Física Quântica I / Mecânica Quântica (2021/22)

Folha de Problemas 1 (prática com matrizes)

Vitor M. Pereira | Universidade do Minho | 19-Feb-2022

— Soluções —

Nota: O primeiro problema será discutido na aula teórico-prática. Os restantes são exercícios suplementares que pretendem familiarizar e praticar outros aspetos de álgebra linear que serão relevantes no decorrer desta unidade curricular.

Problema 1* | Valores e vetores próprios

Considere a matriz seguinte, expressa numa base 3-dimensional, ortogonal e normalizada definida pelos vetores unitários $\{|u_1\rangle, |u_2\rangle, |u_3\rangle\}$:

$$H = \begin{bmatrix} 0 & 0 & i \\ 0 & 1 & 0 \\ -i & 0 & 0 \end{bmatrix}.$$

1. A matriz H é Hermítica? Justifique.

2. Calcule os valores próprios (ou autovalores) e designe-os por E_1, E_2 e E_3.

3. Para cada valor próprio, determine os vetores próprios (autovetores) correspondentes e designe-os $|E_1\rangle$, $|E_2\rangle$, $|E_3\rangle$, respetivamente. Apresente o resultado de modo que o conjunto de vetores $\{|E_1\rangle, |E_2\rangle, |E_3\rangle\}$ seja ortogonal e normalizado à unidade.

4. Considere o seguinte vetor normalizado $|\psi\rangle$ expresso na base $\{|u_i\rangle\}$:

$$|\psi\rangle = \frac{1}{\sqrt{2}}|u_1\rangle + \frac{1}{\sqrt{2}}|u_2\rangle \qquad \text{ou, alternativamente,} \qquad |\psi\rangle \mapsto \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \quad (\text{base } \{|u_i\rangle\}).$$

   Escreva este vetor na base própria de H. Ou seja, determine as constantes χ_1, χ_2 e χ_3 tais que

$$|\psi\rangle = \chi_1|E_1\rangle + \chi_2|E_2\rangle + \chi_3|E_3\rangle, \qquad \text{ou} \qquad |\psi\rangle \mapsto \begin{bmatrix} \chi_1 \\ \chi_2 \\ \chi_3 \end{bmatrix} \quad (\text{base } \{|E_i\rangle\}),$$

   onde $|E_i\rangle$ são os vetores próprios *normalizados* de H obtidos na questão anterior.

5. Mostre que as componentes χ_i obtidas na questão anterior deixam o vetor $|\psi\rangle$ automaticamente normalizado à unidade na nova base $\{|E_i\rangle\}$.

Solution

1. H is an Hermitian matrix because we can see directly that

$$H^\dagger \stackrel{\text{by definition}}{=} \left(H^\top\right)^* = \begin{bmatrix} 0 & 0 & (-i)^* \\ 0 & 1 & 0 \\ i^* & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & i \\ 0 & 1 & 0 \\ -i & 0 & 0 \end{bmatrix} = H.$$

Hence it is Hermitian.

2. The characteristic equation for H can be written as

$$\det(\hat{H} - \lambda\mathbf{1}) = 0 \quad \Leftrightarrow \quad \begin{vmatrix} -\lambda & 0 & i \\ 0 & 1-\lambda & 0 \\ -i & 0 & -\lambda \end{vmatrix} = 0 \quad \Leftrightarrow \quad (1-\lambda)\left(\lambda^2 - 1\right) = 0.$$

The eigenvalues, which are the roots of the characteristic equation, are

$$E_1 = -1, \qquad E_2 = 1, \qquad E_3 = 1.$$

Note that the eigenvalue 1 appears twice (we say it has a “degeneracy of 2” or that it is “doubly degenerate”), because 1 is a double root of the characteristic equation.

3. **Non-degenerate eigenvalue**. Let us start first with the non-degenerate one, $E_1 = -1$, and let’s write the corresponding column representing the associated eigenvector as

$$|E_1\rangle \mapsto \begin{bmatrix} u \\ v \\ w \end{bmatrix},$$

where u, v, w are unknowns, of course, which we determine by replacing the value $\lambda = E_1 = -1$ in the eigenvalue equation:

$$(H - E_1\mathbf{1}) \begin{bmatrix} u \\ v \\ w \end{bmatrix} = 0 \xrightarrow{E_1=-1} \begin{bmatrix} 1 & 0 & i \\ 0 & 2 & 0 \\ -i & 0 & 1 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix} = 0 \quad \Leftrightarrow \quad |E_1\rangle \mapsto \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ i \end{bmatrix}.$$

In the last step, I present already the normalized version of the eigenvector $|E_1\rangle$.

