |+-\rangle, |2\rangle = |-+\rangle\}$ and

$$\boldsymbol{n} = (\sin\theta, 0, \cos\theta),$$

in the *z*-*x* plane, and q is the angle from the z axis. Note that

$$\cos\theta = \frac{\hbar\omega_0}{\sqrt{A^2 + (\hbar\omega_0)^2}}, \qquad \sin\theta = \frac{A}{\sqrt{A^2 + (\hbar\omega_0)^2}}$$

The eigenket of $\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n}$ is defined as

$$\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n}|+\boldsymbol{n}\rangle = |+\boldsymbol{n}\rangle, \qquad \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n}|-\boldsymbol{n}\rangle = -|-\boldsymbol{n}\rangle$$

$$|+\boldsymbol{n}\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix}, \qquad |-\boldsymbol{n}\rangle = \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \end{pmatrix}.$$

under the basis of {$|+-\rangle$, $|-+\rangle$}. Note that

$$\hat{H}_{sub}|\pm\boldsymbol{n}\rangle$$
$$= (-\frac{A}{2} \pm \sqrt{A^2 + (\hbar\omega_0)^2})|\pm\boldsymbol{n}\rangle$$

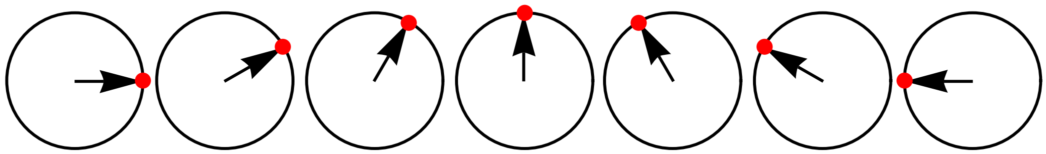
Then there are foue energy states

Eigenvalue	Eigenket
$A/2$	$\lvert ++\rangle$
$A/2$	$\lvert --\rangle$
$(-\frac{A}{2} + \sqrt{A^2 + (\hbar\omega_0)^2})$	$\lvert +\boldsymbol{n}\rangle$
$(-\frac{A}{2} - \sqrt{A^2 + (\hbar\omega_0)^2})$	$\lvert -\boldsymbol{n}\rangle$

---

10. Spin wave

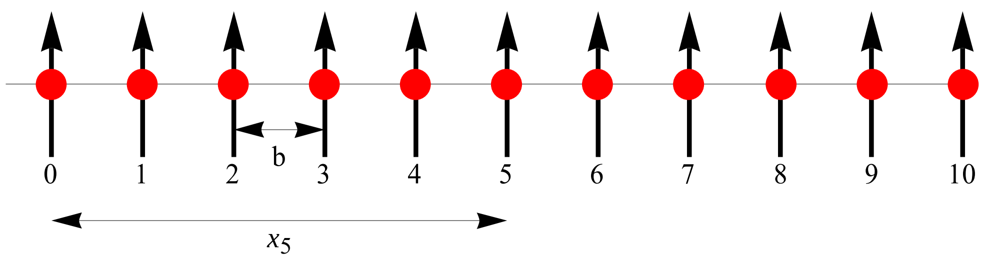
Spin waves are propagating disturbances in the ordering of magnetic materials. These low-lying collective excitations occur in magnetic lattices with continuous symmetry. From the equivalent quasiparticle point of view, spin waves are known as magnons, which are boson modes of the spin lattice that correspond roughly to the phonon excitations of the nuclear lattice. As temperature is increased, the thermal excitation of spin waves reduces a ferromagnet's spontaneous magnetization.



We consider the spin exchange interaction between two adjacent such that

$$\hat{H} = -\frac{J}{2}\sum_{n} \hat{\boldsymbol{\sigma}}_n \cdot \hat{\boldsymbol{\sigma}}_{n+1}$$

With this Hamiltonian we have a complete description of the ferromagnet.



$$\hat{\boldsymbol{\sigma}}_n \cdot \hat{\boldsymbol{\sigma}}_{n+1} = 2\hat{P}_{n,n+1} - 1$$

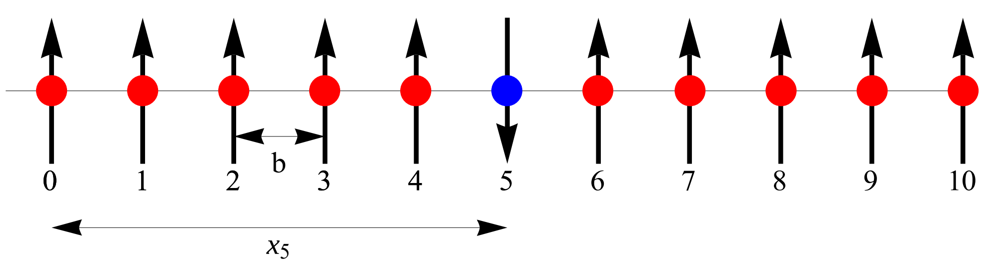
where $\hat{\boldsymbol{\sigma}}_n \cdot \hat{\boldsymbol{\sigma}}_{n+1}$ interchanges the spins of the n-th and (n+1)-th electrons.

For the ground state all spins are up ($\left|+\right\rangle$, so if you exchange a particular pair of spins, one can get back the original state. The ground state is a stationary state: -J/2 for each pair of spins. That is, the energy of the system in the ground state is -J/2 per spin.

It is convenient to measure the energies with respect to the ground state. Our new Hamiltonian is

Using the relation

$$\hat{H} = -J\sum_{n}(\hat{P}_{n,n+1} - \hat{1})$$



With this Hamiltonian, the energy of the ground state is zero. Here we define the state $\left|x_{.n}\right\rangle$ where all the spins except for the one on the spin at x_n.

$$\begin{aligned}\hat{H}\left|x_5\right\rangle &= -J\sum_n (\hat{P}_{n,n+1} - \hat{1})\left|x_5\right\rangle \\ &= -J(\hat{P}_{5,6} - \hat{1})\left|x_5\right\rangle - J(\hat{P}_{4,5} - \hat{1})\left|x_5\right\rangle \\ &= -J(\left|x_6\right\rangle - 2\left|x_5\right\rangle + \left|x_4\right\rangle)\end{aligned}$$

where $\hat{P}_{45}\left|x_5\right\rangle = \left|x_4\right\rangle$, $\hat{P}_{56}\left|x_5\right\rangle = \left|x_6\right\rangle$, $\hat{P}_{78}\left|x_5\right\rangle = \left|x_5\right\rangle$, and . $\hat{P}_{34}\left|x_5\right\rangle = \left|x_5\right\rangle$.

