4. (Quantum Mechanics)

Consider a system of two spin 1/2 particles, labeled a and b, with respective spin operators $\boldsymbol{S}_a$ and $\boldsymbol{S}_b$. We ignore all quantum numbers but those of spin. The particles are in the state $|\Psi\rangle$ of zero total angular momentum, which we consider normalized to $\langle\Psi|\Psi\rangle = 1$. Let $\boldsymbol{n}_a$ and $\boldsymbol{n}_b$ be two independent unit vectors. Compute the expectation value of the product of the spin operators projected onto the directions $\boldsymbol{n}_a$ and $\boldsymbol{n}_b$ respectively, namely $\langle\Psi|\,(\boldsymbol{n}_a \cdot \boldsymbol{S}_a)(\boldsymbol{n}_b \cdot \boldsymbol{S}_b)\,|\Psi\rangle$

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

We present two reasonable ways to solve this problem: First, we show how to solve the problem by a direct calculation. Then we show a more abstract mathematical approach that cuts down on the algebra.

Direct calculation:
To keep this calculation manageable, note the following strategy:

If the problem does not specify a coordinate system, choose the coordinate system in which it is easiest to solve the problem.

This problem does not specify a coordinate system. So let's set the $\hat{\mathbf{z}}$-direction to point in the direction of $\hat{\mathbf{n}}_a$, and let's set the $\hat{\mathbf{x}}$-direction so that $\hat{\mathbf{n}}_b$ points in the xz-plane. In this coordinate system, we have

$$\hat{\mathbf{n}}_a = \hat{\mathbf{z}} \quad \text{and} \quad \hat{\mathbf{n}}_b = \hat{\mathbf{x}} \sin\theta + \hat{\mathbf{z}} \cos\theta \tag{1}$$

since $\hat{\mathbf{n}}_a$ and $\hat{\mathbf{n}}_b$ are unit vectors (with length 1). With this information, we can simplify the expectation value:

$$\begin{aligned} \langle\Psi|(\hat{\mathbf{n}}_a \cdot \mathbf{S}_a)\,(\hat{\mathbf{n}}_b \cdot \mathbf{S}_b)|\Psi\rangle &= \langle\Psi|(\hat{\mathbf{z}} \cdot \mathbf{S}_a)\,((\hat{\mathbf{x}} \sin\theta + \hat{\mathbf{z}} \cos\theta) \cdot \mathbf{S}_b)|\Psi\rangle \\ &= \langle\Psi|S_{a,z}\,(\sin\theta\, S_{b,x} + \cos\theta\, S_{b,z})|\Psi\rangle \end{aligned}$$

For a spin-1/2 particle, $S_i = \frac{\hbar}{2}\sigma_i$, where σ_i is the operator corresponding to the ith Pauli matrix ($i = 1, 2, 3$). Therefore, we can plug in pull out two factors of $\hbar/2$ from the expectation value, to get

$$\begin{aligned} \langle\Psi|(\hat{\mathbf{n}}_a \cdot \mathbf{S}_a)\,(\hat{\mathbf{n}}_b \cdot \mathbf{S}_b)|\Psi\rangle &= \frac{\hbar^2}{4}\,\langle\Psi|\sigma_{a,z}\,(\sin\theta\,\sigma_{b,x} + \cos\theta\,\sigma_{b,z})|\Psi\rangle \\ &= \frac{\hbar^2}{4}\big(\sin\theta\,\langle\Psi|\sigma_{a,z}\sigma_{b,x}|\Psi\rangle + \cos\theta\,\langle\Psi|\sigma_{a,z}\sigma_{b,z}|\Psi\rangle\big) \end{aligned} \tag{2}$$

The next step is to write down the state $|\Psi\rangle$ explicitly. The problem tells us that $|\Psi\rangle$ is the product state of two spin-1/2 particles with zero total angular momentum. You may already know what this state is: It is called the "singlet" state and is given by

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\big[\,|\uparrow\rangle_a\,|\downarrow\rangle_b - |\downarrow\rangle_a\,|\uparrow\rangle_b\,\big] \tag{3}$$

where the first ket in each product state corresponds to particle a, and the second ket corresponds to particle b. (A derivation of this result is at the end of this solution.)

Now, we just need to calculate the expectation values in (2). Recall that for a single spin-1/2 particle, with $c_1\,|\uparrow\rangle + c_2\,|\downarrow\rangle \cong \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$, the Pauli matrices define the action of the Pauli operators on $|\uparrow\rangle$ and $|\downarrow\rangle$:

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \text{so} \quad \sigma_z\,|\uparrow\rangle = |\uparrow\rangle \quad \text{and} \quad \sigma_z\,|\downarrow\rangle = -\,|\downarrow\rangle \tag{4}$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \text{so} \quad \sigma_x\,|\uparrow\rangle = |\downarrow\rangle \quad \text{and} \quad \sigma_x\,|\downarrow\rangle = |\uparrow\rangle \tag{5}$$

