3. (Quantum Mechanics)

Consider a system of two spin-1 particles: $|m_1\rangle$, $|m_2\rangle$, with m_1, $m_2 \in \{-1, 0, 1\}$. The system is governed by the Hamiltonian:

$$H = -\alpha \boldsymbol{S}_1 \cdot \boldsymbol{S}_2 + \beta (S_{1z} + S_{2z})^2$$

where $\boldsymbol{S}_1$ and $\boldsymbol{S}_2$ are the spin operators of the two particles and α, β are positive constants with $\beta > 2\alpha$.

By using the ladder operator $S_- |j, m\rangle = \sqrt{(j+m)(j-m+1)}\hbar |j, m-1\rangle$ or otherwise, find the energies and wavefunctions of the lowest two energy eigenstates. Express these energy eigenstates in the product basis of the two spin-1 particles.

Solution: *Solution by Jonah Hyman (jthyman@g.ucla.edu)*

Most times a quantum mechanics problem talks about two particles with spin, the problem is about addition of angular momentum. Here is some key information about addition of angular momentum:

Addition of angular momentum

Suppose we are adding a spin-j_1 particle to a spin-j_2 particle (this also works for adding orbital and spin angular momentum of a single particle). Let $\mathbf{J}_i$ be the ith angular momentum operator (where $i = 1, 2$ throughout), and define $\mathbf{J} \equiv \mathbf{J}_1 + \mathbf{J}_2$. We can express the state of the system in two different bases:

Original basis: $|m_1\rangle |m_2\rangle$

$$\text{This basis simultaneously diagonalizes} \quad \mathbf{J}_1^2, \ \mathbf{J}_2^2, \ J_{1z}, \ J_{2z} \tag{71}$$

$$\text{Possible quantum numbers:} \quad m_i = -j_i, -j_i + 1, \ldots, j_i - 1, j_i \tag{72}$$

$$\mathbf{J}_i^2 \text{ eigenvalues:} \quad \mathbf{J}_i^2 |m_1\rangle |m_2\rangle = \hbar^2 j_i(j_i + 1) |m_1\rangle |m_2\rangle \tag{73}$$

$$J_{i,z} \text{ eigenvalues:} \quad J_{i,z} |m_1\rangle |m_2\rangle = \hbar m_i |m_1\rangle |m_2\rangle \tag{74}$$

$$\text{Dimension of space:} \quad (2j_1 + 1)(2j_2 + 1) \quad \text{different basis states} \tag{75}$$

Combined basis: $|j, m\rangle$

$$\text{This basis simultaneously diagonalizes} \quad \mathbf{J}_1^2, \ \mathbf{J}_2^2, \ \mathbf{J}^2, \ J_z \tag{76}$$

$$\text{Possible quantum numbers:} \quad j = j_1 + j_2, j_1 + j_2 - 1, \ldots, |j_1 - j_2| \tag{77}$$

$$m = -j, -j + 1, \ldots, j - 1, j \tag{78}$$

$$\mathbf{J}_i^2 \text{ eigenvalues:} \quad \mathbf{J}_i^2 |j, m\rangle = \hbar^2 j_i(j_i + 1) |j, m\rangle \tag{79}$$

$$\mathbf{J}^2 \text{ eigenvalues:} \quad \mathbf{J}^2 |j, m\rangle = \hbar^2 j(j + 1) |j, m\rangle \tag{80}$$

$$J_z \text{ eigenvalues:} \quad J_z |j, m\rangle = \hbar m |j, m\rangle \tag{81}$$

$$\text{Dimension of space:} \quad \sum_{j=|j_1-j_2|}^{j_1+j_2} (2j + 1) = (2j_1 + 1)(2j_2 + 1) \quad \text{different basis states} \tag{82}$$

$$\text{Relation between bases:} \quad m_1 + m_2 = m \tag{83}$$

We also need one weird trick for this problem (and many problems like it), which is so important that it deserves its own box:

Dot product trick:

For addition of angular momentum problems, dot products in the Hamiltonian must be simplified as follows:

$$\mathbf{S}_1 \cdot \mathbf{S}_2 = \frac{1}{2} \left(\mathbf{S}^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2 \right) \quad \text{where } \mathbf{S} \equiv \mathbf{S}_1 + \mathbf{S}_2 \tag{84}$$

To start this problem, apply the dot product trick to the given Hamiltonian:

$$
\begin{aligned}
H &= -\alpha \mathbf{S}_1 \cdot \mathbf{S}_2 + \beta(S_{1z} + S_{2z})^2 \\
&= -\frac{\alpha}{2}\left(\mathbf{S}^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2\right) + \beta(S_{1z} + S_{2z})^2 \\
H &= -\frac{\alpha}{2}\mathbf{S}^2 + \beta S_z^2 + \frac{\alpha}{2}(\mathbf{S}_1^2 + \mathbf{S}_2^2) \quad \text{where } \mathbf{S} \equiv \mathbf{S}_1 + \mathbf{S}_2
\end{aligned}
\tag{85}
$$

This Hamiltonian is now expressed in terms of $\mathbf{S}_1^2$, $\mathbf{S}_2^2$, $\mathbf{S}^2$, and S_z. (76) tell us that the combined basis $|j, m\rangle$ diagonalizes these four operators, so it also diagonalizes the Hamiltonian H. We will therefore work in this basis and search for the lowest two energy eigenstates.

Applying (79), (80), and (81), and bearing in mind that $j_1 = j_2 = 1$ since these are spin-1 particles, we get that

$$
\begin{aligned}
H |j, m\rangle &= -\frac{\alpha}{2}\left[\mathbf{S}^2 |j, m\rangle\right] + \beta\left[S_z^2 |j, m\rangle\right] + \frac{\alpha}{2}\left[\mathbf{S}_1^2 |j, m\rangle + \mathbf{S}_2^2 |j, m\rangle\right] \\
&= -\frac{\alpha}{2}\left[\hbar^2 j(j+1) |j, m\rangle\right] + \beta\left[(\hbar m)^2 |j, m\rangle\right] + \frac{\alpha}{2}\left[\hbar^2(1)(1+1) |j, m\rangle + \hbar^2(1)(1+1) |j, m\rangle\right] \\
&= \hbar^2 \left[-\frac{\alpha}{2}j(j+1) + \beta m^2 + 2\alpha\right] |j, m\rangle
\end{aligned}
\tag{86}
$$

Thus, the energy of the state $|j, m\rangle$ is

$$
E_{j,m} = \hbar^2 \left[-\frac{\alpha}{2}j(j+1) + \beta m^2 + 2\alpha\right]
\tag{87}
$$

Using (77), we can establish that since $j_1 = j_2 = 1$, the possible values of j are $j = 2, 1, 0$. Using (78) to get the possible values of m for each value of j, we can generate a "wedding cake" diagram for the possible eigenstates $|j, m\rangle$:

$$
\begin{array}{lll}
|2, 2\rangle & & \\
|2, 1\rangle & |1, 1\rangle & \\
|2, 0\rangle & |1, 0\rangle & |0, 0\rangle \\
|2, -1\rangle & |1, -1\rangle & \\
|2, -2\rangle & &
\end{array}
\tag{88}
$$

Notice that there are nine states in the diagram, which is equal to $(2j_1 + 1)(2j_2 + 1)$ for $j_1 = j_2 = 1$, as it should be.