Degenerate eigenvalue. The procedure for the other (degenerate) eigenvalue is entirely the same at first:

$$(H - E_n\mathbf{1}) \begin{bmatrix} u \\ v \\ w \end{bmatrix} = 0 \xrightarrow{E_n=+1} \begin{bmatrix} -1 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & -1 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix} = 0 \quad \Leftrightarrow \quad \begin{cases} u = iw \\ \text{any } v \end{cases} \tag{1.1}$$

(note that, indeed, any choice we make for v solves this set of equations). Since v can have any value whatsoever, there is actually an infinite number of solutions at this stage because any vector of the form

$$\begin{bmatrix} iw \\ v \\ w \end{bmatrix}, \qquad \forall\, v, w \in \mathbb{C} \tag{1.2}$$

is an eigenvector of H associated with the eigenvalue $+1$ (this is recurrent every time we are dealing with a degenerate eigenvalue because the eigenvectors associated with a d-degenerate eigenvalue always span a subspace of dimension d). However, since the question asks for a set of *orthogonal* eigenvectors, of the infinite possibilities represented in the solution (1.2) we must *select* two that are orthogonal to each other (we don't have to worry about them being orthogonal also to $|E_1\rangle$, because that is guaranteed by the fact that the matrix is Hermitian *and* $|E_1\rangle$ belongs to a different eigenvalue).

For the first one, let us stick to the simplest possible choice: $v = 0$, in which case the *normalized* eigenvector becomes

$$|E_2\rangle \mapsto \frac{1}{\sqrt{2}} \begin{bmatrix} i \\ 0 \\ 1 \end{bmatrix}.$$

For the second one, we must pick a vector that is still of the form (1.2), but which should be orthogonal to $|E_2\rangle$. In other words we want to find v and w such that

$$\langle E_2|E_3\rangle = \begin{bmatrix} -i & 0 & 1 \end{bmatrix} \begin{bmatrix} iw \\ v \\ w \end{bmatrix} = 0 \qquad \Rightarrow \qquad w = 0, \qquad \forall v.$$

Hence, the normalized eigenvector is

$$|E_3\rangle \mapsto \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}.$$

In summary, one set of orthogonal and normalized eigenvectors of H is thus

$$|E_1\rangle \mapsto \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ i \end{bmatrix}, \qquad |E_2\rangle \mapsto \frac{1}{\sqrt{2}} \begin{bmatrix} i \\ 0 \\ 1 \end{bmatrix}, \qquad |E_3\rangle \mapsto \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}.$$

You can verify explicitly (by substitution, for example) that these satisfy all the requirements: (i) $|E_1\rangle$ is an eigenvector of H associated with eigenvalue $E_1 = -1$, and $|E_2\rangle$, $|E_3\rangle$ are eigenvectors associated with the eigenvalues $E_2 = E_3 = +1$; (ii) all three are mutually orthogonal; (iii) all three are normalized.

4. What's needed here is to write the vector $|\psi\rangle$ in the new basis defined by the three orthonormal eigenvectors of H determined in the previous question. One direct approach is to realize that we can express the vector in question in either basis as

$$|\psi\rangle = \psi_1|u_1\rangle + \psi_2|u_2\rangle + \psi_3|u_3\rangle, \qquad \text{or} \qquad |\psi\rangle = \chi_1|E_1\rangle + \chi_2|E_2\rangle + \chi_3|E_3\rangle$$

Since what we need are the coefficients χ_n, we can readily obtain them by extracting the projection of $|\psi\rangle$ along the three normalized vectors $|E_n\rangle$:

$$\langle E_1|\psi\rangle = \chi_1 \cancelto{1}{\langle E_1|E_1\rangle} + \chi_2 \cancelto{0}{\langle E_1|E_2\rangle} + \chi_3 \cancelto{0}{\langle E_1|E_3\rangle} = \chi_1,$$

where the cancellations occur **because** the three $|E_n\rangle$ that we obtained in the previous question are mutually orthogonal and normalized. Therefore,

$$\chi_1 = \langle E_1|\psi\rangle = \frac{1}{2} \begin{bmatrix} 1 & 0 & -i \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} = \frac{1}{2}.$$

Proceeding analogously to get χ_2 and χ_3 we finally find

$$|\psi\rangle = \frac{1}{2}|E_1\rangle - \frac{i}{2}|E_2\rangle + \frac{1}{\sqrt{2}}|E_3\rangle, \qquad \text{or} \qquad |\psi\rangle \mapsto \begin{bmatrix} \frac{1}{2} \\ \frac{-i}{2} \\ \frac{1}{\sqrt{2}} \end{bmatrix}_{\{|E_i\rangle\}} . \tag{1.3}$$

Note 1: You might have obtained a different result if your choice for the two vectors, $|E_2\rangle$ and $|E_3\rangle$, within the degenerate subspace was different from the one done in the previous question above.

