Physics 916: Homework #5

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Show that in general, any 2×2 matrix M can be represented in terms of the unit matrix, I, and the Pauli matrices. i.e.

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} = a_0 I + \vec{a} \cdot \vec{\sigma}$$

where the expansion coefficients $a_i = \frac{1}{2}Tr\{M\sigma_i\}$

Solution

First I will use a common convention and define σ_0 as the identity operator. So we have:

$$\begin{split} M &= \vec{a} \cdot \vec{\sigma} = a_0 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + a_1 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + a_2 \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + a_3 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ &= \begin{pmatrix} a_0 + a_3 & a_1 - ia_2 \\ a_1 + ia_2 & a_0 - a_3 \end{pmatrix} \\ M_{11} &= a_0 + a_3 \\ M_{12} &= a_1 - ia_2 \\ M_{21} &= a_1 + ia_2 \\ M_{22} &= a_0 - a_3 \end{split}$$

$$a_0 &= \frac{1}{2} Tr \{M\sigma_0\} = \frac{1}{2} Tr \left[\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right] = Tr \left[\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \right] \\ &= \frac{1}{2} \begin{pmatrix} M_{11} + M_{22} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} a_0 + a_3 + a_0 - a_3 \end{pmatrix} \\ &= a_0 \\ a_1 &= \frac{1}{2} Tr \{M\sigma_1\} = \frac{1}{2} Tr \left[\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right] = Tr \left[\begin{pmatrix} M_{12} & M_{11} \\ M_{22} & M_{21} \end{pmatrix} \right] \\ &= \frac{1}{2} \begin{pmatrix} M_{12} + M_{21} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} a_1 - ia_2 + a_1 + ia_2 \end{pmatrix} \\ &= a_1 \\ a_2 &= \frac{1}{2} Tr \{M\sigma_2\} = \frac{1}{2} Tr \left[\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \right] = Tr \left[\begin{pmatrix} iM_{12} & -iM_{11} \\ iM_{22} & -iM_{21} \end{pmatrix} \right] \\ &= \frac{1}{2} \begin{pmatrix} iM_{12} - iM_{21} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} ia_1 - i^2a_2 - ia_1 - i^2a_2 \end{pmatrix} \\ &= a_2 \\ a_3 &= \frac{1}{2} Tr \{M\sigma_3\} = \frac{1}{2} Tr \left[\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right] = Tr \left[\begin{pmatrix} M_{11} & -M_{12} \\ M_{21} & -M_{22} \end{pmatrix} \right] \\ &= \frac{1}{2} \begin{pmatrix} M_{11} - M_{22} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} a_0 + a_3 - a_0 + a_3 \end{pmatrix} \\ &= a_3 \\ &= a_3 \end{aligned}$$

Consider the quantum operator, H, whose matrix representation in the orthonormal basis $\{|u_1\rangle, |u_2\rangle\}$ writes:

$$H = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}$$

where H_{11} and H_{22} are real numbers and $H_{12} = H_{21}^*$. It is thus obvious that H is Hermitian.

- 1. Show that:
- $H = \frac{1}{2}(H_{11} + H_{22})I + \tilde{K} \equiv \frac{1}{2}(H_{11} + H_{22})I + \frac{1}{2}(H_{11} H_{22})K$ where I is the identity operator, and the operators \tilde{K}, K must be determined in terms of the matrix elements of H. Are \tilde{K} and K Hermitian?
- 2. A key result from the decomposition in part 1 is that the operators \tilde{K}, K , and H all have the same eigenvectors $|\psi_{\pm}\rangle$. Let $\tilde{\kappa}_{\pm}, \kappa_{\pm}, E_{\pm}$ be the eigenvalues of \tilde{K}, K , and H. Use the result of part 1 to establish the relation between E_{\pm} and κ_{\pm} , and the relation between E_{\pm} and $\tilde{\kappa}_{\pm}$. Show that these relations allow for a change of the eigenvalue origin.
- 3. Directly solve the secular equations for K and H and determine the corresponding eigenvalues. Check that the relation between E_{\pm} and κ_{\pm} established in part 2 is correct.
- 4. Let us define angles $0 \le \theta \le \pi$ and $0 \le \phi \le 2\pi$ defined as: $\tan \theta = \frac{2|H_{21}|}{H_{11}-H_{22}}$ and $H_{21} = |H_{21}|e^{i\phi}$
- 5. Show that $E_+ + E_- = Tr\{H\}$, and that $E_+E_- = \det H$
- 6. Show that if H has a degenerate spectrum, then it is necessarily proportional to the identity operator.
- 7. Use the operator, $K(\theta, \phi)$ to calculate normalized eigenvectors $|\psi_{\pm}\rangle$ in terms of these angles in the orthonormal basis $\{|u_1\rangle, |u_2\rangle\}$. You must find that the eigenvectors $|\psi_{\pm}\rangle$ are collinear to the eigenvectors $|\pm\rangle$ of the 1/2 spin operator S_u , where u is an arbitrary unit vector defined by these angles.
- 8. Show that $K(\theta = 0, \phi = 0)$ is proportional to the z-component of the Pauli operator, σ_z . What are the corresponding eigenvalues and eigenvectors?
- 9. When $\theta = \pi/2$, the operator K is not finite and we must use \tilde{K} . Show that $\tilde{K}_x \equiv \tilde{K}(\theta = \pi/2, \phi = 0)$ is proportional to the x-component of the Pauli operator, σ_x . What are the corresponding eigenvalues and eigenvectors?
- 10. Show that $\tilde{K}_y \equiv \tilde{K}(\theta = \pi/2, \phi = \pi/2)$ is proportional to the y-component of the Pauli operator, σ_y . What are the corresponding eigenvalues and eigenvectors?
- 11. Calculate the commutator, $[\tilde{K}_x, \tilde{K}_y]$, and show that it is proportional to the z-component of the pauli operator, σ_z .