Inspecting (87), bearing in mind the possible values of j and m, and remembering that α and β are positive, we can see that the lowest possible energy is

$$
E_{2,0} = \hbar^2 \left[-\frac{\alpha}{2}(2)(2+1) + \beta(0)^2 + 2\alpha\right] = -\alpha\hbar^2
\tag{89}
$$

What is the second-lowest energy? The energy $E_{j,m}$ increases if we decrease j or increase the absolute value of m, so there are three possible candidates for the second-lowest energy:

$$
E_{1,0} = \hbar^2 \left[-\frac{\alpha}{2}(1)(1+1) + \beta(0)^2 + 2\alpha\right] = \alpha\hbar^2
\tag{90}
$$

$$
E_{2,1} = \hbar^2 \left[-\frac{\alpha}{2}(2)(2+1) + \beta(1)^2 + 2\alpha\right] = (-\alpha + \beta)\hbar^2
\tag{91}
$$

$$
E_{2,-1} = \hbar^2 \left[-\frac{\alpha}{2}(2)(2+1) + \beta(-1)^2 + 2\alpha\right] = (-\alpha + \beta)\hbar^2
\tag{92}
$$

To determine which of these energies is lower, use the given fact that $\beta > 2\alpha$:

$$
E_{1,0} = \alpha\hbar^2 = (-\alpha + 2\alpha)\hbar^2 < (-\alpha + \beta)\hbar^2 = E_{2,1} = E_{2,-1}
\tag{93}
$$

Thus, the second-lowest energy is $E_{1,0}$. We can write the lowest two energies:

$$\boxed{\text{Lowest energy:} \quad E_{2,0} = -\alpha\hbar^2; \quad \text{Second-lowest energy:} \quad E_{1,0} = \alpha\hbar^2} \tag{94}$$

Now, we need to find the "wavefunctions" (really, the kets) of the two lowest-energy eigenstates. We know that these are the kets $|2,0\rangle$ and $|1,0\rangle$. But the problem asks us to write it in the "product basis of the two spin-1 particles," meaning the original basis $|m_1\rangle|m_2\rangle$. The key to doing this is computing the Clebsch-Gordan coefficients using the following method:

Wedding cake method of computing Clebsch-Gordon coefficients:

$$
\begin{array}{l}
|2,2\rangle \\
|2,1\rangle \quad \longrightarrow |1,1\rangle \\
|2,0\rangle \quad \quad |1,0\rangle \quad \longrightarrow |0,0\rangle \\
|2,-1\rangle \quad \quad |1,-1\rangle \\
|2,-2\rangle
\end{array}
\tag{95}
$$

Start at the $|j,m\rangle$ state with largest m (top of the diagram). For each curvy arrow, use the lowering operators

$$J_- |j,m\rangle = \hbar\sqrt{(j+m)(j-m+1)}\,|j,m-1\rangle \tag{96}$$

$$J_{1-} |m_1\rangle|m_2\rangle = \hbar\sqrt{(j_1+m_1)(j_1-m_1+1)}\,|m_1-1\rangle|m_2\rangle \tag{97}$$

$$J_{2-} |m_1\rangle|m_2\rangle = \hbar\sqrt{(j_2+m_2)(j_2-m_2+1)}\,|m_1\rangle|m_2-1\rangle \tag{98}$$

with $J_- = J_{1-} + J_{2-}$.
For each straight arrow, use the orthogonality of different eigenstates.

We'll now explain how to apply this method in the context of this problem.

To avoid getting stuck in a quagmire of algebra, and to keep the focus on the problem-solving method, we will pre-calculate some values of the proportionality constant $f(j,m) \equiv \sqrt{(j+m)(j-m+1)}$ that appears in the formulas for the lowering operator:

$$
\begin{array}{c|c}
(j,m) & f(j,m) \equiv \sqrt{(j+m)(j-m+1)} \\
\hline
(2,2) & 2 \\
(2,1) & \sqrt{6} \\
(1,1) & \sqrt{2} \\
(1,0) & \sqrt{2}
\end{array}
\tag{99}
$$

Then, in the context of this problem, since we have two spin-1 particles, equations (96)-(98) become

$$S_- |j,m\rangle = \hbar f(j,m)\,|j,m-1\rangle \tag{100}$$

$$S_{1-} |m_1\rangle|m_2\rangle = \hbar\,f(1,m_1)\,|m_1-1\rangle|m_2\rangle \tag{101}$$

$$S_{2-} |m_1\rangle|m_2\rangle = \hbar\,f(1,m_2)\,|m_1\rangle|m_2-1\rangle \tag{102}$$

We are now ready to start working our way through the wedding cake diagram. Our goal is to find expressions for the lowest two energy eigenstates, $|2,0\rangle$ and $|1,0\rangle$ (marked in blue on the diagrams to follow).