Note 2: The notation used in the previous expression where $|E_i\rangle$ appears in subscript,

$$\begin{bmatrix} \cdot \\ \cdot \\ \cdot \end{bmatrix}_{\{|E_i\rangle\}}$$

indicates that the column represents the components of vector $|\psi\rangle$ in the orthonormal basis defined by the vectors $\{|E_1\rangle, |E_2\rangle, |E_3\rangle\}$.

Note: An equivalent approach to this problem is to recall that the two representations are related by a unitary transformation matrix U

$$\begin{bmatrix} \chi_1 \\ \chi_2 \\ \chi_3 \end{bmatrix}_{\{|E_n\rangle\}} = U \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix}_{\{|u_n\rangle\}} ,$$

where, **if** (and only if) the eigenvectors are orthogonal and normalized, $U^\dagger$ is built by placing the eigenvectors of H along each column, i.e.,

$$U^\dagger = \begin{bmatrix} |E_1\rangle & |E_3\rangle & |E_3\rangle \\ \downarrow & \downarrow & \downarrow \\ \downarrow & \downarrow & \downarrow \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{bmatrix} \quad \Rightarrow \quad U = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{-i}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \end{bmatrix}.$$

Therefore,

$$\begin{bmatrix} \chi_1 \\ \chi_2 \\ \chi_3 \end{bmatrix}_{\{|E_n\rangle\}} = U \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix}_{\{|u_n\rangle\}} = U \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{-i}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \\ \frac{-i}{2} \\ \frac{1}{\sqrt{2}} \end{bmatrix}_{\{|E_n\rangle\}}$$

which, of course, is the same obtained in Eq. (1.3).

5. The vector will be normalized if its squared-modulus is 1, which means that the inner product of the vector with itself will be $\langle\psi|\psi\rangle = 1$. Since the basis $\{|E_i\rangle\}$ is orthogonal and normalized, the inner product can be directly computed by multiplying the row and column representation of $|\psi\rangle$ in this basis:

$$\langle\psi|\psi\rangle = \begin{bmatrix} \chi_1^* & \chi_2^* & \chi_3^* \end{bmatrix} \begin{bmatrix} \chi_1 \\ \chi_2 \\ \chi_3 \end{bmatrix} = |\chi_1|^2 + |\chi_2|^2 + |\chi_3|^2$$

Replacing here the values found in the previous question,

$$|\chi_1|^2 + |\chi_2|^2 + |\chi_3|^2 = \left|\frac{1}{2}\right|^2 + \left|\frac{-i}{2}\right|^2 + \left|\frac{1}{\sqrt{2}}\right|^2 = \frac{1}{4} + \frac{1}{4} + \frac{1}{2} = 1.$$

Note: This result is not accidental because of two details: (i) the vector $|\psi\rangle$ was *already* normalized the original basis $\{|u_i\rangle\}$; (ii) when we determined the components χ_i of $|\psi\rangle$ in the new basis $\{|E_i\rangle\}$, we were careful to use *normalized* $|E_i\rangle$ as basis vectors. The result we found here is completely general: the norm of any vector is preserved (doesn't change) in a change of basis, *provided* the new basis is orthonormal. This is equivalent to saying that *any basis change described by a* ***unitary*** *transformation matrix (the matrix U of the previous question) preserves the norm of vectors*.

Problema 2

Considere a matriz

$$H = \begin{bmatrix} \frac{1+i\sqrt{3}}{4} & \frac{\sqrt{3}(1+i)}{2\sqrt{2}} \\ -\frac{\sqrt{3}(1-i)}{2\sqrt{2}} & \frac{1-i\sqrt{3}}{4} \end{bmatrix}.$$

É uma matriz simétrica, Hermítica, ortogonal, unitária, ou nenhuma destas opções?

Solution

It is clearly not symmetric, nor Hermitian because the diagonal elements are not real. For it to be unitary it must hold that $HH^\dagger = I$. We explicitly calculate this:

$$HH^\dagger = \begin{bmatrix} \frac{1+i\sqrt{3}}{4} & \frac{\sqrt{3}(1+i)}{2\sqrt{2}} \\ -\frac{\sqrt{3}(1-i)}{2\sqrt{2}} & \frac{1-i\sqrt{3}}{4} \end{bmatrix} \begin{bmatrix} \frac{1-i\sqrt{3}}{4} & -\frac{\sqrt{3}(1+i)}{2\sqrt{2}} \\ \frac{\sqrt{3}(1-i)}{2\sqrt{2}} & \frac{1+i\sqrt{3}}{4} \end{bmatrix} = \begin{bmatrix} \left(\frac{1}{4}+\frac{6}{8}\right) & 0 \\ 0 & \left(\frac{6}{8}+\frac{1}{4}\right) \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Since $HH^\dagger = I$ the matrix is unitary.