Solution

Since they will be used several times later on in this problem, here are the definitions of the 2×2 Pauli

operators:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

1. If we let the following be true we will have the relation suggested:

$$H_{11} = \frac{1}{2} [H_{11}(1 + K_{11}) + H_{22}(1 - K_{11})]$$

$$H_{22} = \frac{1}{2} [H_{11}(1 + K_{22}) + H_{22}(1 - K_{22})]$$

$$H_{12} = \frac{1}{2} K_{12}(H_{11} - H_{22})$$

$$H_{21} = \frac{1}{2} K_{12}(H_{11} - H_{22})$$

From here we can determine a couple of things about K and \tilde{K}

$$K_{11} = 1, \ K_{22} = -1$$

$$K_{12} = \frac{2}{H_{11} - H_{22}} H_{12} = \frac{2}{H_{11} - H_{22}} H_{21}^* = K_{21}^*$$

So we know the value of the diagonal of K and \tilde{K} and we also know that they are Hermitian.

2. Starting with the relation between E_{\pm} and $\tilde{\kappa}_{\pm}$

$$H |\psi_{\pm}\rangle = \frac{1}{2} (H_{11} + H_{22}) I |\psi_{\pm}\rangle + \tilde{K} |\psi_{\pm}\rangle$$

$$= \frac{1}{2} (H_{11} + H_{22}) |\psi_{\pm}\rangle + \tilde{\kappa}_{\pm} |\psi_{\pm}\rangle$$

$$= E_{\pm} |\psi_{\pm}\rangle$$

$$\Rightarrow E_{\pm} = \frac{1}{2} (H_{11} + H_{22}) + \tilde{\kappa}_{\pm}$$

Now for the relation between E_{\pm} and κ_{\pm}

$$H |\psi_{\pm}\rangle = \frac{1}{2} (H_{11} + H_{22}) I |\psi_{\pm}\rangle + \frac{1}{2} (H_{11} - H_{22}) K |\psi_{\pm}\rangle$$

$$= \frac{1}{2} (H_{11} + H_{22}) |\psi_{\pm}\rangle + \frac{1}{2} (H_{11} - H_{22}) \kappa_{\pm} |\psi_{\pm}\rangle$$

$$= E_{\pm} |\psi_{\pm}\rangle$$

$$\Rightarrow E_{\pm} = \frac{1}{2} (H_{11} + H_{22}) + \frac{1}{2} (H_{11} - H_{22}) \kappa_{\pm}$$

In both of these cases, the eigenvalues are related by a shift by a constant, $\frac{1}{2}(H_{11} + H_{22})$, thus "shifting the origin" of the eigenvalues.

3. Start by solving the secular equation to find the eigenvalues of H

$$\begin{vmatrix} H_{11} - \lambda & H_{12} \\ H_{21} & H_{22} - \lambda \end{vmatrix} = (H_{11} - \lambda)(H_{22} - \lambda) - |H_{12}|^2$$

$$= H_{11}H_{22} + \lambda^2 - \lambda H_{22} - \lambda H_{11} - |H_{12}|^2$$

$$= \lambda^2 - \lambda(H_{11} + H_{22}) + H_{11}H_{22} - |H_{12}|^2$$

$$= 0$$

$$\Rightarrow \lambda = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$= \frac{1}{2}(H_{11} + H_{22}) \pm \frac{1}{2}\sqrt{(H_{11} + H_{22})^2 - 4(H_{11}H_{22} - |H_{12}|^2)}$$

$$= \frac{1}{2}(H_{11} + H_{22}) \pm \frac{1}{2}\sqrt{H_{11}^2 + H_{22}^2 + 2H_{11}H_{22} - 4H_{11}H_{22} + 4|H_{12}|^2}$$

$$= \frac{1}{2}(H_{11} + H_{22}) \pm \frac{1}{2}\sqrt{H_{11}^2 + H_{22}^2 - 2H_{11}H_{22} + 4|H_{12}|^2}$$

$$= \frac{1}{2}(H_{11} + H_{22}) \pm \frac{1}{2}\sqrt{(H_{11} - H_{22})^2 + 4|H_{12}|^2}$$