Therefore, bearing in mind that the σ_a operators act on the first ket and the σ_b operators act on

the second ket, we have

$$\begin{aligned}\sigma_{a,z}\sigma_{b,x}\,|\Psi\rangle &= \frac{1}{\sqrt{2}}\sigma_{a,z}\sigma_{b,x}\big[\,|\uparrow\rangle_a\,|\downarrow\rangle_b - |\downarrow\rangle_a\,|\uparrow\rangle_b\,\big] \\ &= \frac{1}{\sqrt{2}}\big[\sigma_{a,z}\,|\uparrow\rangle_a\;\sigma_{b,x}\,|\downarrow\rangle_b - \sigma_{a,z}\,|\downarrow\rangle_a\;\sigma_{b,x}\,|\uparrow\rangle_b\,\big] \\ &= \frac{1}{\sqrt{2}}\big[\,|\uparrow\rangle_a\,|\uparrow\rangle_b + |\downarrow\rangle_a\,|\downarrow\rangle_b\,\big] \end{aligned} \tag{6}$$

$$\begin{aligned}\sigma_{a,z}\sigma_{b,z}\,|\Psi\rangle &= \frac{1}{\sqrt{2}}\sigma_{a,z}\sigma_{b,z}\big[\,|\uparrow\rangle_a\,|\downarrow\rangle_b - |\downarrow\rangle_a\,|\uparrow\rangle_b\,\big] \\ &= \frac{1}{\sqrt{2}}\big[\sigma_{a,z}\,|\uparrow\rangle_a\;\sigma_{b,z}\,|\downarrow\rangle_b - \sigma_{a,z}\,|\downarrow\rangle_a\;\sigma_{b,z}\,|\uparrow\rangle_b\,\big] \\ &= \frac{1}{\sqrt{2}}\big[\,-|\uparrow\rangle_a\,|\downarrow\rangle_b + |\downarrow\rangle_a\,|\uparrow\rangle_b\,\big] \\ &= -\,|\Psi\rangle \end{aligned} \tag{7}$$

Taking the inner product of (6) and (7) with $\langle\Psi| = \frac{1}{\sqrt{2}}\big[\,\langle\uparrow|_a\,\langle\downarrow|_b - \langle\downarrow|_a\,\langle\uparrow|_b\,\big]$, we get

$$\begin{aligned}\langle\Psi|\sigma_{a,z}\sigma_{b,x}|\Psi\rangle &= \frac{1}{2}\Big[\,\langle\uparrow|_a\,\langle\downarrow|_b - \langle\downarrow|_a\,\langle\uparrow|_b\,\Big]\Big[\,|\uparrow\rangle_a\,|\uparrow\rangle_b + |\downarrow\rangle_a\,|\downarrow\rangle_b\,\Big] \quad \text{restoring particle labels} \\ &= \frac{1}{2}\Big[\,\langle\uparrow|\uparrow\rangle_a\;\langle\downarrow|\uparrow\rangle_b + \langle\uparrow|\downarrow\rangle_a\;\langle\downarrow|\downarrow\rangle_b - \langle\downarrow|\uparrow\rangle_a\,\langle\uparrow|\uparrow\rangle_b - \langle\downarrow|\downarrow\rangle_a\;\langle\uparrow|\downarrow\rangle_b\,\Big] \\ &= 0 \quad \text{since } \langle\uparrow|\downarrow\rangle = \langle\downarrow|\uparrow\rangle = 0 \end{aligned} \tag{8}$$

and

$$\begin{aligned}\langle\Psi|\sigma_{a,z}\sigma_{b,z}|\Psi\rangle &= -\,\langle\Psi|\Psi\rangle \\ &= -1 \quad \text{since } |\Psi\rangle \text{ is normalized} \end{aligned} \tag{9}$$

Plugging the results (8) and (9) into (2), we get

$$\begin{aligned}\langle\Psi|(\hat{\mathbf{n}}_a\cdot\mathbf{S}_a)\,(\hat{\mathbf{n}}_b\cdot\mathbf{S}_b)|\Psi\rangle &= \frac{\hbar^2}{4}\big(\,\sin\theta\,\langle\Psi|\sigma_{a,z}\sigma_{b,x}|\Psi\rangle + \cos\theta\,\langle\Psi|\sigma_{a,z}\sigma_{b,z}|\Psi\rangle\,\big) \\ &= \frac{\hbar^2}{4}\big(\,\sin\theta\,(0) + \cos\theta\,(-1)\big) \\ &= -\frac{\hbar^2}{4}\,\cos\theta \end{aligned} \tag{10}$$

This is an acceptable answer, but it is nicer to write it in a coordinate-independent way. Recall from (1) that θ is the angle between $\hat{\mathbf{n}}_a$ and $\hat{\mathbf{n}}_b$. We can write $\cos\theta$ in terms of the dot product between these two unit vectors, which is a coordinate-independent quantity, using the formula

$$\mathbf{a}\cdot\mathbf{b} = |\mathbf{a}|\,|\mathbf{b}|\,\cos\theta \quad \text{where } \theta \text{ is the angle between } \mathbf{a} \text{ and } \mathbf{b} \tag{11}$$