Problema 3 | Prática com matrizes de Pauli (I)

Considere as três matrizes de Pauli seguintes e ainda a matriz identidade (I), com dimensões 2×2:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

[*Nota: a notação σ_1, σ_2, σ_3 é frequentemente substituída por σ_x, σ_y, σ_z, respetivamente; é também comum encontrar os símbolos τ em vez de σ para as representar.*]

1. Através de cálculo explícito dos produtos relevantes, mostre que o produto de qualquer par destas matrizes se pode escrever de modo compacto como

$$\sigma_\alpha \sigma_\beta = i \sum_{\gamma=1}^{3} \epsilon_{\alpha\beta\gamma} \sigma_\gamma + \delta_{\alpha\beta} I, \qquad \text{where } \alpha, \beta = 1, 2, 3, \tag{3.1}$$

onde $\delta_{\alpha\beta}$ e $\epsilon_{\alpha\beta\gamma}$ representam o *delta de Kronecker delta* e o *símbolo de Levi-Civita*, respetivamente definidos como

$$\delta_{\alpha\beta} = \begin{cases} 1, & \alpha = \beta \\ 0, & \alpha \neq \beta \end{cases}, \qquad \epsilon_{\alpha\beta\gamma} = \begin{cases} 1, & \alpha\beta\gamma = 123,\ 231,\ 312 \\ -1, & \alpha\beta\gamma = 213,\ 132,\ 321 \\ 0, & \text{restantes casos} \end{cases}.$$

2. Mostre que, dado um par de matrizes de Pauli σ_α e σ_β, o seu comutador e anti-comutador se podem escrever, respetivamente, como:

$$[\sigma_\alpha, \sigma_\beta] \overset{\text{def.}}{=} \sigma_\alpha\sigma_\beta - \sigma_\beta\sigma_\alpha = 2i \sum_{\gamma=1}^{3} \epsilon_{\alpha\beta\gamma}\sigma_\gamma, \quad \text{e} \quad \{\sigma_\alpha, \sigma_\beta\} \overset{\text{def.}}{=} \sigma_\alpha\sigma_\beta - \sigma_\beta\sigma_\alpha = 2\delta_{\alpha\beta} I.$$

3. Quando é que duas matrizes de Pauli comutam entre si? E quando anti-comutam?

4. Designemos os dois vetores próprios normalizados da matriz σ_α por $|+\rangle_\alpha$, $|-\rangle_\alpha$. Por exemplo, para σ_3 temos os seguintes vetores próprios

$$|+\rangle_3 \mapsto \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \qquad |-\rangle_3 \mapsto \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \tag{3.2}$$

Calcule os vetores próprios normalizados de σ_1 e σ_2.

Solution

1. Let's calculate those products. First, when $\alpha = \beta$, we can easily show that

$$\sigma_\alpha^2 = \sigma_\beta^2 = \sigma_\gamma^2 = I,$$

hence

$$\sigma_\alpha \sigma_\alpha = I.$$

Now the other ones:

$$\sigma_1\sigma_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = i\sigma_3$$

$$\sigma_2\sigma_1 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = -\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = -i\sigma_3$$

$$\sigma_1\sigma_3 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = -i\sigma_2$$

$$\sigma_3\sigma_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = -\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = i\sigma_2$$

$$\sigma_2\sigma_3 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} = i\sigma_1$$

$$\sigma_3\sigma_2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = -\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} = -i\sigma_1$$

and thus we conclude that the product of any two different matrices i and j can be cast as the third one multiplied by $\pm i$, depending on the cyclic sequence of the three indexes. That is captured by the Levi-Civita symbol $\epsilon_{\alpha\beta\gamma}$:

$$\sigma_\alpha\sigma_\beta = i\sum_{\gamma=1}^{3} \epsilon_{\alpha\beta\gamma}\sigma_\gamma \qquad (\alpha \neq \beta).$$

This is because

$$\sum_{\gamma=1}^{3} \epsilon_{\alpha\beta\gamma}\sigma_\gamma = \epsilon_{\alpha\beta 1}\sigma_1 + \epsilon_{\alpha\beta 2}\sigma_2 + \epsilon_{\alpha\beta 3}\sigma_3$$

and, if $\alpha \neq \beta$, only one of the 3 terms in this sum survives, which is precisely the one multiplying the σ_i for which i is different from both α and β (because this is the only term where all the indices appearing in $\epsilon_{\alpha\beta\gamma}$ are different, which is a prerequisite for it to be nonzero).