Now I'll do the same for the eigenvalues of K. Recall from part 1 that $K_{11}=1,\ K_{22}=-1$

$$\begin{vmatrix} 1 - \lambda & K_{12} \\ K_{21} & -(1+\lambda) \end{vmatrix} = -(1+\lambda)(1-\lambda) - |K_{12}|^2$$

$$= \lambda^2 - 1 - |K_{12}|^2$$

$$= 0$$

$$\Rightarrow \lambda = \pm \sqrt{1 + |K_{12}|^2}$$

Recall from part 1: $K_{12} = \frac{2}{H_{11} - H_{22}} H_{12}$

$$\lambda = \pm \sqrt{1 + \left| \frac{2}{H_{11} - H_{22}} H_{12} \right|^2}$$

$$= \pm \frac{1}{H_{11} - H_{22}} \sqrt{(H_{11} - H_{22})^2 + 4|H_{12}|^2}$$

4. We have:

$$\tan \theta = \frac{2|H_{21}|}{H_{11} - H_{22}}, \ H_{21} = |H_{21}|e^{i\phi}$$

$$\Rightarrow e^{i\phi} \tan \theta = \frac{2H_{21}}{H_{11} - H_{22}}$$

$$K_{21} = e^{i\phi} \tan \theta$$

$$K_{12} = e^{-i\phi} \tan \theta$$

We already established that $K_{11} = 1$ and $K_{22} = -1$, so we have:

$$K = \begin{pmatrix} 1 & e^{-i\phi} \tan \theta \\ e^{i\phi} \tan \theta & -1 \end{pmatrix}$$

Then the eigenvalue can be expressed using the equation in the last part of part 3:

$$\kappa_{\pm} = \pm \sqrt{1 + \left| \frac{2}{H_{11} - H_{22}} H_{12} \right|^2}$$

$$= \pm \sqrt{1 + \left| e^{i\phi} \tan \theta \right|^2}$$

$$= \pm \sqrt{1 + \tan^2 \theta}$$

$$= \pm \sec \theta$$

5. Taking the eigenvalues of H from part 3:

$$E_{+} + E_{-} = \frac{1}{2}(H_{11} + H_{22}) + \frac{1}{2}\sqrt{(H_{11} - H_{22})^{2} + 4|H_{12}|^{2}} + \frac{1}{2}(H_{11} + H_{22}) - \frac{1}{2}\sqrt{(H_{11} - H_{22})^{2} + 4|H_{12}|^{2}}$$

$$= \frac{1}{2}(H_{11} + H_{22}) + \frac{1}{2}(H_{11} + H_{22})$$

$$= H_{11} + H_{22}$$

$$= Tr\{H\}$$

Now to calculate E_+E_- . The form of this will be $(a+b)(a-b)=a^2-b^2$:

$$E_{+}E_{-} = \left(\frac{1}{2}(H_{11} + H_{22})\right)^{2} - \left(\frac{1}{2}\sqrt{(H_{11} - H_{22})^{2} + 4|H_{12}|^{2}}\right)^{2}$$

$$= \frac{1}{4}\left(H_{11}^{2} + H_{22}^{2} + 2H_{11}H_{22}\right) - \frac{1}{4}(H_{11} - H_{22})^{2} - |H_{12}|^{2}$$

$$= \frac{1}{4}\left(H_{11}^{2} + H_{22}^{2} + 2H_{11}H_{22}\right) - \frac{1}{4}(H_{11}^{2} + H_{22}^{2} - 2H_{11}H_{22}) - |H_{12}|^{2}$$

$$= \frac{1}{4}2H_{11}H_{22} - \frac{1}{4}(-2H_{11}H_{22}) - |H_{12}|^{2}$$

$$= H_{11}H_{22} - |H_{12}|^{2}$$

$$= \det H$$

6. Since H is only 2×2 , there are only two eigenvalues, so for it to be degenerate means that the eigenvalues are the same. $\Rightarrow E_{+} = E_{-}$

$$\Rightarrow \frac{1}{2}(H_{11} + H_{22}) + \frac{1}{2}\sqrt{(H_{11} - H_{22})^2 + 4|H_{12}|^2} = \frac{1}{2}(H_{11} + H_{22}) - \frac{1}{2}\sqrt{(H_{11} - H_{22})^2 + 4|H_{12}|^2}$$
$$(H_{11} - H_{22})^2 + 4|H_{12}|^2 = 0$$

For this to be true, $|H_{12}| = 0$. This is because otherwise H_{11} and/or H_{22} would have to be complex, and it was specified in the problem that they are real. Then if $|H_{12}| = 0$, $H_{11} = H_{22}$. This means that H must be proportional to the identity matrix.