Similary,

$$\hat{H}\left|x_n\right\rangle = -J(\left|x_{n+1}\right\rangle - 2\left|x_n\right\rangle + \left|x_{n-1}\right\rangle$$

$$\hat{H}\left|x_{n+1}\right\rangle = -J(\left|x_{n+2}\right\rangle - 2\left|x_{n+1}\right\rangle + \left|x_n\right\rangle$$

Here we consider

$$\left|\psi\right\rangle = \sum_n C_n\left|x_n\right\rangle$$

Eigenvalue problem

$$\hat{H}\left|\psi\right\rangle = E\left|\psi\right\rangle$$

or

$$\sum_n C_n\hat{H}\left|x_n\right\rangle = E\sum_n C_n\left|x_n\right\rangle$$

or

$$\sum_n C_n\hat{H}\left|x_n\right\rangle = E\sum_n C_n\left|x_n\right\rangle$$

or

$$\sum_n (-J)(C_n\left|x_{n+1}\right\rangle - 2C_n\left|x_n\right\rangle + C_n\left|x_{n-1}\right\rangle = E\sum_n C_n\left|x_n\right\rangle$$

or

$$\sum_n (-J)(C_{n-1} - 2C_n + C_{n+1})\left|x_n\right\rangle = E\sum_n C_n \left|x_n\right\rangle$$

or

$$(-J)(C_{n-1} - 2C_n + C_{n+1}) = EC_n$$

Let us take as a trial function

$$C_n = e^{ikx_n}$$

$$(-J)(e^{ik(x_n - b)} - 2e^{ikx_n} + e^{ik(x_n + b)}) = Ee^{ikx_n}$$

$$E = 2J[1 - \cos(kb)] \qquad \text{(energy dispersion)}$$

The difference energy solutions corresponds to "waves" of down spin-called "spin waves."

For kb<<1, E is approximated by

$$E = 2A\frac{k^2b^2}{2} = Ak^2b^2$$

11. Matrix representation of rotation operator for *j* =1.

We are constructing the eigenkets for j = 1. To this end, we start with the basis for j = 1/2.

$$\left|+\boldsymbol{n}\right\rangle = \hat{U}\left|+z\right\rangle = a\left|+z\right\rangle + b\left|-z\right\rangle$$

$$\left|-\boldsymbol{n}\right\rangle = \hat{U}\left|-z\right\rangle = c\left|+z\right\rangle + d\left|-z\right\rangle$$

where

$$a = e^{-i\frac{\phi}{2}}\cos(\frac{\theta}{2}), \qquad b = e^{i\frac{\phi}{2}}\sin(\frac{\theta}{2})$$

$$c = -e^{-i\frac{\phi}{2}}\sin(\frac{\theta}{2}) \qquad d = e^{i\frac{\phi}{2}}\cos(\frac{\theta}{2})$$

$$\left|+\boldsymbol{n}\right\rangle = \begin{pmatrix} e^{-i\frac{\phi}{2}}\cos(\frac{\theta}{2}) \\ e^{i\frac{\phi}{2}}\sin(\frac{\theta}{2}) \end{pmatrix}, \qquad \left|-\boldsymbol{n}\right\rangle = \begin{pmatrix} -e^{-i\frac{\phi}{2}}\sin(\frac{\theta}{2}) \\ e^{i\frac{\phi}{2}}\cos(\frac{\theta}{2}) \end{pmatrix}$$

$$\hat{U} = \begin{pmatrix} e^{-i\frac{\phi}{2}}\cos(\frac{\theta}{2}) & -e^{-i\frac{\phi}{2}}\sin(\frac{\theta}{2}) \\ e^{i\frac{\phi}{2}}\sin(\frac{\theta}{2}) & e^{i\frac{\phi}{2}}\cos(\frac{\theta}{2}) \end{pmatrix}$$

We can write the state

$$\begin{aligned} \left|+\boldsymbol{n},+\boldsymbol{n}\right\rangle &= (a\left|+z\right\rangle + b\left|-z\right\rangle)(a\left|+z\right\rangle + b\left|-z\right\rangle) \\ &= a^2\left|+z,+z\right\rangle + \sqrt{2}ab\frac{1}{\sqrt{2}}(\left|+z,-z\right\rangle + \left|-z,+z\right\rangle) + b^2\left|-z,-z\right\rangle \end{aligned}$$

Similarly

$$\begin{aligned} \left|-\boldsymbol{n},-\boldsymbol{n}\right\rangle &= (c\left|+z\right\rangle + d\left|-z\right\rangle)(c\left|+z\right\rangle + d\left|-z\right\rangle) \\ &= c^2\left|+z,+z\right\rangle + \sqrt{2}cd\frac{1}{\sqrt{2}}(\left|+z,-z\right\rangle + \left|-z,+z\right\rangle) + d^2\left|-z,-z\right\rangle \end{aligned}$$

$$\begin{aligned} \frac{1}{\sqrt{2}}(\left|+\boldsymbol{n},-\boldsymbol{n}\right\rangle + \left|-\boldsymbol{n},+\boldsymbol{n}\right\rangle) &= \sqrt{2}ac\left|+z,+z\right\rangle + (ad+bc)\frac{1}{\sqrt{2}}(\left|+z,-z\right\rangle \\ &\quad + \left|-z,+z\right\rangle) + \sqrt{2}bd\left|-z,-z\right\rangle \end{aligned}$$

Unitary operator $\hat{R}$,

$$\left|+\boldsymbol{n},+\boldsymbol{n}\right\rangle = \left|1,1;\boldsymbol{n}\right\rangle = \hat{R}\left|+z,+z\right\rangle = \hat{R}\left|1,1;z\right\rangle$$

$$\left|-\boldsymbol{n},-\boldsymbol{n}\right\rangle = \left|1,-1;\boldsymbol{n}\right\rangle = \hat{R}\left|-z,-z\right\rangle = \hat{R}\left|1,-1;z\right\rangle$$

$$\frac{\left|+\boldsymbol{n},-\boldsymbol{n}\right\rangle + \left|-\boldsymbol{n},+\boldsymbol{n}\right\rangle}{\sqrt{2}} = \left|1,0;\boldsymbol{n}\right\rangle = \hat{R}\frac{\left|+z,-z\right\rangle + \left|-z,+z\right\rangle}{\sqrt{2}}$$

where

$$|1,1;z\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |1,0;z\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad |1,-1;z\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$\begin{aligned} |+\boldsymbol{n},+\boldsymbol{n}\rangle &== a^2|+z,+z\rangle + \sqrt{2}ab\frac{1}{\sqrt{2}}(|+z,-z\rangle + |-z,+z\rangle) + b^2|-z,-z\rangle \\ &= \begin{pmatrix} a^2 \\ \sqrt{2}ab \\ b^2 \end{pmatrix} \\ &= \begin{pmatrix} R_{11} \\ R_{21} \\ R_{31} \end{pmatrix} \end{aligned}$$

$$\begin{aligned} \frac{1}{\sqrt{2}}(|+\boldsymbol{n},-\boldsymbol{n}\rangle + |-\boldsymbol{n},+\boldsymbol{n}\rangle) &= \sqrt{2}ac|+z,+z\rangle + (ad+bc)\frac{1}{\sqrt{2}}(|+z,-z\rangle \\ &\quad + |-z,+z\rangle) + \sqrt{2}bd|-z,-z\rangle \\ &= \begin{pmatrix} \sqrt{2}ac \\ \dfrac{(ad+bc)}{\sqrt{2}} \\ \sqrt{2}bd \end{pmatrix} \\ &= \begin{pmatrix} R_{12} \\ R_{22} \\ R_{32} \end{pmatrix} \end{aligned}$$

$$\begin{aligned} |-\boldsymbol{n},-\boldsymbol{n}\rangle &= c^2|+z,+z\rangle + \sqrt{2}cd\frac{1}{\sqrt{2}}(|+z,-z\rangle + |-z,+z\rangle) + d^2|-z,-z\rangle \\ &= \begin{pmatrix} c^2 \\ \sqrt{2}cd \\ d^2 \end{pmatrix} \end{aligned}$$