Combining the two cases derived above for $\alpha = \beta$ and $\alpha \neq \beta$ we see that all possibilities can be summarized compactly as

$$\sigma_\alpha\sigma_\beta = i\sum_{\gamma=1}^{3} \epsilon_{\alpha\beta\gamma}\sigma_\gamma + \delta_{\alpha\beta} I.$$

2. From the explicit products calculated in the first question we know that, for example,

$$\sigma_1\sigma_2 = i\sigma_3 \qquad \text{and} \qquad \sigma_2\sigma_1 = -i\sigma_3,$$

and hence

$$[\sigma_1, \sigma_2] = 2i\sigma_3 \qquad \text{and} \qquad \{\sigma_1, \sigma_2\} = 0.$$

The same can be done for all the other pairs by explicitly inspection, and afterwards compactly cast in the form requested in terms of the Kronecker and Levi-Civita symbols.

An alternative approach is to, instead of this explicit inspection, use the compact result derived in the first question:

$$\sigma_\alpha \sigma_\beta = i \sum_\gamma \epsilon_{\alpha\beta\gamma}\sigma_\gamma + \delta_{\alpha\beta} I.$$

Replacing this into $[\sigma_\alpha, \sigma_\beta]$ we obtain

$$\begin{aligned}[\sigma_\alpha, \sigma_\beta] &\overset{\text{def.}}{=} \sigma_\alpha\sigma_\beta - \sigma_\beta\sigma_\alpha = i\sum_\gamma \epsilon_{\alpha\beta\gamma}\sigma_\gamma + \delta_{\alpha\beta} I - \left(i \sum_\gamma \epsilon_{\beta\alpha\gamma}\sigma_\gamma + \delta_{\beta\alpha} I \right) \\ &= i\sum_\gamma \left(\epsilon_{\alpha\beta\gamma} - \epsilon_{\beta\alpha\gamma}\right)\sigma_\gamma = i\sum_\gamma \left(\epsilon_{\alpha\beta\gamma} + \epsilon_{\alpha\beta\gamma}\right)\sigma_\gamma = 2i\sum_\gamma \epsilon_{\alpha\beta\gamma}\sigma_\gamma,\end{aligned}$$

where we used the fact that $\delta_{\alpha\beta} = \delta_{\beta\alpha}$ and $\epsilon_{\alpha\beta\gamma} = -\epsilon_{\beta\alpha\gamma}$, according to their respective definitions. In a similar way, we also get

$$\begin{aligned}\{\sigma_\alpha, \sigma_\beta\} &\overset{\text{def.}}{=} \sigma_\alpha\sigma_\beta + \sigma_\beta\sigma_\alpha \\ &= i\sum_\gamma \epsilon_{\alpha\beta\gamma}\sigma_\gamma + \delta_{\alpha\beta} I + i\sum_\gamma \epsilon_{\beta\alpha\gamma}\sigma_\gamma + \delta_{\beta\alpha} I \\ &= i\sum_\gamma \left(\epsilon_{\alpha\beta\gamma} + \epsilon_{\beta\alpha\gamma}\right)\sigma_\gamma + \left(\delta_{\alpha\beta} + \delta_{\beta\alpha}\right) I \\ &= i\sum_\gamma \left(\epsilon_{\alpha\beta\gamma} - \epsilon_{\alpha\beta\gamma}\right)\sigma_\gamma + \left(\delta_{\alpha\beta} + \delta_{\alpha\beta}\right) I \\ &= 2\delta_{\alpha\beta} I.\end{aligned}$$

3. Since $[\sigma_\alpha, \sigma_\beta] \neq 0$ when $\alpha \neq \beta$, *different* Pauli matrices *do not commute*. On the other hand, $\{\sigma_\alpha, \sigma_\beta\} = 0$ for any pair $\alpha \neq \beta$, and thus any pair of *different* Pauli matrices *anti-commutes*.