7. The eigenvalues of K are $\kappa_{\pm} = \pm \sec \theta$, and K is defined as:

$$K = \begin{pmatrix} 1 & e^{-i\phi} \tan \theta \\ e^{i\phi} \tan \theta & -1 \end{pmatrix}$$

To find the eigenvectors, starting with κ_{+}

$$\begin{pmatrix} 1 - \sec \theta & e^{-i\phi} \tan \theta \\ e^{i\phi} \tan \theta & -(1 + \sec \theta) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$
$$\Rightarrow c_2 = c_1 \frac{\sec \theta - 1}{\tan \theta} e^{i\phi} = c_1 \tan \frac{\theta}{2} e^{i\phi}$$
$$v_+ = \begin{pmatrix} 1 \\ \tan \frac{\theta}{2} e^{i\phi} \end{pmatrix}$$

Now to normalize it:

$$A_{+}^{2}(1 + \tan^{2}\frac{\theta}{2}) = 1$$

$$A_{+} = \sqrt{\frac{1}{1 + \tan^{2}\frac{\theta}{2}}} = \sqrt{\frac{1}{\sec^{2}\frac{\theta}{2}}} = \cos\frac{\theta}{2}$$

For the eigenvalue κ_+ , we have:

$$|\psi_{+}\rangle = \cos\frac{\theta}{2} \begin{pmatrix} 1 \\ \tan\frac{\theta}{2}e^{i\phi} \end{pmatrix}$$

Now for κ_{-}

$$\begin{pmatrix} \sec \theta + 1 & e^{-i\phi} \tan \theta \\ e^{i\phi} \tan \theta & \sec \theta - 1 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$
$$\Rightarrow c_2 = c_1 \frac{\tan \theta}{1 - \sec \theta} e^{i\phi} = -c_1 \cot \frac{\theta}{2} e^{i\phi}$$
$$v_- = \begin{pmatrix} 1 \\ -\cot \frac{\theta}{2} e^{i\phi} \end{pmatrix}$$

Now to normalize it:

$$A_{-}^{2}(1+\cot^{2}\frac{\theta}{2}) = 1$$

$$A_{-} = \sqrt{\frac{1}{1+\cot^{2}\frac{\theta}{2}}} = \sqrt{\frac{1}{\csc^{2}\frac{\theta}{2}}} = \sin\frac{\theta}{2}$$

For the eigenvalue κ_+ , we have:

$$|\psi_{-}\rangle = \sin\frac{\theta}{2} \begin{pmatrix} 1\\ -\cot\frac{\theta}{2}e^{i\phi} \end{pmatrix}$$

8. The operator $K(\theta, \phi)$ is defined in the matrix representation as:

$$K = \begin{pmatrix} 1 & e^{-i\phi} \tan \theta \\ e^{i\phi} \tan \theta & -1 \end{pmatrix}$$

If we let $\theta = \phi = 0$, we have:

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

This is equal to the Pauli matrix, σ_z . The eigenvalues and eigenvectors can be found by solving the charac-

teristic equation:

$$\begin{vmatrix} 1 - \lambda & 0 \\ 0 & -(1 + \lambda) \end{vmatrix} = 0$$

$$\lambda = \pm 1$$

$$\lambda = 1$$

$$\begin{pmatrix} 0 & 0 \\ 0 & -2 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$c_2 = 0$$

$$\Rightarrow v_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\lambda = -1$$

$$\begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$c_1 = 0$$

$$\Rightarrow v_1 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

9. Using the definitions from part 4, we can write:

$$H_{11} - H_{22} = \frac{2|H_{12}|}{\tan \theta}$$

$$\tilde{K} = \frac{1}{2}(H_{11} - H_{22})K = \begin{pmatrix} \frac{|H_{12}|}{\tan \theta} & e^{-i\phi} \tan \theta \frac{|H_{12}|}{\tan \theta} \\ e^{i\phi} \tan \theta \frac{|H_{12}|}{\tan \theta} & -\frac{|H_{12}|}{\tan \theta} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{|H_{12}|}{\tan \theta} & |H_{12}|e^{-i\phi} \\ |H_{12}|e^{i\phi} & -\frac{|H_{12}|}{\tan \theta} \end{pmatrix}$$

For $\theta = \pi/2$ and $\phi = 0$, we have:

$$\tilde{K}_x = |H_{12}| \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \propto \sigma_x$$

Now we use the usual method to find eigenvalues and eigenvectors:

$$\begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda \end{vmatrix} = \lambda^2 - 1 = 0$$
$$\lambda = +1$$

$$\lambda = 1$$

$$\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$c_2 = c_1$$

$$\Rightarrow v_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\lambda = -1$$