Then we have the rotation operator $\hat{R} = \hat{R}_z(\phi)\hat{R}_y(\theta)$

$$\hat{R} = \begin{pmatrix} a^2 & \sqrt{2}ca & c^2 \\ \sqrt{2}ab & ad+bc & \sqrt{2}cd \\ b^2 & \sqrt{2}bd & d^2 \end{pmatrix}$$

or

$$\hat{R} = \begin{pmatrix} \frac{e^{-i\phi}}{2}(1+\cos\theta) & -\frac{e^{-i\phi}}{\sqrt{2}}\sin\theta & \frac{e^{-i\phi}}{2}(1+\cos\theta) \\ \frac{1}{\sqrt{2}}\sin\theta & \cos\theta & -\frac{1}{\sqrt{2}}\sin\theta \\ \frac{e^{i\phi}}{2}(1-\cos\theta) & \frac{e^{i\phi}}{\sqrt{2}}\sin\theta & \frac{e^{i\phi}}{2}(1+\cos\theta) \end{pmatrix}$$

which is the same as the matrix of $\hat{R} = \exp(-\frac{i}{\hbar}\hat{J}_z\phi)\exp(-\frac{i}{\hbar}\hat{J}_y\theta)$

12. Two spin state using KroneckProduct

We discuss the above discussion by using the KroneckerProduct.

$$\hat{S}_x^T = \hat{S}_{x1} \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{S}_{x2}$$

$$\hat{S}_y^T = \hat{S}_{y1} \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{S}_{y2}$$

$$\hat{S}_z^T = \hat{S}_{z1} \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{S}_{z2}$$

(a)

$$\begin{aligned} \left(\hat{S}_x^T\right)^2 + \left(\hat{S}_y^T\right)^2 + \left(\hat{S}_z^T\right)^2 &= (\hat{S}_{x1} \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{S}_{x2})(\hat{S}_{x1} \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{S}_{x2}) \\ &\quad + (\hat{S}_{y1} \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{S}_{y2})(\hat{S}_{y1} \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{S}_{y2}) \\ &\quad + (\hat{S}_{z1} \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{S}_{z2})(\hat{S}_{z1} \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{S}_{z2}) \\ &= (\hat{S}_{x1}{}^2 \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{S}_{x2}{}^2 + 2\hat{S}_{x1} \otimes \hat{S}_{x2}) \\ &\quad + (\hat{S}_{y1}{}^2 \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{S}_{y2}{}^2 + 2\hat{S}_{y1} \otimes \hat{S}_{y2}) \\ &\quad + (\hat{S}_{z1}{}^2 \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{S}_{z2}{}^2 + 2\hat{S}_{z1} \otimes \hat{S}_{z2}) \\ &= (\hat{S}_{x1}{}^2 + \hat{S}_{y1}{}^2 + \hat{S}_{z1}{}^2) \otimes \hat{1}_2 + \hat{1}_1 \otimes (\hat{S}_{x2}{}^2 + \hat{S}_{y2}{}^2 + \hat{S}_{z2}{}^2) + 2(\hat{S}_{x1} \otimes \hat{S}_{x2} \\ &\quad + \hat{S}_{y1} \otimes \hat{S}_{y2} + \hat{S}_{z1} \otimes \hat{S}_{z2}) \end{aligned}$$

where

$$\hat{S}_{x1}{}^2 + \hat{S}_{y1}{}^2 + \hat{S}_{z1}{}^2 = \frac{\hbar^2}{4}(\hat{\sigma}_{x1}{}^2 + \hat{\sigma}_{y1}{}^2 + \hat{\sigma}_{z1}{}^2) = \frac{3\hbar^2}{4}\hat{1}_1$$

$$\hat{S}_{x2}{}^2 + \hat{S}_{y2}{}^2 + \hat{S}_{z2}{}^2 = \frac{\hbar^2}{4}(\hat{\sigma}_{x2}{}^2 + \hat{\sigma}_{y2}{}^2 + \hat{\sigma}_{z2}{}^2) = \frac{3\hbar^2}{4}\hat{1}_2$$

Then we have

$$\begin{aligned}\hat{\boldsymbol{S}}^2 &= \left(\hat{S}_x^T\right)^2 + \left(\hat{S}_y^T\right)^2 + \left(\hat{S}_z^T\right)^2 \\ &= \frac{3\hbar^2}{4}\hat{1}_1 \otimes \hat{1}_2 + \hat{1}_1 \otimes \frac{3\hbar^2}{4}\hat{1}_1 + 2(\hat{S}_{x1} \otimes \hat{S}_{x2} \\ &\quad + \hat{S}_{y1} \otimes \hat{S}_{y2} + \hat{S}_{z1} \otimes \hat{S}_{z2}) \\ &= \frac{3\hbar^2}{2}\hat{1}_1 \otimes \hat{1}_2 + \frac{\hbar^2}{2}(\hat{\sigma}_{x1} \otimes \hat{\sigma}_{x2} + \hat{\sigma}_{y1} \otimes \hat{\sigma}_{y2} + \hat{\sigma}_{z1} \otimes \hat{\sigma}_{z2})\end{aligned}$$

and

$$\hat{S}_z = \hat{S}_{z1} \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{S}_{z2} = \frac{\hbar}{2}(\hat{\sigma}_{z1} \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{\sigma}_{z2})$$

((**Note**)) Alternative method (simpler method)
After the calculation of

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

this expression can be rewritten

$$\hat{\boldsymbol{S}}^2 = \frac{3\hbar^2}{2}\hat{1}_1 \otimes \hat{1}_2 + \frac{\hbar^2}{2}(\hat{\sigma}_{x1} \otimes \hat{\sigma}_{x2} + \hat{\sigma}_{y1} \otimes \hat{\sigma}_{y2} + \hat{\sigma}_{z1} \otimes \hat{\sigma}_{z2})$$

using the Kronecker product $\otimes$.

The matrix of $\hat{\boldsymbol{S}}^2$ is expressed by

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

under the basis of { $|+,+\rangle, |+-\rangle, |-,+\rangle, |-,-\rangle$ }. The matrix of $\hat{S}_z$ is expressed by

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

under the basis of { $|+,+\rangle, |+-\rangle, |-,+\rangle, |-,-\rangle$ }.

$$\begin{aligned}\hat{\boldsymbol{S}}^2(|+\rangle \otimes |+\rangle) &= [\frac{3\hbar^2}{2}\hat{1}_1 \otimes \hat{1}_2 + \frac{\hbar^2}{2}(\hat{\sigma}_{x1} \otimes \hat{\sigma}_{x2} + \hat{\sigma}_{y1} \otimes \hat{\sigma}_{y2} + \hat{\sigma}_{z1} \otimes \hat{\sigma}_{z2})](|+\rangle \otimes |+\rangle)] \\ &= \frac{3\hbar^2}{2}|+\rangle \otimes |+\rangle + \frac{\hbar^2}{2}[|-\rangle \otimes |-\rangle - |-\rangle \otimes |-\rangle + |+\rangle \otimes |+\rangle] \\ &= 2\hbar^2 |+\rangle \otimes |+\rangle\end{aligned}$$