For the two unit vectors $\hat{\mathbf{n}}_a$ and $\hat{\mathbf{n}}_b$, $|\hat{\mathbf{n}}_a| = |\hat{\mathbf{n}}_b| = 1$, so

$$\hat{\mathbf{n}}_a\cdot\hat{\mathbf{n}}_b = \cos\theta \tag{12}$$

Plugging this into (10), we get the final answer

$$\boxed{\langle\Psi|(\hat{\mathbf{n}}_a\cdot\mathbf{S}_a)\,(\hat{\mathbf{n}}_b\cdot\mathbf{S}_b)|\Psi\rangle = -\frac{\hbar^2}{4}\,(\hat{\mathbf{n}}_a\cdot\hat{\mathbf{n}}_b)} \tag{13}$$

Mathematical approach:
In this approach, we exploit some symmetries and transformation properties of the expectation value to avoid most of the algebra. The key is to consider the expectation value to be a scalar function g of the vectors $\hat{\mathbf{n}}_a$ and $\hat{\mathbf{n}}_b$. While we are interested in the case in which $\hat{\mathbf{n}}_a$ and $\hat{\mathbf{n}}_b$ are unit vectors, we will loosen the definition of this function to allow them to be any vectors (which we'll call $\mathbf{n}$ and $\mathbf{m}$, without the hats):

$$g(\mathbf{n},\mathbf{m}) \equiv \langle\Psi|(\mathbf{n}\cdot\mathbf{S}_a)\,(\mathbf{m}\cdot\mathbf{S}_b)|\Psi\rangle \tag{14}$$

We can write this in Einstein summation notation, where $i,j = 1,2,3$:

$$g(\mathbf{n},\mathbf{m}) = \langle\Psi|(n_i\,S_{a,i})\,(m_j\,S_{b,j})|\Psi\rangle \tag{15}$$

What properties of $g(\mathbf{n},\mathbf{m})$ can we identify?

Linearity:
First, since the inner product is a linear function in its second argument, $g(\mathbf{n},\mathbf{m})$ is linear in $\mathbf{n}$:

$$\begin{aligned} g(c\,\mathbf{n}+\mathbf{m},\mathbf{q}) &= \langle\Psi|((c\,n_i+m_i)\;S_{a,i})\,(q_j\,S_{b,j})|\Psi\rangle \\ &= c\,\langle\Psi|(n_i\,S_{a,i})\,(q_j\,S_{b,j})|\Psi\rangle + \langle\Psi|(m_i\,S_{a,i})\,(q_j\,S_{b,j})|\Psi\rangle \\ &= c\,g(\mathbf{n},\mathbf{q}) + g(\mathbf{m},\mathbf{q}) \quad \text{for } c \text{ a scalar, } \mathbf{n},\ \mathbf{m}, \text{ and } \mathbf{q} \text{ vectors} \end{aligned} \tag{16}$$

By an analogous argument, $g(\mathbf{n},\mathbf{m})$ is also linear in $\mathbf{m}$:

$$g(\mathbf{n},c\,\mathbf{m}+\mathbf{q}) = c\,g(\mathbf{n},\mathbf{m}) + g(\mathbf{n},\mathbf{q}) \tag{17}$$

Symmetry:
To derive this property, we need to write down the state $|\Psi\rangle$ explicitly. The problem tells us that $|\Psi\rangle$ is the product state of two spin-1/2 particles with zero total angular momentum. You may already know what this state is: It is called the "singlet" state and is given by

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\big[\,|\uparrow\rangle_a\,|\downarrow\rangle_b - |\downarrow\rangle_a\,|\uparrow\rangle_b\,\big] \tag{18}$$

where the first ket in each product state corresponds to particle a, and the second ket corresponds to particle b. (A derivation of this result is at the end of this solution.)

Note that if we swap the labels a and b, $|\Psi\rangle$ picks up a minus sign. In other words, if we let W be the operator that swaps the labels a and b,

$$\begin{aligned} |W\Psi\rangle &= \frac{1}{\sqrt{2}}\big[\,|\uparrow\rangle_b\,|\downarrow\rangle_a - |\downarrow\rangle_b\,|\uparrow\rangle_a\,\big] \\ &= -\frac{1}{\sqrt{2}}\big[\,|\uparrow\rangle_a\,|\downarrow\rangle_b - |\downarrow\rangle_a\,|\uparrow\rangle_b\,\big] \\ &= -\,|\Psi\rangle \end{aligned} \tag{19}$$

We will now show how this property tells us that the function $g(\mathbf{n},\mathbf{m})$ is symmetric:

$$\begin{aligned} g(\mathbf{n},\mathbf{m}) &= \langle\Psi|(\mathbf{n}\cdot\mathbf{S}_a)\,(\mathbf{m}\cdot\mathbf{S}_b)|\Psi\rangle \quad \text{by definition of } g \\ &= \langle W\Psi|(\mathbf{n}_b\cdot\mathbf{S}_a)\,(\mathbf{m}\cdot\mathbf{S}_b)|W\Psi\rangle \quad \text{since } |W\Psi\rangle = -\,|\Psi\rangle \\ &= \langle\Psi|W\,(\mathbf{n}\cdot\mathbf{S}_a)\,(\mathbf{m}\cdot\mathbf{S}_b)\,W|\Psi\rangle \end{aligned} \tag{20}$$