$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$c_2 = -c_1$$

 $\Rightarrow v_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\ -1 \end{pmatrix}$

$$\tilde{K} = \begin{pmatrix} \frac{|H_{12}|}{\tan \theta} & |H_{12}|e^{-i\phi} \\ |H_{12}|e^{i\phi} & -\frac{|H_{12}|}{\tan \theta} \end{pmatrix}$$

$$\tilde{K}(\pi/2, \pi/2) = \begin{pmatrix} 0 & |H_{12}|e^{-i\pi/2} \\ |H_{12}|e^{i\pi/2} & 0 \end{pmatrix}$$

$$e^{i\pi/2} = \cos(\pi/2) + i\sin(\pi/2) = i$$

$$e^{-i\pi/2} = \cos(\pi/2) - i\sin(\pi/2) = -i$$

$$\Rightarrow \tilde{K}(\pi/2, \pi/2) = |H_{12}| \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \propto \sigma_y$$

Now we use the usual method to find eigenvalues and eigenvectors:

$$\begin{vmatrix} -\lambda & -i \\ i & -\lambda \end{vmatrix} = \lambda^2 + i^2 = 0$$
$$\lambda = +1$$

$$\lambda = 1$$

$$\begin{pmatrix} -1 & -i \\ i & -1 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$c_2 = ic_1$$

$$\Rightarrow v_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}$$

$$\lambda = -1$$

$$\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$c_2 = -ic_1$$

$$\Rightarrow v_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

$$\begin{split} [\tilde{K}_{x}, \tilde{K}_{y}] = & \tilde{K}_{x} \tilde{K}_{y} - \tilde{K}_{y} \tilde{K}_{x} \\ \tilde{K}_{x} \tilde{K}_{y} = & |H_{12}|^{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = & |H_{12}|^{2} \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \\ \tilde{K}_{y} \tilde{K}_{x} = & |H_{12}|^{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = & |H_{12}|^{2} \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \\ [\tilde{K}_{x}, \tilde{K}_{y}] = & |H_{12}|^{2} \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} - & |H_{12}|^{2} \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \\ = & |H_{12}|^{2} \begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix} \\ = & 2i|H_{12}|^{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \propto \sigma_{z} \end{split}$$

The spin operator, S of an electron is pointing in any direction and is related to the Pauli matrices as $S = \frac{\hbar}{2} \sigma$ in the orthonormal basis $\{ |+\rangle, |-\rangle \}$ for S_z .

- 1. Write down the matrix for S_x , S_y , S_z , S_u . Are they Hermitian?
- 2. Determine the eigenvalues of each component for the spin operator.
- 3. Determine the eigenvectors of each component for the spin operator.
- 4. Show that $[S_x, S_y] = i\hbar S_z$, $[S_y, S_z] = i\hbar S_x$, $[S_z, S_x] = i\hbar S_y$
- 5. Show that $[S^2, S] = 0$

Solution

1. For S_x, S_y, S_z , we simply plug in the Pauli matrices.

$$S_x = \frac{\hbar}{2}\sigma_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1\\ 1 & 0 \end{pmatrix}$$

$$S_y = \frac{\hbar}{2}\sigma_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i\\ i & 0 \end{pmatrix}$$

$$S_z = \frac{\hbar}{2}\sigma_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0\\ 0 & -1 \end{pmatrix}$$

To find S_u we use the definition: $S_u = \mathbf{S} \cdot \mathbf{u}$, where \mathbf{u} is the unit vector in 3-dimensional space.

$$\begin{split} S_{u} &= \mathbf{S} \cdot \mathbf{u} = S_{x} u_{x} + S_{y} u_{y} + S_{z} u_{z} \\ &= \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \sin \theta \cos \phi + \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \sin \theta \sin \phi + \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cos \theta \\ &= \frac{\hbar}{2} \begin{pmatrix} \cos \theta & \sin \theta \cos \phi - i \sin \theta \sin \phi \\ \sin \theta \cos \phi + i \sin \theta \sin \phi & \cos \theta \end{pmatrix} \\ &= \frac{\hbar}{2} \begin{pmatrix} \cos \theta & \sin \theta (\cos \phi - i \sin \phi) \\ \sin \theta (\cos \phi + i \sin \phi) & \cos \theta \end{pmatrix} \\ &= \frac{\hbar}{2} \begin{pmatrix} \cos \theta & e^{-i\phi} \sin \theta \\ e^{i\phi} \sin \theta & \cos \theta \end{pmatrix} \end{split}$$

Each of these matrices is symmetric except for the two cases with complex parts, S_y , S_u , but in both of those matrices, $S_{21} = S_{12}^*$, so these are all Hermitian.

