Physics 916: Homework #5

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Problem 1

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:

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

$$a_0 &= \frac{1}{2} Tr \{M\sigma_0\} = \frac{1}{2} Tr \left[\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right] = Tr \left[\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \right] \\ &= \frac{1}{2} (M_{11} + M_{22}) = \frac{1}{2} (a_0 + a_3 + a_0 - a_3) \\ &= a_0 \end{split}$$

$$a_1 &= \frac{1}{2} Tr \{M\sigma_1\} = \frac{1}{2} Tr \left[\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right] = Tr \left[\begin{pmatrix} M_{12} & M_{11} \\ M_{22} & M_{21} \end{pmatrix} \right] \\ &= \frac{1}{2} (M_{12} + M_{21}) = \frac{1}{2} (a_1 - ia_2 + a_1 + ia_2) \\ &= a_1 \end{split}$$

$$a_2 &= \frac{1}{2} Tr \{M\sigma_2\} = \frac{1}{2} Tr \left[\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \right] = Tr \left[\begin{pmatrix} iM_{12} & -iM_{11} \\ iM_{22} & -iM_{21} \end{pmatrix} \right] \\ &= \frac{1}{2} (iM_{12} - iM_{21}) = \frac{1}{2} (ia_1 - i^2a_2 - ia_1 - i^2a_2) \\ &= a_2 \end{split}$$

$$a_3 &= \frac{1}{2} Tr \{M\sigma_3\} = \frac{1}{2} Tr \left[\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right] = Tr \left[\begin{pmatrix} M_{11} & -M_{12} \\ M_{21} & -M_{22} \end{pmatrix} \right] \\ &= \frac{1}{2} (M_{11} - M_{22}) = \frac{1}{2} (a_0 + a_3 - a_0 + a_3) \\ &= a_3 \end{split}$$

Problem 2

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.

Solution

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

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

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

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

$$= 0$$

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

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

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

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

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

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: $K_{12} = \frac{2}{H_{11} - H_{22}} H_{12}$

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

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

Problem 3

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.

$$S_{u} = \mathbf{S} \cdot \mathbf{u} = S_{x} u_{x} + S_{y} u_{y} + S_{z} u_{z}$$

$$= \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \sin \theta \cos \phi + \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \sin \theta \sin \phi + \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cos \theta$$

$$= \frac{\hbar}{2} \begin{pmatrix} \cos \theta & \sin \theta \cos \phi - i \sin \theta \sin \phi \\ \sin \theta \cos \phi + i \sin \theta \sin \phi & \cos \theta \end{pmatrix}$$

$$= \frac{\hbar}{2} \begin{pmatrix} \cos \theta & \sin \theta (\cos \phi - i \sin \phi) \\ \sin \theta (\cos \phi + i \sin \phi) & \cos \theta \end{pmatrix}$$

$$= \frac{\hbar}{2} \begin{pmatrix} \cos \theta & e^{-i\phi} \sin \theta \\ e^{i\phi} \sin \theta & \cos \theta \end{pmatrix}$$

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

$$\begin{split} 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}{2} \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_z S_x - S_x S_z &= \frac{\hbar^2}{4} \begin{pmatrix} 0 & 1 \\ 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_x, S_x] = i\hbar S_y \\ \Rightarrow [S_x, S_x] = i\hbar S_y \\ \end{cases}$$

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.