Starting point: $|2, 2\rangle$

Recall that $m_1 + m_2 = m$ (by (83)). In this case, $m = 2$. Since we have two spin-1 particles, m_1 and m_2 can be at most 1 (by (72)). Thus, the only possible original eigenket that can contribute to the combined eigenket $|2, 2\rangle$ is $|1\rangle |1\rangle$. We can set the normalization of $|2, 2\rangle$ so that the prefactor is zero, getting

$$|2, 2\rangle = |1\rangle |1\rangle \tag{103}$$

Lowering operator: $|2, 2\rangle \curvearrowright |2, 1\rangle$
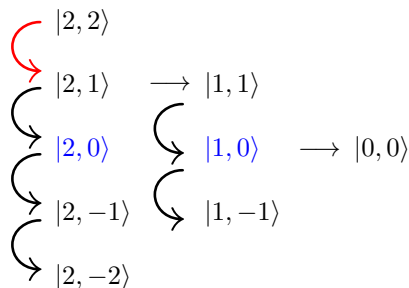
Lowering $|2, 2\rangle$ with the S_- lowering operator for total angular momentum and applying table (99), we get

$$S_- |2, 2\rangle = \hbar f(2, 2) |2, 2 - 1\rangle = 2\hbar |2, 1\rangle \tag{104}$$

But $S_- = S_{1-} + S_{2-}$, so we can also use this to lower in the original basis:

$$
\begin{aligned}
S_- |2, 2\rangle &= (S_{1-} + S_{2-}) |2, 2\rangle \\
&= (S_{1-} + S_{2-}) |1\rangle |1\rangle \quad \text{by our earlier calculation of } |2, 2\rangle \text{ in the original basis (103)} \\
&= S_{1-} |1\rangle |1\rangle + S_{2-} |1\rangle |1\rangle \\
&= \hbar f(1, 1) |0\rangle |1\rangle + \hbar f(1, 1) |1\rangle |0\rangle \quad \text{by (97) and (98)} \\
&= \hbar\sqrt{2} |0\rangle |1\rangle + \hbar\sqrt{2} |1\rangle |0\rangle \quad \text{by table (99)}
\end{aligned} \tag{105}
$$

Setting (104) and (105) equal to one another, we get

$$2\hbar |2, 1\rangle = S_- |2, 2\rangle = \hbar\sqrt{2} |0\rangle |1\rangle + \hbar\sqrt{2} |1\rangle |0\rangle$$

Simplifying, we get an expression for $|2, 1\rangle$ in the original basis:

$$|2, 1\rangle = \frac{1}{\sqrt{2}} |0\rangle |1\rangle + \frac{1}{\sqrt{2}} |1\rangle |0\rangle \tag{106}$$

Note that this expression is correctly normalized, which is a useful check that our work is correct. (We could have skipped calculating the overall constant in (104) and used the normalization to calculate it. Calculating the overall constant is a useful algebra check, though, so we have opted to include it.)

Lowering operator: $|2, 1\rangle \curvearrowright |2, 0\rangle$
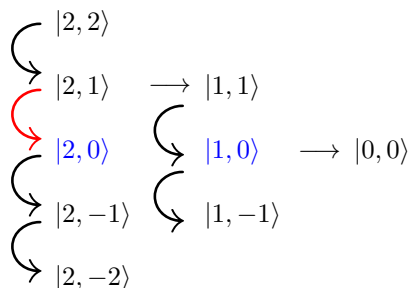
This is exactly the same process. Lowering $|2, 1\rangle$ with the S_- lowering operator for total angular momentum and using table (99), we get

$$S_- |2, 1\rangle = \hbar f(2, 1) |2, 1 - 1\rangle = \sqrt{6}\hbar |2, 0\rangle \tag{107}$$