2. We find the eigenvalues in the usual way by solving the characteristic equation. For S_x :

$$\begin{vmatrix} -\lambda & \hbar/2 \\ \hbar/2 & -\lambda \end{vmatrix} = \lambda^2 - \frac{\hbar^2}{4} = 0 \Rightarrow \lambda = \pm \hbar/2$$

For S_y :

$$\begin{vmatrix} -\lambda & -i\hbar/2 \\ i\hbar/2 & -\lambda \end{vmatrix} = \lambda^2 + i^2 \frac{\hbar^2}{4} = \lambda^2 - \frac{\hbar^2}{4} = 0 \Rightarrow \lambda = \pm \hbar/2$$

For S_x :

$$\begin{vmatrix} \hbar/2 - \lambda & 0 \\ 0 & \hbar/2 - \lambda \end{vmatrix} = -\left(\frac{\hbar}{2} + \lambda\right) \left(\frac{\hbar}{2} - \lambda\right) = 0 \Rightarrow \lambda = \pm \hbar/2$$

So each of the spin operators has the same eigenvalues.

3. For each of the spin operators, plug the eigenvalues calculated in the last part into the eigenvalue equation and calculate the eigenvectors.

For $S_x, \lambda = +1$ (leaving off the factors of $\hbar/2$ since they don't matter here):

$$\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$c_2 = c_1$$

$$\vec{v}_{\lambda=+1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\1 \end{pmatrix}$$

For $S_x, \lambda = -1$:

$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$c_2 = -c_1$$

$$\vec{v}_{\lambda=-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\ -1 \end{pmatrix}$$

For $S_y, \lambda = +1$:

$$\begin{pmatrix} -1 & -i \\ i & -1 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$c_2 = ic$$

$$\vec{v}_{\lambda=+1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\i \end{pmatrix}$$

For $S_y, \lambda = -1$:

$$\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$c_2 = -ic_1$$

$$\vec{v}_{\lambda=-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\ -i \end{pmatrix}$$

For $S_z, \lambda = +1$:

$$\begin{pmatrix} 0 & 0 \\ 0 & -2 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$c_2 = 0$$

$$\vec{v}_{\lambda=+1} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

For $S_z, \lambda = -1$:

$$\begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$c_1 = 0$$

$$\vec{v}_{\lambda=+1} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

4. Use the matrix definitions given in part 1 to explicitly calculate the commutators

$$S_{x}S_{y} = \frac{\hbar^{2}}{4} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{\hbar^{2}}{4} \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$$

$$S_{y}S_{x} = \frac{\hbar^{2}}{4} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar^{2}}{4} \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$$

$$S_{x}S_{y} - S_{y}S_{x} = \frac{\hbar^{2}}{4} \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} - \frac{\hbar^{2}}{4} \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$$

$$= \frac{\hbar^{2}}{4} \begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix} = \frac{i\hbar^{2}}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$= i\hbar \left(\frac{\hbar}{2}\sigma_{z}\right)$$

$$\Rightarrow [S_{x}, S_{y}] = i\hbar S_{z}$$

$$S_{y}S_{z} = \frac{\hbar^{2}}{4} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar^{2}}{4} \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$$

$$S_{z}S_{y} = \frac{\hbar^{2}}{4} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{\hbar^{2}}{4} \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$$

$$= \frac{\hbar^{2}}{4} \begin{pmatrix} 0 & 2i \\ 2i & 0 \end{pmatrix} = \frac{i\hbar^{2}}{4} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$= i\hbar \left(\frac{\hbar}{2}\sigma_{x}\right)$$

$$\Rightarrow [S_{y}, S_{z}] = i\hbar S_{x}$$

$$S_{z}S_{x} = \frac{\hbar^{2}}{4} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar^{2}}{4} \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$$

$$S_{x}S_{z} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar^{2}}{4} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

$$= \frac{\hbar^{2}}{4} \begin{pmatrix} 0 & 2 \\ -2 & 0 \end{pmatrix} = \frac{i\hbar^{2}}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$= i\hbar \left(\frac{\hbar}{2}\sigma_{y}\right)$$

$$\Rightarrow [S_{z}, S_{z}] = i\hbar S_{y}$$

$$\Rightarrow [S_{z}, S_{z}] = i\hbar S_{y}$$

5. To start with, calculate S^2

$$S = \begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{pmatrix}$$

$$S^2 = \frac{\hbar^2}{4} \begin{pmatrix} \sigma_x & \sigma_y & \sigma_z \end{pmatrix} \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{pmatrix}$$

$$= \frac{\hbar^2}{4} [\sigma_x^2 + \sigma_y^2 + \sigma_z^2]$$

$$= \frac{\hbar^2}{4} [I + I + I]$$

$$= \frac{3\hbar^2}{4} I$$

For each of the Pauli matrices, $\sigma_i^2 = I$, the identity matrix. So now we know:

$$\left[\boldsymbol{S}^{2},\boldsymbol{S}\right] \propto \left[I,\boldsymbol{S}\right] =0$$

Because the identity matrix commutes with everything.