$$\begin{aligned}\hat{\boldsymbol{S}}^2(|-\rangle \otimes |-\rangle) &= [\frac{3\hbar^2}{2}\hat{1}_1 \otimes \hat{1}_2 + \frac{\hbar^2}{2}(\hat{\sigma}_{x1} \otimes \hat{\sigma}_{x2} + \hat{\sigma}_{y1} \otimes \hat{\sigma}_{y2} + \hat{\sigma}_{z1} \otimes \hat{\sigma}_{z2})](|-\rangle \otimes |-\rangle)] \\ &= \frac{3\hbar^2}{2}|-\rangle \otimes |-\rangle + \frac{\hbar^2}{2}[|+\rangle \otimes |+\rangle - |+\rangle \otimes |+\rangle + |-\rangle \otimes |-\rangle] \\ &= 2\hbar^2 |-\rangle \otimes |-\rangle\end{aligned}$$

$$\begin{aligned}\hat{\boldsymbol{S}}^2(|+\rangle \otimes |-\rangle) &= [\frac{3\hbar^2}{2}\hat{1}_1 \otimes \hat{1}_2 + \frac{\hbar^2}{2}(\hat{\sigma}_{x1} \otimes \hat{\sigma}_{x2} + \hat{\sigma}_{y1} \otimes \hat{\sigma}_{y2} + \hat{\sigma}_{z1} \otimes \hat{\sigma}_{z2})](|+\rangle \otimes |-\rangle)] \\ &= \frac{3\hbar^2}{2}|+\rangle \otimes |-\rangle + \frac{\hbar^2}{2}[2|-\rangle \otimes |+\rangle - |+\rangle \otimes |-\rangle] \\ &= \hbar^2[|+\rangle \otimes |-\rangle + |-\rangle \otimes |+\rangle]\end{aligned}$$

$$\begin{aligned}\hat{\boldsymbol{S}}^2(|-\rangle \otimes |+\rangle) &= [\frac{3\hbar^2}{2}\hat{1}_1 \otimes \hat{1}_2 + \frac{\hbar^2}{2}(\hat{\sigma}_{x1} \otimes \hat{\sigma}_{x2} + \hat{\sigma}_{y1} \otimes \hat{\sigma}_{y2} + \hat{\sigma}_{z1} \otimes \hat{\sigma}_{z2})](|-\rangle \otimes |+\rangle)] \\ &= \frac{3\hbar^2}{2}|-\rangle \otimes |+\rangle + \frac{\hbar^2}{2}[2|+\rangle \otimes |-\rangle - |-\rangle \otimes |+\rangle] \\ &= \hbar^2[|+\rangle \otimes |-\rangle + |-\rangle \otimes |+\rangle]\end{aligned}$$

$(|+\rangle \otimes |+\rangle)$ is the eigenket of $\hat{\boldsymbol{S}}^2$ with the eigenvalue $2\hbar^2$ ($S = 1$)

$(|-\rangle \otimes |-\rangle)$ is the eigenket of $\hat{\boldsymbol{S}}^2$ with the eigenvalue $2\hbar^2$ ($S = 1$)

We now consider the operator $\hat{\boldsymbol{S}}^2$ under the basis $\{|+\rangle \otimes |-\rangle,\ |-\rangle \otimes |+\rangle\}$. The matrix $\left(\hat{\boldsymbol{S}}^2\right)_{sub}$ can be expressed by

$$\left(\hat{\boldsymbol{S}}^2\right)_{sub} = \hbar^2 \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \hbar^2 [\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}] = \hbar^2 (\hat{\sigma}_x + \hat{1})$$

Then we have

$$\left(\hat{\boldsymbol{S}}^2\right)_{sub} |+x\rangle = \hbar^2 (\hat{\sigma}_x + \hat{1}) |+x\rangle = 2\hbar^2 |+x\rangle$$

$$\left(\hat{\boldsymbol{S}}^2\right)_{sub} |-x\rangle = \hbar^2 (\hat{\sigma}_x + \hat{1}) |-x\rangle = 0 |+x\rangle$$

where

$$|+x\rangle \rightarrow \frac{1}{\sqrt{2}} [|+\rangle \otimes |-\rangle + |-\rangle \otimes |+\rangle] \qquad \text{eigenvalue: } 2\hbar^2 \qquad (S = 1)$$

$$|-x\rangle \rightarrow \frac{1}{\sqrt{2}} [|+\rangle \otimes |-\rangle - |-\rangle \otimes |+\rangle] \qquad \text{eigenvalue: } 0\hbar^2 \qquad (S = 0)$$

We note that

$$\begin{aligned} \hat{S}_z (|+\rangle \otimes |+\rangle) &= \frac{\hbar}{2} (\hat{\sigma}_{z1} \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{\sigma}_{z2}) (|+\rangle \otimes |+\rangle) \\ &= \hbar (|+\rangle \otimes |+\rangle) \end{aligned}$$

$$\begin{aligned} \hat{S}_z (|-\rangle \otimes |-\rangle) &= \frac{\hbar}{2} (\hat{\sigma}_{z1} \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{\sigma}_{z2}) (|-\rangle \otimes |-\rangle) \\ &= -\hbar (|-\rangle \otimes |-\rangle) \end{aligned}$$

$$\begin{aligned} \hat{S}_z \frac{[|+\rangle \otimes |-\rangle + |-\rangle \otimes |+\rangle)}{\sqrt{2}} &= \frac{\hbar}{2} (\hat{\sigma}_{z1} \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{\sigma}_{z2}) \frac{[|+\rangle \otimes |-\rangle + |-\rangle \otimes |+\rangle)}{\sqrt{2}} \\ &= \frac{\hbar}{2\sqrt{2}} (\hat{\sigma}_{z1} \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{\sigma}_{z2}) |+\rangle \otimes |-\rangle \\ &\quad + \frac{\hbar}{2\sqrt{2}} (\hat{\sigma}_{z1} \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{\sigma}_{z2}) |-\rangle \otimes |+\rangle \\ &= 0 \end{aligned}$$

$$\hat{S}_z \frac{[|+\rangle \otimes |-\rangle - |-\rangle \otimes |+\rangle)}{\sqrt{2}} = \frac{\hbar}{2}(\hat{\sigma}_{z1} \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{\sigma}_{z2}) \frac{[|+\rangle \otimes |-\rangle - |-\rangle \otimes |+\rangle)}{\sqrt{2}}$$

$$= \frac{\hbar}{2\sqrt{2}}(\hat{\sigma}_{z1} \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{\sigma}_{z2})|+\rangle \otimes |-\rangle$$

$$- \frac{\hbar}{2\sqrt{2}}(\hat{\sigma}_{z1} \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{\sigma}_{z2})|-\rangle \otimes |+\rangle$$

$$= 0$$

((**Summary**))

$|\, j = 1, m = 1\rangle = (|+\rangle \otimes |+\rangle)$:

The eigenket of $\hat{\boldsymbol{S}}^2$ with the eigenvalue $2\hbar^2$ ($S = 1$)
The eigenket of $\hat{S}_z$ with the eigenvalue $\hbar$

$$|\, j = 1, m = 0\rangle = \frac{1}{\sqrt{2}}[|+\rangle \otimes |-\rangle + |-\rangle \otimes |+\rangle]$$