But $S_- = S_{1-} + S_{2-}$, so we can also lower in the original basis:

$$\begin{aligned}
S_- |2, 1\rangle &= (S_{1-} + S_{2-}) |2, 1\rangle \\
&= (S_{1-} + S_{2-}) \left(\frac{1}{\sqrt{2}} |1\rangle |0\rangle + \frac{1}{\sqrt{2}} |0\rangle |1\rangle \right) \quad \text{by (106)} \\
&= \frac{1}{\sqrt{2}} \left(S_{1-} |1\rangle |0\rangle + S_{2-} |1\rangle |0\rangle + S_{1-} |0\rangle |1\rangle + S_{2-} |0\rangle |1\rangle \right) \\
&= \frac{\hbar}{\sqrt{2}} \left(f(1, 1) |0\rangle |0\rangle + f(1, 0) |1\rangle |-1\rangle + f(1, 0) |-1\rangle |1\rangle + f(1, 1) |0\rangle |0\rangle \right) \\
&= \frac{\hbar}{\sqrt{2}} \left(\sqrt{2} |0\rangle |0\rangle + \sqrt{2} |1\rangle |-1\rangle + \sqrt{2} |-1\rangle |1\rangle + \sqrt{2} |0\rangle |0\rangle \right) \quad \text{by table (99)} \\
&= \hbar \left(|1\rangle |-1\rangle + 2 |0\rangle |0\rangle + |-1\rangle |1\rangle \right) \tag{108}
\end{aligned}$$

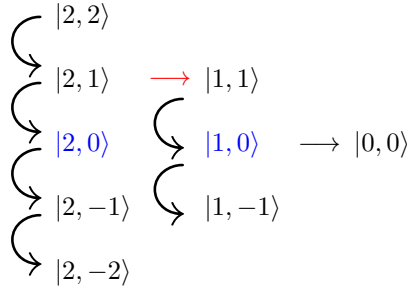Setting (107) and (108) equal to one another, we get

$$\sqrt{6}\hbar |2, 0\rangle = S_- |2, 1\rangle = \hbar \left(|1\rangle |-1\rangle + 2 |0\rangle |0\rangle + |-1\rangle |1\rangle \right)$$

Simplifying, we get an expression of $|2, 0\rangle$ in the original basis:

$$\boxed{|2, 0\rangle = \frac{1}{\sqrt{6}} |1\rangle |-1\rangle + \frac{2}{\sqrt{6}} |0\rangle |0\rangle + \frac{1}{\sqrt{6}} |-1\rangle |1\rangle} \tag{109}$$

As before, this state is correctly normalized.

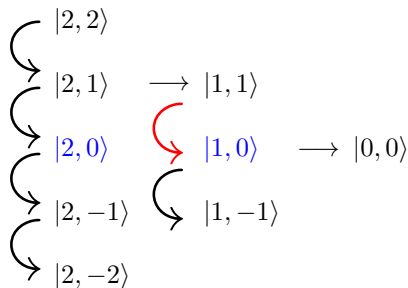**Orthogonality:** $|2, 1\rangle \curvearrowright |1, 1\rangle$

Since $m_1 + m_2 = m$ and $m_i = -1, 0, 1$, we know that $|1, 1\rangle$ must be the sum of $|1\rangle |0\rangle$ and $|0\rangle |1\rangle$. But since $|j, m\rangle$ is an orthonormal basis, $|1, 1\rangle$ must be orthogonal to $|2, 1\rangle$. Recall our expression for $|2, 1\rangle$ in the original basis (106)

$$|2, 1\rangle = \frac{1}{\sqrt{2}} |0\rangle |1\rangle + \frac{1}{\sqrt{2}} |1\rangle |0\rangle$$

There is only one vector that is orthogonal to this one, and (up to an overall phase) we can set it equal to $|1, 1\rangle$:

$$|1, 1\rangle = \frac{1}{\sqrt{2}} |0\rangle |1\rangle - \frac{1}{\sqrt{2}} |1\rangle |0\rangle \tag{110}$$