4. If we denote the eigenvalues by λ, for σ_1 we have that

$$\det\left(\sigma_1 - \lambda I\right) = 0 \quad \Leftrightarrow \quad \begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda \end{vmatrix} = 0 \quad \Leftrightarrow \quad \lambda^2 = 1 \quad \Leftrightarrow \quad \lambda = \pm 1.$$

The corresponding eigenvectors of σ_1 will be columns of the form

$$|+\rangle_1 \to \begin{bmatrix} u \\ v \end{bmatrix}, \qquad |-\rangle_1 \to \begin{bmatrix} w \\ z \end{bmatrix}$$

which we can write compactly as

$$|\lambda\rangle_1 \to \begin{bmatrix} u_\lambda \\ v_\lambda \end{bmatrix}, \qquad \text{where } \lambda = \pm 1.$$

We obtain u_λ, v_λ directly from the definition of eigenvector:

$$(\sigma_1 - \lambda)\,|\lambda\rangle_1 = 0 \quad \Leftrightarrow \quad \begin{bmatrix} -\lambda & 1 \\ 1 & -\lambda \end{bmatrix} \begin{bmatrix} u_\lambda \\ v_\lambda \end{bmatrix} = 0 \quad \Leftrightarrow \quad \begin{cases} -\lambda u_\lambda + v_\lambda & = 0 \\ u_\lambda - \lambda v_\lambda & = 0 \end{cases}$$

These two equations yield the condition

$$u_\lambda = \lambda v_\lambda,$$

and one possible solution is then to choose $v_\lambda = A$ and $u_\lambda = \lambda A$, or

$$|\lambda\rangle_1 \to A \begin{bmatrix} \lambda \\ 1 \end{bmatrix},$$

where A is a free parameter (i.e., $\forall A \in \mathbb{Z}$, the $|\lambda\rangle_1$ above is an eigenvector of σ_1 belonging to the eigenvalue λ). But since we want the *normalized* eigenvectors, the value of A cannot be completely arbitrary, because we must have

$$\langle\lambda|\lambda\rangle = 1 \quad \Leftrightarrow \quad 1 = |A|^2 \begin{bmatrix} \lambda & 1 \end{bmatrix} \begin{bmatrix} \lambda \\ 1 \end{bmatrix} \quad \Leftrightarrow \quad 1 = |A|^2 \left(\lambda^2 + 1\right).$$

But since the eigenvalues are $\lambda = \pm 1$, it follows that A can be chosen as

$$A = \frac{1}{\sqrt{2}},$$

and the complete, normalized eigenvectors read

$$|+\rangle_1 \to \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}}|+\rangle_3 + \frac{1}{\sqrt{2}}|-\rangle_3,$$

$$|-\rangle_1 \to \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \frac{1}{\sqrt{2}}|+\rangle_3 - \frac{1}{\sqrt{2}}|-\rangle_3.$$

Now for σ_2, proceeding exactly as above:

$$\det\left(\sigma_2 - \lambda I\right) = 0 \quad \Leftrightarrow \quad \begin{vmatrix} -\lambda & -i \\ i & -\lambda \end{vmatrix} = 0 \quad \Leftrightarrow \quad \lambda^2 = 1 \quad \Leftrightarrow \quad \lambda = \pm 1.$$

The corresponding eigenvectors will be again denoted

$$|\lambda\rangle_2 \to \begin{bmatrix} u_\lambda \\ v_\lambda \end{bmatrix},$$

and the definition of eigenvector requires that

$$\sigma_2|\lambda\rangle_2 = \lambda|\lambda\rangle_2 \quad \Leftrightarrow \quad \begin{cases} -\lambda u_\lambda - i v_\lambda & = 0 \\ i u_\lambda - \lambda v_\lambda & = 0 \end{cases} \quad \Leftrightarrow \quad u_\lambda = -i\lambda v_\lambda.$$

One possible choice is then

$$|\lambda\rangle_1 \to A \begin{bmatrix} -i\lambda \\ 1 \end{bmatrix}.$$

But since the constant A is (again) arbitrary, we can also write this as

$$|\lambda\rangle_2 \to A \begin{bmatrix} -i\lambda \\ 1 \end{bmatrix} = A\left(-i\lambda\right) \begin{bmatrix} 1 \\ i\lambda \end{bmatrix} = B \begin{bmatrix} 1 \\ i\lambda \end{bmatrix}.$$

(this last step is not that important, and is done here only to obtain the eigenvectors of σ_2 in a form visually similar to the ones of σ_1). The normalization constant B is obtained from

$$\langle\lambda|\lambda\rangle = 1 \quad \Leftrightarrow \quad 1 = |B|^2 \begin{bmatrix} 1 & -i\lambda \end{bmatrix} \begin{bmatrix} 1 \\ i\lambda \end{bmatrix} \quad \Leftrightarrow \quad 1 = |B|^2 \left(1 + \lambda^2\right),$$

and thus

$$B = \frac{1}{\sqrt{2}}.$$

The complete, normalized eigenvectors are then

$$|+\rangle_2 \to \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} = \frac{1}{\sqrt{2}}|+\rangle_3 + \frac{i}{\sqrt{2}}|-\rangle_3,$$

$$|-\rangle_2 \to \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix} = \frac{1}{\sqrt{2}}|+\rangle_3 - \frac{i}{\sqrt{2}}|-\rangle_3.$$