The eigenket of $\hat{\boldsymbol{S}}^2$ with the eigenvalue $2\hbar^2$ ($S = 1$)
The eigenket of $\hat{S}_z$ with the eigenvalue $0\hbar$

$$|\, j = 1, m = -1\rangle = |-\rangle \otimes |-\rangle$$

The eigenket of $\hat{\boldsymbol{S}}^2$ with the eigenvalue $2\hbar^2$ ($S = 1$)
The eigenket of $\hat{S}_z$ with the eigenvalue -$\hbar$

$$|\, j = 0, m = 0\rangle = \frac{1}{\sqrt{2}}[|+\rangle \otimes |-\rangle - |-\rangle \otimes |+\rangle]$$

The eigenket of $\hat{\boldsymbol{S}}^2$ with the eigenvalue $0\hbar^2$ ($S = 0$)
The eigenket of $\hat{S}_z$ with the eigenvalue $0\hbar$

((**Mathematica**))

```
Clear["Global`*"];
exp_* := exp /. {Complex[re_, im_] ⧴ Complex[re, -im]};
ψ1 = (1
      0);
ψ2 = (0
      1);
σx = PauliMatrix[1];
σy = PauliMatrix[2];
σz = PauliMatrix[3];
I2 = IdentityMatrix[2];
I8 = IdentityMatrix[8];
ϕ1 = KroneckerProduct[ψ1, ψ1];
ϕ2 = KroneckerProduct[ψ1, ψ2];
ϕ3 = KroneckerProduct[ψ2, ψ1];
ϕ4 = KroneckerProduct[ψ2, ψ2];
ST1 = 1/2 (KroneckerProduct[σx, σx] + KroneckerProduct[σy, σy]
      + KroneckerProduct[σz, σz]) + 3/2 KroneckerProduct[I2, I2];
Sz = 1/2 (KroneckerProduct[σz, I2] + KroneckerProduct[I2, σz]);

ST1 // MatrixForm
```

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

```
Sz // MatrixForm
```

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

```
eq1 = Eigensystem[ST1] // Simplify
```

```
{{2, 2, 2, 0},
 {{0, 0, 0, 1}, {0, 1, 1, 0}, {1, 0, 0, 0}, {0, -1, 1, 0}}}
```

```
χ1 = eq1[[2, 3]]; χ2 = eq1[[2, 2]]; χ3 = eq1[[2, 1]];
χ4 = -eq1[[2, 4]];
```

```
eq2 = Orthogonalize[{χ1, χ2, χ3, χ4}]
```

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

```
Φ1 = eq2[[1]]; Φ2 = eq2[[2]]; Φ3 = Normalize[eq2[[3]]];
Φ4 = eq2[[4]];
```

```
Sz // MatrixForm
```

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

```
Sz.Φ1 - Φ1
```

```
{0, 0, 0, 0}
```

```
Sz.Φ2
```

{0, 0, 0, 0}

```
Sz.Φ3 + Φ3
```

{0, 0, 0, 0}

```
Sz.Φ4
```

{0, 0, 0, 0}

```
Φ1 // MatrixForm
```

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

```
Φ2 // MatrixForm
```

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

```
Φ3 // MatrixForm
```

$$\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

```
Φ4 // MatrixForm
```

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

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APPENDIX

A1. Eigenvalues and eigenkets for the two spins with S = 1/2: The use of KroneckerProduct for the calculation

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

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

These operators can be rewritten as

$$\hat{\boldsymbol{S}}^2 \to \frac{\hbar^2}{2}(3\hat{1}\otimes\hat{1} + \hat{\sigma}_x \otimes \hat{\sigma}_x + \hat{\sigma}_y \otimes \hat{\sigma}_y + \hat{\sigma}_z \otimes \hat{\sigma}_z)$$

$$\hat{S}_z \to \frac{\hbar}{2}(\hat{\sigma}_z \otimes \hat{1} + \hat{1} \otimes \hat{\sigma}_z)$$

The matrix of $\hat{\boldsymbol{S}}^2$ is obtained with the use of the Mathematica, as

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

The matrix of $\hat{S}_z$ is obtained as

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

A2. Eigenvalues and eigenkets for the Dirac spi n exchange operator: The use of KroneckerProduct for the calculation

The Dirac spin exchange operator is defined by

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

This operator can be rewritten as

$$\hat{P}_{12} \to \frac{1}{2}(\hat{1} \otimes \hat{1} + \hat{\sigma}_x \otimes \hat{\sigma}_x + \hat{\sigma}_y \otimes \hat{\sigma}_y + \hat{\sigma}_z \otimes \hat{\sigma}_z)$$

where $\hat{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

The matrix of $\hat{P}_{12}$ is obtained with the use of the Mathematica, as

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

Note that

$$\hat{\boldsymbol{S}}^2 = \hbar^2(\hat{1} \otimes \hat{1} + \hat{P}_{12})$$

Eigenvalue problem:

Eigenvalues, eigenkets

```
{{-1, 1, 1, 1}, {{0, -1, 1, 0}, {0, 0, 0, 1}, {0, 1, 1, 0}, {1, 0, 0, 0}}}
```

Eigenvalues of $\hat{P}_{12}$,	Eigenkets
1	$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$

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

1 $\qquad \begin{pmatrix}0\\0\\0\\1\end{pmatrix}$

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

((**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];

P12 = 1/2 (KroneckerProduct[σx, σx] + KroneckerProduct[σy, σy]
     + KroneckerProduct[σz, σz] + KroneckerProduct[I2, I2]);

P12 // MatrixForm
```

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

```
eq1 = Eigensystem[P12] // Simplify
```

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

```
χ1 = eq1[[2, 4]]; χ2 = eq1[[2, 3]]; χ3 = eq1[[2, 2]];
χ4 = eq1[[2, 1]];
```

```
eq2 = Orthogonalize[{χ1, χ2, χ3, χ4}]
```

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

