1 Pauli Matrices

\[
\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]  

(1.1)

1.1 Compute the commutators and anticommutators of the Pauli matrices.

We shall compute the commutators and anticommutators by first deducing a general formula for products of Pauli matrices. Note that each of the Pauli matrix squares to the \(2 \times 2\) identity matrix.

\[
\sigma_i^2 = 1
\]  

(1.2)

Secondly, multiplying two different Pauli matrices gives the third one up to a factor of \(\pm i\).

\[
\sigma_1 \sigma_2 = i \sigma_3 \\
\sigma_2 \sigma_3 = i \sigma_1 \\
\sigma_3 \sigma_1 = i \sigma_2 \\
\sigma_2 \sigma_1 = -i \sigma_3 \\
\sigma_3 \sigma_2 = -i \sigma_1 \\
\sigma_1 \sigma_3 = -i \sigma_2
\]  

(1.3)

Equivalently, for \(i \neq j\), we can write

\[
\sigma_i \sigma_j = i \epsilon_{ijk} \sigma_k
\]  

(1.4)

where \(\epsilon_{ijk}\) is the totally antisymmetric Levi-Civita symbol with \(\epsilon_{123} = +1\), and we are using the summation convention wherein any repeated index on one side of an equation is implicitly summed over. The above formula can be combined with the \(i = j\) case to obtain\(^1\)

\[
\sigma_i \sigma_j = 1 \delta_{ij} + i \epsilon_{ijk} \sigma_k
\]  

(1.5)

Next, we can use this to compute the general commutator

\[
[\sigma_i, \sigma_j] = \sigma_i \sigma_j - \sigma_j \sigma_i \\
= (1 \delta_{ij} + i \epsilon_{ijk} \sigma_k) - (1 \delta_{ji} + i \epsilon_{jik} \sigma_k)
\]  

(1.6)

Using the fact that \(\delta_{ij} = \delta_{ji}\) and \(\epsilon_{ijk} = -\epsilon_{jik}\), this can be simplified to

\[
[\sigma_i, \sigma_j] = 2i \epsilon_{ijk} \sigma_k
\]  

(1.7)

The anticommutator can be similarly evaluated to find

\[
\{\sigma_i, \sigma_j\} = \sigma_i \sigma_j + \sigma_j \sigma_i \\
= 1 \delta_{ij} + i \epsilon_{ijk} \sigma_k + 1 \delta_{ji} + i \epsilon_{jik} \sigma_k \\
= 21 \delta_{ij}
\]  

(1.8)

\(^1\)Note that the identity matrix \(I_2\) is often omitted from this formula to write \(\sigma_i \sigma_j = \delta_{ij} + i \epsilon_{ijk} \sigma_k\).
1.2 Which of the Pauli matrices are unitary and which ones are Hermitian?

From the matrix expressions above it is clear that all the Pauli matrices are Hermitian

\[ \sigma_i^\dagger = \sigma_i \]  

(1.9)

Furthermore, since we have already observed that the Pauli matrices square to the identity matrix, this implies that

\[ 1 = \sigma_i^2 = \sigma_i \sigma_i^\dagger \]  

(1.10)

(Note that there is no implicit sum here. The expression holds for every value of the index \(i\).) Hence, each of the Pauli matrices are also unitary.

1.3 Find the eigenvalues and eigenvectors of the Pauli matrices.

Since the Pauli matrices square to the identity matrix, their eigenvalues must square to 1. Hence, the eigenvalues of the Pauli matrices must be

\[ \lambda_{\pm}^i = \pm 1 \]  

(1.11)

Let us begin by working out the eigenvector for the first Pauli matrix corresponding to eigenvalue +1, the equation we need to solve is

\[
\begin{pmatrix}
0 & 1 \\
1 & 0
\end{pmatrix}
\begin{pmatrix}
a \\
b
\end{pmatrix} = +1
\begin{pmatrix}
a \\
b
\end{pmatrix}
\]  