Let us consider two Stern-Gerlach experiments where the first one prepares the atoms in a state and the second one measures a spin physical quantity. Here, the state of the 1/2 spin system is prepared such that the spin is pointing down along \hat{u} in the x-z plane.

- 1. Immediately before measurement, what is the state $|\psi\rangle$ of the system in the basis of eigenvectors of S_z ?
- 2. What is the probability that a measurement of spin along the z-axis will find $-\hbar/2$? What is the state of the system immediately after measurement?
- 3. What is the probability that a measurement of spin along the z-axis will find $+\hbar/2$? What is the state of the system immediately after measurement?
- 4. What is the probability that spin down along the y-axis? What is the state of the system immediately after measurement?
- 5. What is the probability for spin up along the x-axis? What is the state of the system immediately after the measurement?
- 6. What is the probability that a measurement of spin along the u-axis will find $-\hbar/2$?
- 7. What is the probability that a measurement of spin along the u-axis will find $+\hbar/2$?

8.

Solution

1. In the S_z basis, with the spin known to be in the x-z plane ($\phi = 0$), we can write:

$$|+\rangle_u = \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{pmatrix}, \ |-\rangle_u = \begin{pmatrix} -\sin \frac{\theta}{2} \\ \cos \frac{\theta}{2} \end{pmatrix}$$

Since the state is prepared to be in the down state along \hat{u} , so the state before measurement would be:

$$|\psi\rangle = |-\rangle_u = -\sin\frac{\theta}{2}|+\rangle + \cos\frac{\theta}{2}|-\rangle$$

2. Since we are starting in the state, $|-\rangle_u$, the probability of finding it in the $-\hbar/2$ state is:

$$\mathcal{P} = \left| \left\langle - \right| + \right\rangle_u \right|^2 = \cos^2 \frac{\theta}{2}$$

Immediately following this measurement, the state of the system is spin down in S_z .

3. Since we are starting in the state, $|-\rangle_u$, the probability of finding it in the $+\hbar/2$ state is:

$$\mathcal{P} = \left| \left\langle + \right| + \right\rangle_u \right|^2 = \sin^2 \frac{\theta}{2}$$

Immediately following this measurement, the state of the system is spin up in S_z .

4. Since the spin is along \hat{u} which is only in the x-z plane, there is zero probability that the spin will

be found along the y-axis.

$$\begin{aligned} |+\rangle_x &= \frac{1}{\sqrt{2}} [|+\rangle + |-\rangle] \\ \mathcal{P}_{x+} &= \frac{1}{2} |\langle +|\psi\rangle + \langle -|\psi\rangle|^2 \\ &= \frac{1}{2} \left(-\sin\frac{\theta}{2} + \cos\frac{\theta}{2} \right)^2 \\ &= \frac{1}{2} \left(\sin^2\frac{\theta}{2} + \cos^2\frac{\theta}{2} - 2\sin\frac{\theta}{2}\cos\frac{\theta}{2} \right) \\ &= \frac{1}{2} - \sin\frac{\theta}{2}\cos\frac{\theta}{2} \end{aligned}$$

- 6. The probability is 100% since we prepared the system in the down u-direction to begin with.
- 7. Since the system is set up in the state down along \hat{u} , the probability to find it up along \hat{u} is zero.
- 8. Calculate the mean value $\langle \psi | S_z | \psi \rangle$ by two methods. First by using statistical analysis where the incident beam contains N silver atoms, and the direct calculation of the matrix element. How does this result compare with classical prediction?

$$\langle \psi | S_z | \psi \rangle = \frac{\hbar}{2} \left(-\sin \frac{\theta}{2} - \cos \frac{\theta}{2} \right) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} -\sin \frac{\theta}{2} \\ \cos \frac{\theta}{2} \end{pmatrix}$$
$$= \frac{\hbar}{2} \left(-\sin \frac{\theta}{2} - \cos \frac{\theta}{2} \right) \begin{pmatrix} -\sin \frac{\theta}{2} \\ -\cos \frac{\theta}{2} \end{pmatrix}$$
$$= \frac{\hbar}{2} \sin^2 \frac{\theta}{2} - \cos^2 \frac{\theta}{2}$$
$$= -\frac{\hbar}{2} \cos \theta$$

Consider a spin 1/2 particle placed in a magnetic field $\vec{B} = (B_x \quad 0 \quad B_z) = \frac{B_0}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 \end{pmatrix}$ in the orthonormal basis $\{|+\rangle, |-\rangle\}$ for S_z .

- 1. Calculate the matrix representing the Hamiltonian H of the system.
- 2. Calculate the eigenvalues and eigenvectors of H.
- 3. The system at time t = 0 is in the state $|-\rangle$. What values can be found if the energy is measured, and with what probabilities?
- 4. Calculate the state vector $|\psi(t)\rangle$ at time t. At this instant, S_x is measured; what is the mean value of the results that can be obtained? Give a geometrical interpretation of your results.