```
Φ1 = eq2[[1]]; Φ2 = eq2[[2]]; Φ3 = -Normalize[eq2[[4]]];
Φ4 = eq2[[3]];
```

```
P12.ϕ1 - ϕ1
```

{{0}, {0}, {0}, {0}}

```
P12.ϕ2 - ϕ3
```

{{0}, {0}, {0}, {0}}

```
P12.ϕ3 - ϕ2
```

{{0}, {0}, {0}, {0}}

```
P12.ϕ4 - ϕ4
```

{{0}, {0}, {0}, {0}}

```
Φ1 // MatrixForm
```

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

```
Φ2 // MatrixForm
```

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

```
Φ3 // MatrixForm
```

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

```
Φ4 // MatrixForm
```

$$\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

A.3 Example for the use of KroneckerProduct

We consider the Hamiltonian given by the form of tensor product

$$\hat{H} = J(\hat{\sigma}_x \otimes \hat{\sigma}_x + \hat{\sigma}_y \otimes \hat{\sigma}_y + \hat{\sigma}_z \otimes \hat{\sigma}_z) - \mu_1 B(\hat{\sigma}_z \otimes \hat{1}) - \mu_2 B(\hat{1} \otimes \hat{\sigma}_z)$$

Using the Mathematica, we have the matrix of $\hat{H}$ as

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

We use the Mathematica program "Eigensystem in order to get the eigenvalues and eigenkets.

(1) The eigen value: $J - (\mu_1 + \mu_2)B$

The eigenket; $\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$

When $B = 0$, the energy is J.

(2) The eigenvalue: $J + (\mu_1 + \mu_2)B$

The eigenket; $\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$

When $B = 0$, the energy is J.

(3) Eigenvalue: $-J - \sqrt{4J^2 + (\mu_1 - \mu_2)^2 B^2}$

The eigenket: $\begin{pmatrix} 0 \\ \dfrac{-(\mu_1 - \mu_2)B - \sqrt{4J^2 + (\mu_1 - \mu_2)^2 B^2}}{2J} \\ 1 \\ 0 \end{pmatrix}$

When $B = 0$, the energy is $-3J$.

(4) Eigenvalue: $-J + \sqrt{4J^2 + (\mu_1 - \mu_2)^2 B^2}$

The eigenket $\begin{pmatrix} 0 \\ \dfrac{-(\mu_1 - \mu_2)B + \sqrt{4J^2 + (\mu_1 - \mu_2)^2 B^2}}{2J} \\ 1 \\ 0 \end{pmatrix}$

When $B = 0$, the energy is J.

A4. Eigenvalue problem for the exchange interaction (general case)

We consider the Hamiltonian given by the form of tensor product

$$\hat{H} = h_x \hat{\sigma}_x \otimes \hat{\sigma}_x + h_y \hat{\sigma}_y \otimes \hat{\sigma}_y + h_z \hat{\sigma}_z \otimes \hat{\sigma}_z$$

Using the Mathematica, we have the matrix of $\hat{H}$ as

$$\hat{H} = \begin{pmatrix} h_z & 0 & 0 & h_x - h_y \\ 0 & -h_z & h_x + h_y & 0 \\ 0 & h_x + h_y & -h_z & 0 \\ h_x - h_y & 0 & 0 & h_z \end{pmatrix}$$

(1) Eigenvalue: $h_x + h_y - h_z$, Eigenket: $\frac{1}{\sqrt{2}}[|+-\rangle + |-+\rangle]$.

(2) Eigenvalue: $-h_x - h_y - h_z$, Eigenket: $\frac{1}{\sqrt{2}}[|+-\rangle - |-+\rangle]$.

(3) Eigenvalue: $h_x - h_y + h_z$, Eigenket: $\frac{1}{\sqrt{2}}[|++\rangle + |--\rangle]$.

(4) Eigenvalue: $-h_x + h_y + h_z$, Eigenket: $\frac{1}{\sqrt{2}}[|++\rangle - |--\rangle]$.

We note that these eigenkets correspond to the four Bell's states.

APPENDIX B KroneckerProduct

B-1 Formula

$$(\hat{A} \otimes \hat{B})(\hat{C} \otimes \hat{D}) = (\hat{A}\hat{C}) \otimes (B\hat{D})$$

$$(\hat{A} \otimes \hat{B})(|\psi_1\rangle \otimes |\psi_2\rangle) = \hat{A}|\psi_1\rangle \otimes \hat{B}|\psi_2\rangle$$

$$\hat{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}, \quad \hat{B} = \begin{pmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{pmatrix}$$

$$\hat{A} \otimes \hat{B} = \begin{pmatrix} a_{11}\hat{B} & a_{12}\hat{B} & a_{13}\hat{B} \\ a_{21}\hat{B} & a_{22}\hat{B} & a_{23}\hat{B} \\ a_{31}\hat{B} & a_{32}\hat{B} & a_{33}\hat{B} \end{pmatrix}$$

B2 The expression for the magnitude of the total spin angular momentum (two spin system) with the KroneckerProduct

The magnitude of the total spin angular momentum is obtained as follows.

$$
\begin{aligned}
(\hat{\sigma}_{x1}\otimes\hat{1}_2+\hat{1}_1\otimes\hat{\sigma}_{x2})(\hat{\sigma}_{x1}\otimes\hat{1}_2+\hat{1}_1\otimes\hat{\sigma}_{x2}) &= (\hat{\sigma}_{x1}\otimes\hat{1}_2)(\hat{\sigma}_{x1}\otimes\hat{1}_2)+(\hat{1}_1\otimes\hat{\sigma}_{x2})(\hat{\sigma}_{x1}\otimes\hat{1}_2) \\
&\quad +(\hat{\sigma}_{x1}\otimes\hat{1}_2)(\hat{1}_1\otimes\hat{\sigma}_{x2})+(\hat{1}_1\otimes\hat{\sigma}_{x2})(\hat{1}_1\otimes\hat{\sigma}_{x2}) \\
&= \hat{\sigma}_{x1}{}^2\otimes\hat{1}_2{}^2+\hat{\sigma}_{x1}\otimes\hat{\sigma}_{x2}+\hat{\sigma}_{x1}\otimes\hat{\sigma}_{x2}+\hat{1}_1{}^2\otimes\hat{\sigma}_{x2}{}^2 \\
&= 2(\hat{1}_1\otimes\hat{1}_2+\hat{\sigma}_{x1}\otimes\hat{\sigma}_{x2})
\end{aligned}
$$

Then

$$
\begin{aligned}
\hat{\boldsymbol{\sigma}}_{tot}{}^2 &= \sum_{i=x,y,z}(\hat{\sigma}_{i1}\otimes\hat{1}_2+\hat{1}_1\otimes\hat{\sigma}_{i2})(\hat{\sigma}_{i1}\otimes\hat{1}_2+\hat{1}_1\otimes\hat{\sigma}_{i2}) \\
&= 6\hat{1}_1\otimes\hat{1}_2+2(\hat{\sigma}_{x1}\otimes\hat{\sigma}_{x2}+\hat{\sigma}_{y1}\otimes\hat{\sigma}_{y2}+\hat{\sigma}_{z1}\otimes\hat{\sigma}_{z2})
\end{aligned}
$$

Using the Dirac exchange operator

$$
\hat{P}_{12}=\frac{1}{2}(\hat{1}_1\otimes\hat{1}_2+\hat{\sigma}_{x1}\otimes\hat{\sigma}_{x2}+\hat{\sigma}_{y1}\otimes\hat{\sigma}_{y2}+\hat{\sigma}_{z1}\otimes\hat{\sigma}_{z2})
$$

we have

$$
\hat{\boldsymbol{\sigma}}_{tot}{}^2=4\hat{1}_1\otimes\hat{1}_2+4\hat{P}_{12}, \qquad \text{or} \qquad \hat{\boldsymbol{S}}_{tot}{}^2=\hbar^2(\hat{1}_1\otimes\hat{1}_2+\hat{P}_{12})
$$

where $\hat{1}$ is the identity matrix of 4 x 4, and $\hat{1}_1$ and $\hat{1}_2$ are the identity matrix of 2 x 2. Note that

$$
\hat{1}=\hat{1}_1\otimes\hat{1}_2=\begin{pmatrix}1&0\\0&1\end{pmatrix}\otimes\begin{pmatrix}1&0\\0&1\end{pmatrix}=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}
$$

$$
\hat{\sigma}_{x1}\otimes\hat{\sigma}_{x2}=\begin{pmatrix}0&1\\1&0\end{pmatrix}\otimes\begin{pmatrix}0&1\\1&0\end{pmatrix}=\begin{pmatrix}0&0&0&1\\0&0&1&0\\0&1&0&0\\1&0&0&0\end{pmatrix}
$$

$$\hat{\sigma}_{y1} \otimes \hat{\sigma}_{y2} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$

$$\hat{\sigma}_{z1} \otimes \hat{\sigma}_{z2} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Then we get