The operator in the middle of this expectation value corresponds to swapping the labels a and b, performing the operator $(\mathbf{n}\cdot\mathbf{S}_a)\,(\mathbf{m}\cdot\mathbf{S}_b)$, and then swapping the labels a and b again. This

double-swap of the labels is equivalent to just swapping the labels in the operator. Therefore, this is equivalent to performing the single operator $(\mathbf{n}\cdot\mathbf{S}_b)\,(\mathbf{m}\cdot\mathbf{S}_a)$:

$$\begin{aligned} g(\mathbf{n},\mathbf{m}) &= \langle\Psi|(\mathbf{n}\cdot\mathbf{S}_b)\,(\mathbf{m}\cdot\mathbf{S}_a)|\Psi\rangle \\ &= \langle\Psi|(\mathbf{m}\cdot\mathbf{S}_a)\,(\mathbf{n}\cdot\mathbf{S}_b)|\Psi\rangle \quad \text{since operators on } a \text{ commute with operators on } b \\ &= g(\mathbf{m},\mathbf{n}) \end{aligned} \tag{21}$$

This establishes that $g(\mathbf{n},\mathbf{m})$ is symmetric in its two arguments.

Invariance under rotations:
Let's suppose we change our coordinate system by rotating the $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ axes simultaneously to new directions $\hat{\mathbf{x}}'$, $\hat{\mathbf{y}}'$, and $\hat{\mathbf{z}}'$. There are several things that could change under this change of coordinates:

- The vectors $\mathbf{n}$ and $\mathbf{m}$. For example, suppose the primed and unprimed coordinate systems differ by a 90° rotation about the $\hat{\mathbf{z}}$-axis. In this case, if $\mathbf{n}=\hat{\mathbf{x}}$, then $\mathbf{n}'=\hat{\mathbf{y}}'$.
- The vectorial angular momentum operators $\mathbf{S}_a$ and $\mathbf{S}_b$. For example, suppose the primed and unprimed coordinate systems differ by a 90° rotation about the $\hat{\mathbf{z}}$-axis. In this case, if $\mathbf{S}_a = S_{a,x}\hat{\mathbf{x}}$, then $\mathbf{S}'_a = S_{a,y'}\hat{\mathbf{y}}'$.
- The state $|\Psi\rangle$. For example, suppose the primed and unprimed coordinate systems differ by a 90° rotation about the $\hat{\mathbf{z}}$-axis. In this case, if the state $|\Psi\rangle$ is a product state of two spin-x eigenstates with positive eigenvalue, $|\Psi\rangle = |+x\rangle_a\,|+x\rangle_b$, then the state $|\Psi\rangle'$ is a product state of two spin-y' eigenstates with positive eigenvalue, $|\Psi\rangle' = |+y'\rangle_a\,|+y'\rangle_b$.

Which of these things actually change under this change of coordinates? The operator $(\mathbf{n}\cdot\mathbf{S}_a)\,(\mathbf{m}\cdot\mathbf{S}_b)$ is independent of the coordinate system that we choose (since it is written in a coordinate-independent way, as the dot product of two vectors).

In addition, the state $|\Psi\rangle$ is also coordinate-independent, since it has zero total angular momentum. States with zero angular momentum have complete spherical symmetry, so they are unchanged under rotations of the coordinate axes. (One way to remember this is to recall that the spherical harmonic for zero total angular momentum, $Y_{00}(\theta,\varphi)$, is constant in both spherical coordinates θ and φ. It is therefore spherically symmetric.)

Since all parts of the scalar function $g(\mathbf{n},\mathbf{m}) \equiv \langle\Psi|(\mathbf{n}\cdot\mathbf{S}_a)\,(\mathbf{m}\cdot\mathbf{S}_b)|\Psi\rangle$ are coordinate-independent, $g(\mathbf{n},\mathbf{m})$ must also be coordinate-independent. In other words, $g(\mathbf{n},\mathbf{m})$ is invariant under rotations of the coordinate system.

So far, we have identified that $g(\mathbf{n},\mathbf{m})$ is linear, symmetric, and invariant under rotations. What scalar functions of two vectors satisfy these three properties? One such function is the dot product $\mathbf{n}\cdot\mathbf{m}$. Any scalar multiple of the dot product, $A\,(\mathbf{n}\cdot\mathbf{m})$ for scalar A, also satisfies these three properties. It turns out that this is the entire class of functions that satisfy these properties, and here is a rough justification:

Claim. Suppose that $g(\mathbf{n},\mathbf{m})$, a function of two three-dimensional real vectors, satisfies the following three properties:

- *Linearity:* $g(c\,\mathbf{n}+\mathbf{m},\mathbf{q}) = c\,g(\mathbf{n},\mathbf{q})+g(\mathbf{m},\mathbf{q})$ and $g(\mathbf{n},c\,\mathbf{m}+\mathbf{p}) = c\,g(\mathbf{n},\mathbf{m})+g(\mathbf{n},\mathbf{q})$ for scalar c and vectors $\mathbf{n}$, $\mathbf{m}$, and $\mathbf{q}$.
- *Symmetry:* $g(\mathbf{n},\mathbf{m}) = g(\mathbf{m},\mathbf{n})$ for vectors $\mathbf{n}$, $\mathbf{m}$.