Solution

1. The Hamiltonian of a particle of spin 1/2 in a magnetic field is:

$$\begin{split} H &= -\vec{\mu} \cdot \vec{B} \\ \vec{\mu} &= \gamma \vec{S} \\ \Rightarrow H &= -\gamma \vec{S} \cdot \vec{B} \\ &= -\gamma (S_x B_x + S_y B_y + S_z B_z) \\ &= -\frac{\gamma B_0 \hbar}{2\sqrt{2}} \begin{bmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{bmatrix} \\ &= -\frac{\gamma B_0 \hbar}{2\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \end{split}$$

2. By the usual means, calculate eigenvalues then eigenvectors:

$$\begin{vmatrix} 1 - \lambda & 1 \\ 1 & -(1+\lambda) \end{vmatrix} = -(1+\lambda)(1-\lambda) - 1 = 0$$
$$= -(1-\lambda^2) - 1 = \lambda^2 - 2 = 0$$
$$\Rightarrow \lambda = \pm \sqrt{2}$$

So the eigenvalues of H are:

$$E_{\pm} = \mp \frac{\gamma B_0 \hbar}{2} = \pm \frac{\omega_0 \hbar}{2}$$

where ω_0 is the Larmor frequency.

Now plug in these values to calculate the eigenvectors.

$$\lambda = +\sqrt{2}$$

$$\begin{pmatrix} 1 - \sqrt{2} & 1\\ 1 & -(1 + \sqrt{2}) \end{pmatrix} \begin{pmatrix} c_1\\ c_2 \end{pmatrix} = \begin{pmatrix} 0\\ 0 \end{pmatrix}$$

$$\lambda = -\sqrt{2}$$

$$\begin{pmatrix} 1 + \sqrt{2} & 1\\ 1 & -\sqrt{2} - 1 \end{pmatrix} \begin{pmatrix} c_1\\ c_2 \end{pmatrix} = \begin{pmatrix} 0\\ 0 \end{pmatrix}$$

$$v_{+} = \begin{pmatrix} 1\\ \sqrt{2} - 1 \end{pmatrix}$$
$$v_{-} = \begin{pmatrix} 1\\ -\sqrt{2} - 1 \end{pmatrix}$$

3. At t=0 the system is in the $|-\rangle$ state, meaning v_{-} from the last step.

$$|\psi(0)\rangle = \begin{pmatrix} 0\\1 \end{pmatrix} = |-\rangle$$

To find the possible energies, we simply apply the Hamiltonian operator that was calculated in part 1.

$$H |\psi(0)\rangle = -\frac{\gamma B_0 \hbar}{2\sqrt{2}} \begin{pmatrix} 1 & 1\\ 1 & -1 \end{pmatrix} \begin{pmatrix} 0\\ 1 \end{pmatrix}$$
$$= -\frac{\gamma B_0 \hbar}{2\sqrt{2}} \begin{pmatrix} 1\\ -1 \end{pmatrix}$$
$$= -\frac{\gamma B_0 \hbar}{2\sqrt{2}} |+\rangle + \frac{\gamma B_0 \hbar}{2\sqrt{2}} |-\rangle$$
$$E_{\pm} = \mp \frac{\gamma B_0 \hbar}{2\sqrt{2}}$$

But since the system is in the $|-\rangle$ state, there is zero possibility of finding it to have $E=E_+$ and a 100% probability to find it to have energy $E=E_-$ state.

$$\begin{split} |\psi(t)\rangle &= -\frac{\gamma B_0 \hbar}{2\sqrt{2}} e^{-i\omega_0 t} \left| + \right\rangle + \frac{\gamma B_0 \hbar}{2\sqrt{2}} e^{i\omega_0 t} \left| - \right\rangle \\ &= -\frac{\gamma B_0 \hbar}{2\sqrt{2}} \begin{pmatrix} e^{-i\omega_0 t} \\ -e^{i\omega_0 t} \end{pmatrix} \\ \langle S_x \rangle &= \langle \psi(t) | S_x | \psi(t) \rangle \\ &= \left(\frac{\gamma B_0 \hbar}{2\sqrt{2}} \right)^2 \left(e^{i\omega_0 t} - e^{-i\omega_0 t} \right) \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} e^{-i\omega_0 t} \\ -e^{i\omega_0 t} \end{pmatrix} \\ &= \frac{\gamma^2 B_0^2 \hbar^3}{16} \left(e^{i\omega_0 t} - e^{-i\omega_0 t} \right) \begin{pmatrix} -e^{i\omega_0 t} \\ e^{-i\omega_0 t} \end{pmatrix} \\ &= -\frac{\gamma^2 B_0^2 \hbar^3}{8} \cos 2\omega_0 t \end{split}$$