(1.12)

where \(a, b\) are arbitrary complex numbers. This simplifies to a single equation

\[ b = a \]  

(1.13)

Hence any vector of the form

\[ a \begin{pmatrix} 1 \\ 1 \end{pmatrix} \]  

(1.14)

is an eigenvector. For convenience, we shall also choose to normalize the eigenvector and write

\[ |\lambda_+^1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \]  

(1.15)

Using this procedure, we can evaluate the rest of the eigenvectors, which turn out to be

\[ |\lambda_-^1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad |\lambda_-^2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}, \quad |\lambda_-^3\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}, \quad |\lambda_+^2\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\lambda_+^3\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \]  

(1.16)

1.4 Add the identity matrix \(\sigma_0 = 1\) to these three and show that any 2 \(\times\) 2 matrix can be written in the form

\[ M = \sum_{i=0}^{3} \alpha_i \sigma_i \]
for some complex $\alpha^i$. Under what conditions on $\alpha^i$ is $M$ unitary? Under what conditions is $M$ Hermitian?

Consider a general complex matrix

$$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$  \hspace{1cm} (1.17)$$

To demonstrate that this can be written as a linear combination of Pauli matrices above, we will simply solve for the $\alpha^i$ in terms of the components of the matrix. Expanding out the linear combination, we need to solve the equation

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} \alpha^0 + \alpha^3 \alpha^1 - i\alpha^2 \\ \alpha^1 + i\alpha^2 \alpha^0 - \alpha^3 \end{pmatrix}$$  \hspace{1cm} (1.18)$$

These equations can be straightforwardly solved to obtain

$$\begin{align*}
\alpha^0 &= (a + d)/2 \\
\alpha^3 &= (a - d)/2 \\
\alpha^1 &= (b + c)/2 \\
\alpha^2 &= i(b - c)/2
\end{align*}$$  \hspace{1cm} (1.19)$$

Since this solution clearly exists and is unique (being a solution to a system of linear equations with as many variables as equations), every complex matrix can be uniquely written as the above linear combination.

The Hermitian conjugate of $M$ is given by

$$M^\dagger = \sum_{i=0}^{3} \alpha^i \sigma_i$$  \hspace{1cm} (1.20)$$

since the Pauli matrices are Hermitian. For $M$ to be Hermitian, we need

$$\sum_{i=0}^{3} \alpha^i \sigma_i = \sum_{i=0}^{3} \alpha^i \sigma_i$$  \hspace{1cm} (1.21)$$

Since the expansion in terms of Pauli matrices is unique, this must imply

$$\alpha^i = \alpha^i$$  \hspace{1cm} (1.22)$$

i.e., the coefficients in the expansion must be real.

For $M$ to be unitary, we need instead

$$M^\dagger M = 1 \quad \text{and} \quad MM^\dagger = 1$$  \hspace{1cm} (1.23)$$

Expanding out the product, we find

$$M^\dagger M = (\alpha^0 \mathbf{1} + \alpha^i \sigma_i)(\alpha^0 \mathbf{1} + \alpha^j \sigma_j)$$  \hspace{1cm} (1.24)$$
where repeated indices are implicitly summed over from 1 to 3. Expanding out the product we find

\[ M^\dagger M = |\alpha^0|^2 \mathbf{1} + \alpha^0 \alpha^i \sigma_i + \alpha^0 \alpha^i \sigma_i \sigma_j + \alpha^i \sigma_i \sigma_j \]
\[ = |\alpha^0|^2 \mathbf{1} + (\alpha^0 \alpha^i + \alpha^0 \alpha^i \sigma_i + \alpha^i \sigma_i + i\epsilon_{ijk} \sigma_k) \]
\[ = \left( \sum_{i=0}^{3} |\alpha^i|^2 \right) \mathbf{1} + \left( \alpha^0 \alpha^k + \alpha^0 \alpha^k + i\epsilon_{ijk} \alpha^i \alpha^j \right) \sigma_k \quad (1.25) \]