- *Invariance under rotations:* $g(\mathbf{n}, \mathbf{m})$ is invariant under simultaneous rotations of the coordinate axes.

Then, $g(\mathbf{n}, \mathbf{m}) = A\ (\mathbf{n} \cdot \mathbf{m})$ for a constant scalar A.

Justification:
First, we can show that $g(\hat{\mathbf{x}}, \hat{\mathbf{y}}) = 0$. Rotating the coordinate axes by 90° about the $\hat{\mathbf{z}}$-axis takes $\hat{\mathbf{x}} \to \hat{\mathbf{y}}$ and $\hat{\mathbf{y}} \to -\hat{\mathbf{x}}$. Therefore, we can write

$$\begin{aligned} g(\hat{\mathbf{x}}, \hat{\mathbf{y}}) &= g(\hat{\mathbf{y}}, -\hat{\mathbf{x}}) \quad \text{by rotation invariance} \\ &= -g(\hat{\mathbf{y}}, \hat{\mathbf{x}}) \quad \text{by linearity} \\ &= -g(\hat{\mathbf{x}}, \hat{\mathbf{y}}) \quad \text{by symmetry} \end{aligned} \tag{22}$$

Since $g(\hat{\mathbf{x}}, \hat{\mathbf{y}})$ is equal to its negative, we must have $g(\hat{\mathbf{x}}, \hat{\mathbf{y}}) = 0$. By rotation invariance and symmetry, this implies that

$$g(\hat{\mathbf{x}}, \hat{\mathbf{y}}) = g(\hat{\mathbf{x}}, \hat{\mathbf{z}}) = g(\hat{\mathbf{y}}, \hat{\mathbf{z}}) = g(\hat{\mathbf{y}}, \hat{\mathbf{x}}) = g(\hat{\mathbf{z}}, \hat{\mathbf{x}}) = g(\hat{\mathbf{z}}, \hat{\mathbf{y}}) = 0 \tag{23}$$

Now, define $A \equiv g(\hat{\mathbf{x}}, \hat{\mathbf{x}})$. By rotation invariance, this implies that

$$g(\hat{\mathbf{x}}, \hat{\mathbf{x}}) = g(\hat{\mathbf{y}}, \hat{\mathbf{y}}) = g(\hat{\mathbf{z}}, \hat{\mathbf{z}}) = A \tag{24}$$

Now, consider arbitrary vectors

$$\mathbf{n} = n_x \hat{\mathbf{x}} + n_y \hat{\mathbf{y}} + n_z \hat{\mathbf{z}} \quad \text{and} \quad \mathbf{m} = m_x \hat{\mathbf{x}} + m_y \hat{\mathbf{y}} + m_z \hat{\mathbf{z}} \tag{25}$$

We can then write

$$\begin{aligned} g(\mathbf{n}, \mathbf{m}) &= gf(n_x \hat{\mathbf{x}} + n_y \hat{\mathbf{y}} + n_z \hat{\mathbf{z}},\ m_x \hat{\mathbf{x}} + m_y \hat{\mathbf{y}} + m_z \hat{\mathbf{z}}) \\ &= n_x\, m_x\, g(\hat{\mathbf{x}}, \hat{\mathbf{x}}) + n_y\, m_y\, g(\hat{\mathbf{y}}, \hat{\mathbf{y}}) + n_z\, m_z\, g(\hat{\mathbf{z}}, \hat{\mathbf{z}}) \\ &\quad + n_x\, m_y\, g(\hat{\mathbf{x}}, \hat{\mathbf{y}}) + n_y\, m_z\, g(\hat{\mathbf{y}}, \hat{\mathbf{z}}) + n_z\, m_x\, g(\hat{\mathbf{z}}, \hat{\mathbf{x}}) \\ &\quad + n_y\, m_x\, g(\hat{\mathbf{y}}, \hat{\mathbf{x}}) + n_z\, m_y\, g(\hat{\mathbf{z}}, \hat{\mathbf{y}}) + n_x\, m_z\, g(\hat{\mathbf{x}}, \hat{\mathbf{z}}) \quad \text{by linearity} \\ &= n_x\, m_x\, A + n_y\, m_y\, A + n_z\, m_z\, A \quad \text{by (23) and (24)} \\ &= A\ (\mathbf{n} \cdot \mathbf{m}) \quad \text{by the definition of the dot product} \end{aligned} \tag{26}$$

Thus, $g(\mathbf{n}, \mathbf{m}) = A\ (\mathbf{n} \cdot \mathbf{m})$ for a constant scalar A.