Problema 4 | Prática com matrizes de Pauli (II)

Para trabalhar problemas relacionados com spin 1/2 (que consideraremos em breve) é útil introduzir um "vetor" de matrizes de Pauli, definido como a seguinte combinação linear

$$\boldsymbol{\sigma} \equiv \sigma_x \boldsymbol{u}_x + \sigma_y \boldsymbol{u}_y + \sigma_z \boldsymbol{u}_z,$$

onde $\sigma_{x,y,z}$ são as três matrizes definidas no Problema anterior e $\boldsymbol{u}_i$ são vetores unitários paralelos aos três eixos Cartesianos. Dado um vetor arbitrário $\boldsymbol{n} = n_x \boldsymbol{u}_x + n_y \boldsymbol{u}_y + n_z \boldsymbol{u}_z$ no espaço Cartesiano (n_i são números), mas normalizado segundo $\boldsymbol{n}.\boldsymbol{n} = 1$, é possível gerar uma matriz de Pauli (2×2) mais geral através do produto interno

$$\boldsymbol{n} \cdot \boldsymbol{\sigma} = n_x \sigma_x + n_y \sigma_y + n_z \sigma_z.$$

1. Partindo desta última definição de $\boldsymbol{n} \cdot \boldsymbol{\sigma}$, mostre que

   $$(\boldsymbol{n} \cdot \boldsymbol{\sigma})^{2p} = I, \qquad \text{e que} \qquad (\boldsymbol{n} \cdot \boldsymbol{\sigma})^{2p+1} = \boldsymbol{n} \cdot \boldsymbol{\sigma}, \qquad (p \in \mathbb{N}).$$

   (*sugestão: apenas precisa de calcular* $(\boldsymbol{n} \cdot \boldsymbol{\sigma})^2$ *para provar ambos* os resultados.)

2. Usando estas duas identidades, mostre que

   $$e^{i\gamma \boldsymbol{n} \cdot \boldsymbol{\sigma}} = I \cos\gamma + i\,(\boldsymbol{n} \cdot \boldsymbol{\sigma}) \sin\gamma.$$

   (*sugestão: relembre a expansão de Taylor relativa a cada uma das funções que aqui aparecem.*)

3. Calcule os autovalores da matriz $\boldsymbol{n} \cdot \boldsymbol{\sigma}$.

4. Expressando o vetor unitário $\boldsymbol{n}$ em termos do seu ângulo polar e azimutal,

   $$\boldsymbol{n} = \sin\theta \cos\phi\, \boldsymbol{u}_x + \sin\theta \sin\phi\, \boldsymbol{u}_y + \cos\theta\, \boldsymbol{u}_z,$$

   calcule os autovetores normalizados de $\boldsymbol{n} \cdot \boldsymbol{\sigma}$, e mostre que os podemos escrever como:

   $$|+\rangle_{\boldsymbol{n}} \mapsto \begin{bmatrix} \cos\frac{\theta}{2} e^{-i\phi/2} \\ \\ \sin\frac{\theta}{2} e^{i\phi/2} \end{bmatrix}, \qquad |-\rangle_{\boldsymbol{n}} \mapsto \begin{bmatrix} -\sin\frac{\theta}{2} e^{-i\phi/2} \\ \\ \cos\frac{\theta}{2} e^{i\phi/2} \end{bmatrix}.$$

Solution

1. Let us first calculate $(\boldsymbol{n} \cdot \boldsymbol{\sigma})^2$, keeping in mind that, since $\boldsymbol{n}$ is a unit vector, it means that $n_x^2 + n_y^2 + n_z^2 = 1$.