Similarly for the other equation, we find

\[ M^\dagger M = \left( \sum_{i=0}^{3} |\alpha^i|^2 \right) \mathbf{1} + \left( \alpha^0 \alpha^k + \alpha^0 \alpha^k + i\epsilon_{ijk} \alpha^i \alpha^j \right) \sigma_k \quad (1.26) \]

The conditions required for the above expressions to evaluate to the identity matrix are then

\[ \sum_{i=0}^{3} |\alpha^i|^2 = 1 \]
\[ \left( \alpha^0 \alpha^k + \alpha^0 \alpha^k + i\epsilon_{ijk} \alpha^i \alpha^j \right) = 0 \quad \forall \ k = 1, 2, 3 \]
\[ \left( \alpha^0 \alpha^k + \alpha^0 \alpha^k + i\epsilon_{ijk} \alpha^i \alpha^j \right) = 0 \quad \forall \ k = 1, 2, 3 \quad (1.27) \]

The second and third equations above can be simplified further by writing

\[ \beta^k = \beta^{k*} = \alpha^0 \alpha^k + \alpha^0 \alpha^k \]
\[ \gamma^k = i\epsilon_{ijk} \alpha^i \alpha^j \]
\[ -\gamma^{k*} = i\epsilon_{ijk} \alpha^i \alpha^j \quad (1.28) \]

and observing that the equations reduce to

\[ \beta^k + \gamma^k = 0 \]
\[ \beta^k - \gamma^{k*} = 0 \quad (1.29) \]

Taking the conjugate of the second equation above and adding to and subtracting from the first results in

\[ \beta^k = 0, \quad \gamma^k = 0 \quad (1.30) \]

which, upon expanding out, reduce to

\[ \alpha^0 \alpha^k + \alpha^0 \alpha^k = 0 \]
\[ i\epsilon_{ijk} \alpha^i \alpha^j = 0 \quad (1.31) \]

Another way of obtaining conditions on the coefficients that would make \( M \) unitary is to directly compute its inverse and equate it to its Hermitian conjugate. The inverse of any \( 2 \times 2 \) matrix is given by the following formula

\[ \begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} \quad (1.32) \]
For the matrix $M$ in the Pauli matrix expansion, the determinant is given by

$$\det M = (\alpha^0 + \alpha^3)(\alpha^0 - \alpha^3) - (\alpha^1 + i\alpha^2)(\alpha^1 - i\alpha^2) = (\alpha^0)^2 - (\alpha^1)^2 - (\alpha^2)^2 - (\alpha^3)^2$$

(1.33)

So the inverse is

$$M^{-1} = \frac{1}{(\alpha^0)^2 - (\alpha^1)^2 - (\alpha^2)^2 - (\alpha^3)^2} \begin{pmatrix} \alpha^0 - \alpha^3 & -\alpha^1 + i\alpha^2 \\ -\alpha^1 - i\alpha^2 & \alpha^0 + \alpha^3 \end{pmatrix}$$

(1.34)

We now equate this to $M^\dagger$ to obtain the equation

$$\frac{1}{(\alpha^0)^2 - (\alpha^1)^2 - (\alpha^2)^2 - (\alpha^3)^2} \begin{pmatrix} \alpha^0 - \alpha^3 & -\alpha^1 + i\alpha^2 \\ -\alpha^1 - i\alpha^2 & \alpha^0 + \alpha^3 \end{pmatrix} \begin{pmatrix} \alpha^0* + \alpha^3* & \alpha^1* + i\alpha^2* \\ \alpha^1* - i\alpha^2* & \alpha^0* - \alpha^3* \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

(1.35)

The four equations obtained by equating the components of the above matrices are equivalent to the four equations that we obtained earlier by computing $M^\dagger M$.