Now that we know the form of $g(\mathbf{n}, \mathbf{m})$, all we need to do is find the scalar A. To do so, we can choose the easiest possible values for $\mathbf{n}$ and $\mathbf{m}$ and evaluate $g(\mathbf{n}, \mathbf{m})$. The easiest possible values for $\mathbf{n}$ and $\mathbf{m}$ are $\mathbf{n} = \mathbf{m} = \hat{\mathbf{z}}$. Then, we have

$$\begin{aligned} g(\hat{\mathbf{z}}, \hat{\mathbf{z}}) &= \langle \Psi | S_{a,z} S_{b,z} | \Psi \rangle \quad \text{by definition of } g(\mathbf{n}, \mathbf{m}) \\ &= \frac{\hbar^2}{4} \langle \Psi | \sigma_{a,z} \sigma_{b,z} | \Psi \rangle \quad \text{since for a spin-1/2 particle, } S_i = \frac{\hbar}{2} \sigma_i \end{aligned} \tag{27}$$

Recall that for a single spin-1/2 particle, with $c_1 |\uparrow\rangle + c_2 |\downarrow\rangle \cong \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$, the Pauli matrices define the action of the Pauli operators on $|\uparrow\rangle$ and $|\downarrow\rangle$:

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \text{so} \quad \sigma_z |\uparrow\rangle = |\uparrow\rangle \quad \text{and} \quad \sigma_z |\downarrow\rangle = -|\downarrow\rangle \tag{28}$$

Therefore, bearing in mind that the σ_a operators act on the first ket and the σ_b operators act on the second ket, we have

$$\begin{aligned}
\sigma_{a,z}\sigma_{b,z}\,|\Psi\rangle &= \frac{1}{\sqrt{2}}\sigma_{a,z}\sigma_{b,z}\big[\,|\uparrow\rangle_a\,|\downarrow\rangle_b - |\downarrow\rangle_a\,|\uparrow\rangle_b\,\big] \quad \text{by (18)} \\
&= \frac{1}{\sqrt{2}}\big[\sigma_{a,z}\,|\uparrow\rangle_a\;\sigma_{b,z}\,|\downarrow\rangle_b - \sigma_{a,z}\,|\downarrow\rangle_a\;\sigma_{b,z}\,|\uparrow\rangle_b\,\big] \\
&= \frac{1}{\sqrt{2}}\big[-|\uparrow\rangle_a\,|\downarrow\rangle_b + |\downarrow\rangle_a\,|\uparrow\rangle_b\,\big] \\
&= -\,|\Psi\rangle
\end{aligned} \tag{29}$$

Taking the inner product with $\langle\Psi|$, we get

$$\begin{aligned}
\langle\Psi|\sigma_{a,z}\sigma_{b,z}|\Psi\rangle &= -\,\langle\Psi|\Psi\rangle \\
&= -1 \quad \text{since } |\Psi\rangle \text{ is normalized}
\end{aligned} \tag{30}$$

Plugging this into (27), we get

$$g(\hat{\mathbf{z}},\hat{\mathbf{z}}) = -\frac{\hbar^2}{4} \tag{31}$$

But we also know that $g(\mathbf{n},\mathbf{m}) = A\;(\mathbf{n}\cdot\mathbf{m})$, so

$$g(\hat{\mathbf{z}},\hat{\mathbf{z}}) = A\,\hat{\mathbf{z}}\cdot\hat{\mathbf{z}} = A \tag{32}$$

Therefore, $A = -\frac{\hbar^2}{4}$, meaning that

$$g(\mathbf{n},\mathbf{m}) = -\frac{\hbar^2}{4}\;(\mathbf{n}\cdot\mathbf{m}) \tag{33}$$

Restoring the unit vectors $\hat{\mathbf{n}}_a$ and $\hat{\mathbf{n}}_b$, we get our answer

$$\boxed{g(\hat{\mathbf{n}}_a,\hat{\mathbf{n}}_b) \equiv \langle\Psi|(\hat{\mathbf{n}}_a\cdot\mathbf{S}_a)\,(\hat{\mathbf{n}}_b\cdot\mathbf{S}_b)|\Psi\rangle = -\frac{\hbar^2}{4}\,(\hat{\mathbf{n}}_a\cdot\hat{\mathbf{n}}_b)} \tag{34}$$

At first glance, this mathematical approach seems far more complicated than the direct calculation. However, once you get some practice, it is actually pretty easy to see that $g(\hat{\mathbf{n}}_a,\hat{\mathbf{n}}_b)$, which is defined by $\langle\Psi|(\hat{\mathbf{n}}_a\cdot\mathbf{S}_a)\,(\hat{\mathbf{n}}_b\cdot\mathbf{S}_b)|\Psi\rangle$, satisfies the three properties of a dot product (linearity, symmetry, and invariance under rotations). From there, you immediately know that $g(\hat{\mathbf{n}}_a,\hat{\mathbf{n}}_b)$ is proportional to the dot product $\hat{\mathbf{n}}_a\cdot\hat{\mathbf{n}}_b$. Then, all you need to do is find the constant prefactor A, which is a relatively straightforward calculation.