Lowering operator: $|1,1\rangle \curvearrowright |1,0\rangle$

$$
\begin{array}{l}
|2,2\rangle \\
|2,1\rangle \quad \longrightarrow \quad |1,1\rangle \\
|2,0\rangle \qquad\quad |1,0\rangle \quad \longrightarrow \quad |0,0\rangle \\
|2,-1\rangle \qquad |1,-1\rangle \\
|2,-2\rangle
\end{array}
$$

Lowering $|1,1\rangle$ with the S_- lowering operator for total angular momentum and using table (99), we get

$$S_- |1,1\rangle = \hbar f(1,1) |2, 1-1\rangle = \sqrt{2}\hbar |1,0\rangle \tag{111}$$

But $S_- = S_{1-} + S_{2-}$, so we can also lower in the original basis:

$$
\begin{aligned}
S_- |1,1\rangle &= (S_{1-} + S_{2-}) |1,1\rangle \\
&= (S_{1-} + S_{2-}) \left(\frac{1}{\sqrt{2}} |1\rangle |0\rangle - \frac{1}{\sqrt{2}} |0\rangle |1\rangle \right) \quad \text{by (106)} \\
&= \frac{1}{\sqrt{2}} \left(S_{1-} |1\rangle |0\rangle + S_{2-} |1\rangle |0\rangle - S_{1-} |0\rangle |1\rangle - S_{2-} |0\rangle |1\rangle \right) \\
&= \frac{\hbar}{\sqrt{2}} \left(f(1,1) |0\rangle |0\rangle + f(1,0) |1\rangle |-1\rangle - f(1,0) |-1\rangle |1\rangle - f(1,1) |0\rangle |0\rangle \right) \\
&= \frac{\hbar}{\sqrt{2}} \left(\sqrt{2} |0\rangle |0\rangle + \sqrt{2} |1\rangle |-1\rangle - \sqrt{2} |-1\rangle |1\rangle - \sqrt{2} |0\rangle |0\rangle \right) \quad \text{by table (99)} \\
&= \hbar \left(|1\rangle |-1\rangle - |-1\rangle |1\rangle \right) \tag{112}
\end{aligned}
$$

Setting (111) and (112) equal to one another, we get

$$\sqrt{2}\hbar |1,0\rangle = S_- |1,1\rangle = \hbar \left(|1\rangle |-1\rangle - |-1\rangle |1\rangle \right)$$

Simplifying, we get an expression of $|1,0\rangle$ in the original basis:

$$\boxed{ |1,0\rangle = \frac{1}{\sqrt{2}} |1\rangle |-1\rangle - \frac{1}{\sqrt{2}} |-1\rangle |1\rangle } \tag{113}$$

As before, this state is correctly normalized.

Putting everything together, we have

$$\boxed{ \text{Lowest-energy state:} \quad |2,0\rangle = \frac{1}{\sqrt{6}} |1\rangle |-1\rangle + \frac{2}{\sqrt{6}} |0\rangle |0\rangle + \frac{1}{\sqrt{6}} |-1\rangle |1\rangle \quad \text{and} \quad E_{2,0} = -\alpha\hbar^2 }$$

$$\boxed{ \text{Second-lowest-energy state:} \quad |1,0\rangle = \frac{1}{\sqrt{2}} |1\rangle |-1\rangle - \frac{1}{\sqrt{2}} |-1\rangle |1\rangle \quad \text{and} \quad E_{1,0} = \alpha\hbar^2 }$$

Sometimes, in order to emphasize that both particles are spin-1, the state $|m_1\rangle |m_2\rangle$ is written $|1, m_1\rangle |1, m_2\rangle$.

Angular momentum problems are very frequent on the comp. For more practice, try 2021 Q1, 2017 Q3, and 2015 Q4. For a special challenge, try 2015 Q6 and 2011 Q4.