2 Take an orthonormal basis $\{|0\rangle, |1\rangle\}$ for a two-dimensional Hilbert space. With respect to this basis, we have three operators that correspond to the Pauli matrices. Assume that this basis is an eigenbasis for $\sigma_3$ with eigenvalues $+1, -1$ respectively. Write each of these Pauli matrices in “ket-bra” notation.

To begin with, consider a general matrix $M$ with components $M_{ij}$ corresponding to an operator $\hat{M}$ in an ordered orthonormal basis $\{|i\rangle\}$. The components of the matrix can be written in terms of the operator in the following manner

$$M_{ij} = \langle i | \hat{M} | j \rangle$$

(2.1)

Since this basis is orthonormal, the above expression implies an expansion for the operator given by

$$\hat{M} = \sum_{i,j} M_{ij} |i\rangle \langle j|$$

(2.2)

We can use this expansion to write the operators $\hat{\sigma}_i$ corresponding to each Pauli matrix in ket-bra notation. First, we need to figure out which matrix elements correspond to which basis vector. For this, observe that the $(1, 1)$ component of $\sigma_3$ is $+1$, which is the eigenvalue for $|0\rangle$, while the $(2, 2)$ component is $-1$, the eigenvalue for $|1\rangle$. Hence $|0\rangle$ corresponds to the matrix index 1 and $|1\rangle$ corresponds to the index 2. The operators corresponding to the Pauli matrices will have the following expansion determined by their components

$$\hat{\sigma}_1 = (\sigma_1)_{11} |0\rangle \langle 0| + (\sigma_1)_{12} |0\rangle \langle 1| + (\sigma_1)_{21} |1\rangle \langle 0| + (\sigma_1)_{22} |1\rangle \langle 1|$$

(2.3)

More explicitly, we have

$$\hat{\sigma}_1 = |0\rangle \langle 1| + |1\rangle \langle 0|$$

$$\hat{\sigma}_2 = -i |0\rangle \langle 1| + i |1\rangle \langle 0|$$

$$\hat{\sigma}_3 = |0\rangle \langle 0| - |0\rangle \langle 0|$$

(2.4)
3 Matrix/Operator Exponentiation

3.1 What is the Taylor series definition of $e^x$?

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} = 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \cdots$$  \hspace{1cm} (3.1)

3.2 Take the generator of rotations in two dimensions given by

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

The operator $1 + \epsilon T$ generates an infinitesimal rotation of the vector $(x, y)^T$ by angle $\epsilon$. To get a finite rotation, we will want to exponentiate the matrix using the Taylor series definition. Evaluate $e^{\theta T}$ using the Taylor series definition above.

The Taylor series definition for the exponent gives

$$e^{\theta T} = \sum_{n=0}^{\infty} \frac{\theta^n}{n!} T^n$$  \hspace{1cm} (3.2)

where $T^n = T \cdot T \cdots T$ is a product of $n$ copies of the matrix $T$. In order to evaluate this series, first observe that $T$ is proportional to a Pauli matrix

$$T = i\sigma_2$$  \hspace{1cm} (3.3)

and hence

$$T^2 = -1$$  \hspace{1cm} (3.4)

The third power is then

$$T^3 = -T$$  \hspace{1cm} (3.5)

while the fourth power is

$$T^4 = -T^2 = 1$$  \hspace{1cm} (3.6)

The terms in the exponential series hence split up into two different series, one proportional to 1 and the other proportional to $T$. Explicitly, we have

$$e^{\theta T} = \left(1 - \frac{\theta^2}{2!} + \frac{\theta^4}{4!} - \cdots \right) 1 + \left(\theta - \frac{\theta^3}{3!} + \frac{\theta^5}{5!} - \cdots \right) T$$  \hspace{1cm} (3.7)

The two series in parenthesis are now familiar - they are simply the series definitions for cosine and sine respectively. Hence, we have

$$e^{\theta T} = \cos \theta 1 + \sin \theta T = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix}$$  \hspace{1cm} (3.8)