$$\hat{\sigma}_{x1} \otimes \hat{\sigma}_{x2} + \hat{\sigma}_{y1} \otimes \hat{\sigma}_{y2} + \hat{\sigma}_{z1} \otimes \hat{\sigma}_{z2} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\begin{aligned} \hat{P}_{12} &= \frac{1}{2}(\hat{1}_1 \otimes \hat{1}_2 + \hat{\sigma}_{x1} \otimes \hat{\sigma}_{x2} + \hat{\sigma}_{y1} \otimes \hat{\sigma}_{y2} + \hat{\sigma}_{z1} \otimes \hat{\sigma}_{z2}) \\ &= \frac{1}{2}\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \end{aligned}$$

APPENDIX
Example: Zeeman effect of positron and electron (spin 1/2).

The spin-dependent Hamiltonian of an electron (1) positron (2) system in the presence of a uniform magnetic field (B) in the z-direction can be written as

$$\hat{H} = A\hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2 + \frac{eB}{mc}(\hat{S}_{1z} - \hat{S}_{2z})$$

where $\hat{\boldsymbol{S}}_1 = \frac{\hbar}{2}\hat{\boldsymbol{\sigma}}_1$ (spin of electron) and $\hat{\boldsymbol{S}}_2 = \frac{\hbar}{2}\hat{\boldsymbol{\sigma}}_2$ (spin of positron). Note that the Dirac spin exchange operator is given by $\hat{P}_{12} = \frac{1}{2}(\hat{1} + \hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2)$. We consider the four states given by $|+\rangle_1 |+\rangle_2 = |+,+\rangle$, $|+,-\rangle$, $|-,+\rangle$, $|-,-\rangle$,

(a) Calculate $\hat{H}|+,+\rangle$, $\hat{H}|+,-\rangle$, $\hat{H}|-,+\rangle$, and $\hat{H}|-,-\rangle$.

(b) Find the matrix of $\hat{H}$ (4x4 matrix) under the basis of $|+,+\rangle$, $|+,-\rangle$, $|-,+\rangle$, $|-,-\rangle$.

(c) Solve the eigenvalues and eigenkets of the Hamiltonian.

(d) Make a plot of the energy eigenvalues as a function of *B*.

((**Solution**))
(a), (b)

We introduce the Dirac spin exchange operator:

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

or

$$\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2 = 2\hat{P}_{12} - \hat{1}$$

The spin Hamiltonian $\hat{H}$ is given by

$$\hat{H} = A\hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2 + \frac{eB}{mc}(\hat{S}_{1z} - \hat{S}_{2z}) = \frac{A}{4}\hbar^2 \hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2 + \frac{e\hbar B}{2mc}(\hat{\sigma}_{1z} - \hat{S}_{2z})$$

or

$$\hat{H} = \frac{A}{4}\hbar^2(2\hat{P}_{12} - \hat{1}) + \frac{e\hbar B}{2mc}(\hat{\sigma}_{1z} - \hat{\sigma}_{2z})$$

Then we get

$$\begin{aligned}
\hat{H}|+-\rangle &= \frac{A}{4}\hbar^2[2|-+\rangle - |+-\rangle + \frac{e\hbar B}{mc}|+-\rangle \\
&= \frac{A}{2}\hbar^2|-+\rangle - \frac{A}{4}\hbar^2|+-\rangle + \frac{e\hbar B}{mc}|+-\rangle \\
&= \frac{A}{2}\hbar^2|-+\rangle + (-\frac{A}{4}\hbar^2 + \frac{e\hbar B}{mc})|+-\rangle
\end{aligned}$$

$$\hat{H}|-+\rangle = \frac{A}{4}\hbar^2(2\hat{P}_{12} - \hat{1})|-+\rangle + \frac{e\hbar B}{2mc}(\hat{\sigma}_{1z} - \hat{\sigma}_{2z})|-+\rangle$$
$$= \frac{A}{4}\hbar^2[2|+-\rangle - |-+\rangle] - \frac{e\hbar B}{mc}|-+\rangle$$
$$= \frac{A}{2}\hbar^2|+-\rangle - (\frac{A}{4}\hbar^2 + \frac{e\hbar B}{mc})|-+\rangle$$

$$\hat{H}|++\rangle = \frac{A}{4}\hbar^2(2\hat{P}_{12} - \hat{1})|++\rangle + \frac{e\hbar B}{2mc}(\hat{\sigma}_{1z} - \hat{\sigma}_{2z})|++\rangle$$
$$= \frac{A}{4}\hbar^2[2|++\rangle - |++\rangle]$$
$$= \frac{A}{4}\hbar^2|++\rangle$$

$$\hat{H}|--\rangle = \frac{A}{4}\hbar^2(2\hat{P}_{12} - \hat{1})|--\rangle + \frac{e\hbar B}{2mc}(\hat{\sigma}_{1z} - \hat{\sigma}_{2z})|--\rangle$$
$$= \frac{A}{4}\hbar^2|--\rangle$$

The matrix of $\hat{H}$ is given by

$$\hat{H} = \begin{pmatrix} \frac{A}{4}\hbar^2 & 0 & 0 & 0 \\ 0 & -\frac{A}{4}\hbar^2 + \frac{e\hbar B}{mc} & \frac{A}{2}\hbar^2 & 0 \\ 0 & \frac{A}{2}\hbar^2 & -\frac{A}{4}\hbar^2 - \frac{e\hbar B}{mc} & 0 \\ 0 & 0 & 0 & \frac{A}{4}\hbar^2 \end{pmatrix}$$

(c)

$|++\rangle$ is the eigenket of $\hat{H}$ with the eigenvalue $\frac{A}{4}\hbar^2$.

$|--\rangle$ is the eigenket of $\hat{H}$ with the eigenvalue $\frac{A}{4}\hbar^2$.

We now consider the matrix of $\hat{H}$ under the subspace of $|+-\rangle$ and $|-+\rangle$.

$$\hat{H}_{sub} = \begin{pmatrix} -\frac{A}{4}\hbar^2 + \frac{e\hbar B}{mc} & \frac{A}{2}\hbar^2 \\ \frac{A}{2}\hbar^2 & -\frac{A}{4}\hbar^2 - \frac{e\hbar B}{mc} \end{pmatrix}$$
$$= \frac{A}{2}\hbar^2\hat{\sigma}_x + \frac{e\hbar B}{mc}\hat{\sigma}_z - \frac{A}{4}\hbar^2\hat{1}$$
$$= \hbar^2\sqrt{\left(\frac{A}{2}\right)^2 + \left(\frac{eB}{mc\hbar}\right)^2}\,\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n} - \frac{A}{4}\hbar^2\hat{1}$$

where $\boldsymbol{n}$ is the unit vector in the z-x plane; $\boldsymbol{n} = (\sin\theta, 0, \cos\theta)$

$$\cos\theta = \frac{\frac{e\hbar B}{mc\hbar}}{\sqrt{\left(\frac{A}{2}\right)^2 + \left(\frac{eB}{mc\hbar}\right)^2}}, \qquad \sin\theta = \frac{\frac{A}{2}}{\sqrt{\left(\frac{A}{2}\right)^2 + \left(\frac{eB}{mc\hbar}\right)^2}}$$

Note that

$$\hat{H}_{sub}\left|+\boldsymbol{n}\right\rangle = (\hbar^2\sqrt{\left(\frac{A}{2}\right)^2 + \left(\frac{eB}{mc\hbar}\right)^2}\,\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n} - \frac{A}{4}\hbar^2\hat{1})\left|+\boldsymbol{n}\right\rangle$$
$$= \hbar^2(\sqrt{\left(\frac{A}{2}\right)^2 + \left(\frac{eB}{mc\hbar}\right)^2} - \frac{A}{4})\left|+\boldsymbol{n}\right\rangle$$

$$\hat{H}_{sub}\left|-\boldsymbol{n}\right\rangle = (\hbar^2\sqrt{\left(\frac{A}{2}\right)^2 + \left(\frac{eB}{mc\hbar}\right)^2}\,\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n} - \frac{A}{4}\hat{1})\left|-\boldsymbol{n}\right\rangle$$
$$= \hbar^2(-\sqrt{\left(\frac{A}{2}\right)^2 + \left(\frac{eB}{mc\hbar}\right)^2} - \frac{A}{4}\hat{1})\left|+\boldsymbol{n}\right\rangle$$

Energy eigenvalue: $\hbar^2(\sqrt{\left(\frac{A}{2}\right)^2 + \left(\frac{eB}{mc\hbar}\right)^2} - \frac{A}{4})$ Eigenstate $\begin{pmatrix} 0 \\ \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \\ 0 \end{pmatrix}$

Energy eigenvalue: $\hbar^2[-\sqrt{\left(\frac{A}{2}\right)^2+\left(\frac{eB}{mc\hbar}\right)^2}-\frac{A}{4}]$ Eigenstate $\begin{pmatrix} 0 \\ \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \\ 0 \end{pmatrix}$

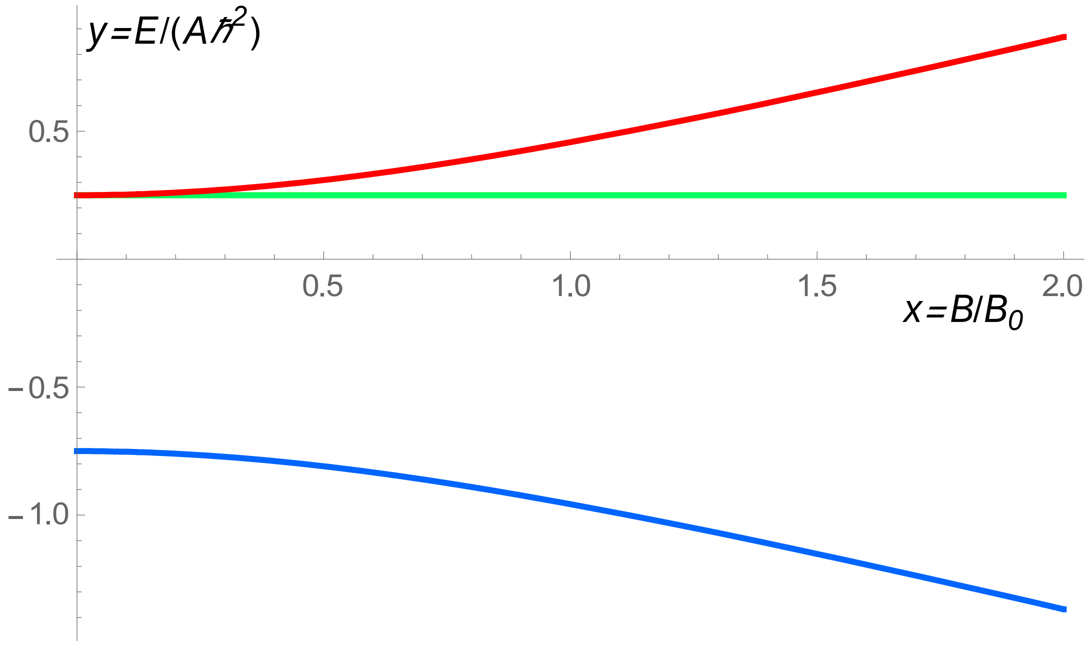

Fig. Plot of energy levels ($y = E/(A\hbar^2)$ as a function of $x = \frac{B}{B_0}$ with $B_0 = \frac{Amc\hbar}{2e}$

((**Another solution**)) KroneckerProduct (Mathematica)