It is also instructive to see how some aspects of the direct calculation rely on the mathematical properties of the setup. In particular, the invariance of the setup under rotations is precisely the reason we can set the unit vectors $\hat{\mathbf{n}}_a$ and $\hat{\mathbf{n}}_b$ to point in the directions given by (1).

Deriving the spin-1/2 Clebsch-Gordan coefficients:
Here is how we derive the expression (18) for the state $|\Psi\rangle$. First, note a few facts 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: $|m_1\rangle\,|m_2\rangle$

$$\text{This basis simultaneously diagonalizes} \quad \mathbf{J}_1^2,\ \mathbf{J}_2^2,\ J_{1z},\ J_{2z} \tag{35}$$

$$\text{Possible quantum numbers:} \quad m_i = -j_i, -j_i+1, \ldots, j_i-1, j_i \tag{36}$$

$$\mathbf{J}_i^2 \text{ eigenvalues:} \quad \mathbf{J}_i^2\,|m_1\rangle\,|m_2\rangle = \hbar^2 j_i(j_i+1)\,|m_1\rangle\,|m_2\rangle \tag{37}$$

$$J_{i,z} \text{ eigenvalues:} \quad J_{i,z}\,|m_1\rangle\,|m_2\rangle = \hbar\, m_i\,|m_1\rangle\,|m_2\rangle \tag{38}$$

$$\text{Dimension of space:} \quad (2j_1+1)(2j_2+1) \quad \text{different basis states} \tag{39}$$

Combined basis: $|j, m\rangle$

$$\text{This basis simultaneously diagonalizes} \quad \mathbf{J}_1^2,\ \mathbf{J}_2^2,\ \mathbf{J}^2,\ J_z \tag{40}$$

$$\text{Possible quantum numbers:} \quad j = j_1+j_2, j_1+j_2-1, \ldots, |j_1-j_2| \tag{41}$$

$$m = -j, -j+1, \ldots, j-1, j \tag{42}$$

$$\mathbf{J}_i^2 \text{ eigenvalues:} \quad \mathbf{J}_i^2\,|j,m\rangle = \hbar^2 j_i(j_i+1)\,|j,m\rangle \tag{43}$$

$$\mathbf{J}^2 \text{ eigenvalues:} \quad \mathbf{J}^2\,|j,m\rangle = \hbar^2 j(j+1)\,|j,m\rangle \tag{44}$$

$$J_z \text{ eigenvalues:} \quad J_z\,|j,m\rangle = \hbar m\,|j,m\rangle \tag{45}$$

$$\text{Dimension of space:} \quad \sum_{j=|j_1-j_2|}^{j_1+j_2} (2j+1) = (2j_1+1)(2j_2+1) \quad \text{different basis states} \tag{46}$$

$$\text{Relation between bases:} \quad m_1 + m_2 = m \tag{47}$$

Since particles a and b are spin-1/2 particles, then the spin quantum number s_i associated with each particle is equal to 1/2. We need to add these two spin-1/2 particles.

First, let's determine the possible values of j and m. By (41), the possible values of j are

$$j = s_1 + s_2, \ldots, |s_1 - s_2| = 1 \text{ and } 0 \tag{48}$$

We can use (42) to find the possible values of m for each possible value of j. For $j = 1$, the possible values of m are equal to

$$j = 1: \qquad m = 1, 0, -1 \tag{49}$$

For $j = 0$, the only possible value of m is zero:

$$j = 0: \qquad m = 0 \tag{50}$$

We can now draw a "wedding cake" diagram for the possible values of j and m for this system of two spin-1/2 particles:

$$\begin{array}{ccc} |1,1\rangle & & \\ |1,0\rangle & \qquad & |0,0\rangle \\ |1,-1\rangle & & \end{array} \tag{51}$$

Note that as we expect for two spin-1/2 particles, the total number of spin states is $2 \times 2 = 4$. For the specific case of two spin-1/2 particles, the three states $|1,1\rangle$, $|1,0\rangle$, and $|1,-1\rangle$ are referred to as the "triplet," and the state $|0,0\rangle$ is referred to as the "singlet."

The state we are interested in is the singlet state $|\Psi\rangle = |0,0\rangle$, since this state has zero total angular momentum ($j = 0$).

Here is the appropriate method:

Wedding cake method of computing Clebsch-Gordon coefficients:

$$\begin{array}{l} \curvearrowright\ |1,1\rangle \\ \curvearrowright\ |1,0\rangle \quad \longrightarrow\ |0,0\rangle \\ \curvearrowright\ |1,-1\rangle \end{array} \tag{52}$$

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

$$J_- |j,m\rangle = \hbar\sqrt{(j+m)(j-m+1)}\,|j,m-1\rangle \tag{53}$$

$$J_{1-} |m_1\rangle |m_2\rangle = \hbar\sqrt{(j_1+m_1)(j_1-m_1+1)}\,|m_1-1\rangle |m_2\rangle \tag{54}$$

$$J_{2-} |m_1\rangle |m_2\rangle = \hbar\sqrt{(j_2+m_2)(j_2-m_2+1)}\,|m_1\rangle |m_2-1\rangle \tag{55}$$

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:

(j,m)	$f(j,m) \equiv \sqrt{(j+m)(j-m+1)}$
$(1,1)$	$\sqrt{2}$
$(1,0)$	$\sqrt{2}$
$(1/2,1/2)$	1

(56)

Then, in the context of this problem, since we have two spin-1/2 particles, equations (53)-(55) become

$$S_- |j,m\rangle = \hbar f(j,m)\,|j,m-1\rangle \tag{57}$$

$$S_{1-} |m_1\rangle |m_2\rangle = \hbar\, f(1/2,m_1)\,|m_1-1\rangle |m_2\rangle \tag{58}$$

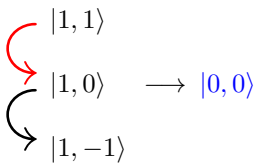
$$S_{2-} |m_1\rangle |m_2\rangle = \hbar\, f(1/2,m_2)\,|m_1\rangle |m_2-1\rangle \tag{59}$$

We are now ready to start working our way through the wedding cake diagram:

Starting point: $|1,1\rangle$
Recall that $m_1 + m_2 = m$ (by (47)). In this case, $m = 1$. Since we have two spin-1 particles, m_1 and m_2 can be at most 1/2 (by (36)). Thus, the only possible original eigenket that can contribute to the combined eigenket $|1,1\rangle$ is $|\uparrow\rangle |\uparrow\rangle$ (recall that $|\uparrow\rangle$ has $m_i = 1/2$). We can set the normalization of $|1,1\rangle$ so that the prefactor is equal to 1, getting

$$|1,1\rangle = |\uparrow\rangle |\uparrow\rangle \tag{60}$$

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



Lowering $|1,1\rangle$ with the S_- lowering operator for total angular momentum and applying table (56), we get

$$S_- |1,1\rangle = \hbar f(1,1) |1,\, 1-1\rangle = \sqrt{2}\hbar |1,0\rangle \tag{61}$$

But $S_- = S_{1-} + S_{2-}$, so we can also use perform this lowering operation in the original basis (recalling that $|\downarrow\rangle$ has $m_i = -1/2$):

$$\begin{aligned} S_- |1,1\rangle &= (S_{1-} + S_{2-}) |1,1\rangle \\ &= (S_{1-} + S_{2-}) |\uparrow\rangle |\uparrow\rangle \quad \text{by our earlier calculation of } |1,1\rangle \text{ in the original basis (60)} \\ &= S_{1-} |\uparrow\rangle |\uparrow\rangle + S_{2-} |\uparrow\rangle |\uparrow\rangle \\ &= \hbar\, f(1/2,1/2) |\downarrow\rangle |\uparrow\rangle + \hbar\, f(1/2,1/2) |\uparrow\rangle |\downarrow\rangle \quad \text{by (54) and (55)} \\ &= \hbar\, |\downarrow\rangle |\uparrow\rangle + \hbar\, |\uparrow\rangle |\downarrow\rangle \quad \text{by table (56)} \end{aligned} \tag{62}$$

Setting (61) and (62) equal to one another, we get

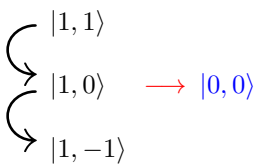
$$\sqrt{2}\hbar |1,0\rangle = S_- |1,1\rangle = \hbar\, |\downarrow\rangle |\uparrow\rangle + \hbar\, |\uparrow\rangle |\downarrow\rangle$$

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

$$|1,0\rangle = \frac{1}{\sqrt{2}} \big[\, |\uparrow\rangle |\downarrow\rangle + |\downarrow\rangle |\uparrow\rangle \,\big] \tag{63}$$

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 (61) and used the normalization to calculate it. Calculating the overall constant is a useful algebra check, though, so we have opted to include it.)

Orthogonality: $|1,0\rangle \to |0,0\rangle$



Since $m_1 + m_2 = m$ and $m_i = 1/2, -1/2$, we know that $|0,0\rangle$ must be the sum of $|\uparrow\rangle |\downarrow\rangle$ and $|\uparrow\rangle |\downarrow\rangle$. But since $|j,m\rangle$ is an orthonormal basis, $|0,0\rangle$ must be orthogonal to $|1,0\rangle$. Recall our expression for $|1,0\rangle$ in the original basis (63)

$$|1,0\rangle = \frac{1}{\sqrt{2}} \big[\, |\uparrow\rangle |\downarrow\rangle + |\downarrow\rangle |\uparrow\rangle \,\big]$$

There is only one vector that is orthogonal to this one, and (up to an overall phase) we can set it equal to $|0,0\rangle$:

$$|\Psi\rangle = |0,0\rangle = \frac{1}{\sqrt{2}} \big[\, |\uparrow\rangle |\downarrow\rangle - |\downarrow\rangle |\uparrow\rangle \,\big] \tag{64}$$

This completes the derivation of the singlet state in the original basis.

The coefficients which relate the combined basis to the original basis are known as "Clebsch-Gordan coefficients." For small values of j, you can look them up in a table (just make sure you know how to read such a table first).