```
Clear["Global`*"];
σx = (0 1
      1 0);
σy = (0 -ⅈ
      ⅈ  0);
σz = (1  0
      0 -1);
I2 = IdentityMatrix[2];

H1 =
  A/4 ℏ^2 (KroneckerProduct[σx, σx] +
      KroneckerProduct[σy, σy]
      + KroneckerProduct[σz, σz]) +
   (e1 B)/(2 m c) KroneckerProduct[σz, I2] -
   (e1 B)/(2 m c) KroneckerProduct[I2, σz];

H1 // MatrixForm
```

$$\begin{pmatrix} \frac{A\hbar^2}{4} & 0 & 0 & 0 \\ 0 & \frac{B\,e1}{c\,m} - \frac{A\hbar^2}{4} & \frac{A\hbar^2}{2} & 0 \\ 0 & \frac{A\hbar^2}{2} & -\frac{B\,e1}{c\,m} - \frac{A\hbar^2}{4} & 0 \\ 0 & 0 & 0 & \frac{A\hbar^2}{4} \end{pmatrix}$$

eq1 = Eigensystem[H1] // Simplify

$$\left\{\left\{\frac{A\hbar^2}{4}, \frac{A\hbar^2}{4}, -\frac{A\,c\,m\,\hbar^2 + 2\sqrt{4\,B^2\,e1^2 + A^2\,c^2\,m^2\,\hbar^4}}{4\,c\,m},\right.\right.$$

$$\left. -\frac{A\hbar^2}{4} + \frac{\sqrt{4\,B^2\,e1^2 + A^2\,c^2\,m^2\,\hbar^4}}{2\,c\,m}\right\},$$

$$\left\{\{0, 0, 0, 1\}, \{1, 0, 0, 0\},\right.$$

$$\left\{0, \frac{2\,B\,e1 - \sqrt{4\,B^2\,e1^2 + A^2\,c^2\,m^2\,\hbar^4}}{A\,c\,m\,\hbar^2}, 1, 0\right\},$$

$$\left.\left.\left\{0, \frac{2\,B\,e1 + \sqrt{4\,B^2\,e1^2 + A^2\,c^2\,m^2\,\hbar^4}}{A\,c\,m\,\hbar^2}, 1, 0\right\}\right\}\right\}$$

```
E1[i_] := 1/(A ℏ^2) eq1[[1, i]] /. {B → x (A c m ℏ^2)/(2 e1)} //
  Simplify[#, {A > 0, c > 0, m > 0, ℏ > 0}] &
```

```
E1[3]
```

$$\frac{1}{4}\left(-1-2\sqrt{1+x^2}\right)$$

```
E1[1]
```

$$\frac{1}{4}$$

```
E1[4]
```

$$\frac{1}{4}\left(-1+2\sqrt{1+x^2}\right)$$

```
E1[2]
```

$$\frac{1}{4}$$

```
f1 = Plot[{E1[1], E1[2], E1[3], E1[4]}, {x, 0, 2},
  PlotStyle → {{Hue[0.2], Thick},
    {Hue[0.4], Thick}, {Hue[0.6], Thick},
    {Hue[0.0], Thick}} ];
f2 =
 Graphics[
  {Text[Style["y=E/(Aħ^2)", Italic, 12, Black],
    {0.2, 0.9}],
   Text[Style["x=B/B0", Italic, 12, Black],
    {1.8, -0.2}]}];
Show[f1, f2]
```