   One possible solution strategy is to explicitly take the matrix $\boldsymbol{n} \cdot \boldsymbol{\sigma}$,

   $$\boldsymbol{n} \cdot \boldsymbol{\sigma} = \begin{pmatrix} n_z & n_x - i n_y \\ n_x + i n_y & -n_z \end{pmatrix},$$

and square it, which would be done as follows:

$$
\begin{aligned}
(\boldsymbol{n}\cdot\boldsymbol{\sigma})^2 &= \begin{bmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{bmatrix}\begin{bmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{bmatrix} \\
&= \begin{bmatrix} n_z^2 + (n_x - in_y)(n_x + in_y) & n_z(n_x - in_y) - n_z(n_x - in_y) \\ n_z(n_x + in_y) - n_z(n_x + in_y) & (n_x + in_y)(n_x - in_y) + n_z^2 \end{bmatrix} \\
&= \begin{bmatrix} n_x^2 + n_y^2 + n_z^2 & 0 \\ 0 & n_x^2 + n_y^2 + n_z^2 \end{bmatrix} \\
&= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}
\end{aligned}
$$

We hence conclude that the square of this matrix is just the identity:

$$(\boldsymbol{n}\cdot\boldsymbol{\sigma})^2 = I$$

An alternative solution strategy uses the results derived in the previous problem for products, commutators, and anti-commutators of Pauli matrices, and does not require explicit matrix multiplications. Expanding $(\boldsymbol{n}\cdot\boldsymbol{\sigma})^2 = (n_x\sigma_x + n_y\sigma_y + n_z\sigma_z)^2$ leads to

$$
\begin{aligned}
(\boldsymbol{n}\cdot\boldsymbol{\sigma})^2 &= (n_x\sigma_x + n_y\sigma_y + n_z\sigma_z)(n_x\sigma_x + n_y\sigma_y + n_z\sigma_z) \\
&= n_x^2\sigma_x^2 + n_y^2\sigma_y^2 + n_z^2\sigma_z^2 + n_xn_y\sigma_x\sigma_y + n_xn_z\sigma_x\sigma_z + n_yn_x\sigma_y\sigma_x \\
&\quad + n_yn_z\sigma_y\sigma_z + n_zn_x\sigma_z\sigma_x + n_zn_y\sigma_z\sigma_y \\
&= \left(n_x^2 + n_y^2 + n_z^2\right) I + n_xn_y(\sigma_x\sigma_y + \sigma_y\sigma_x) + n_xn_z(\sigma_x\sigma_z + \sigma_z\sigma_x) + n_yn_z(\sigma_y\sigma_z + \sigma_z\sigma_y) \\
&= I + n_xn_y\{\sigma_x, \sigma_y\} + n_xn_z\{\sigma_x, \sigma_z\} + n_yn_z\{\sigma_y, \sigma_z\}
\end{aligned}
$$

using the results obtained in the previous problem for the anti-commutators:

$$
\begin{aligned}
&= I + n_xn_y \times 0 + n_xn_z \times 0 + n_yn_z \times 0 \\
&= I
\end{aligned}
$$

From here we can immediately conclude that all even powers of $\boldsymbol{n}\cdot\boldsymbol{\sigma}$ correspond to the identity, because

$$(\boldsymbol{n}\cdot\boldsymbol{\sigma})^{2p} = \overbrace{(\boldsymbol{n}\cdot\boldsymbol{\sigma})^2(\boldsymbol{n}\cdot\boldsymbol{\sigma})^2\cdots(\boldsymbol{n}\cdot\boldsymbol{\sigma})^2}^{p\text{ times}} = I^p = I.$$

Likewise, any odd power can be written as

$$(\boldsymbol{n}\cdot\boldsymbol{\sigma})^{2p+1} = (\boldsymbol{n}\cdot\boldsymbol{\sigma})^{2p}(\boldsymbol{n}\cdot\boldsymbol{\sigma}) = I(\boldsymbol{n}\cdot\boldsymbol{\sigma}) = \boldsymbol{n}\cdot\boldsymbol{\sigma}.$$

2. Using the Taylor series expansion of the exponential function

$$e^{i\gamma\boldsymbol{n}\cdot\boldsymbol{\sigma}} = \sum_{m=0}^{\infty}\frac{i^m\gamma^m}{m!}\,(\boldsymbol{n}\cdot\boldsymbol{\sigma})^m,$$

we can split this sum into one term involving only even powers and another with only odd powers:

$$e^{i\gamma \boldsymbol{n}\cdot\boldsymbol{\sigma}} = \sum_{m \text{ even}} \frac{i^m \gamma^m}{m!} \, (\boldsymbol{n}\cdot\boldsymbol{\sigma})^m + \sum_{m \text{ odd}} \frac{i^m \gamma^m}{m!} \, (\boldsymbol{n}\cdot\boldsymbol{\sigma})^m \, .$$

From the result above regarding the powers of $\boldsymbol{n}\cdot\boldsymbol{\sigma}$ it simplifies to

$$e^{i\gamma \boldsymbol{n}\cdot\boldsymbol{\sigma}} = I \sum_{m \text{ even}} \frac{i^m \gamma^m}{m!} + (\boldsymbol{n}\cdot\boldsymbol{\sigma}) \sum_{m \text{ odd}} \frac{i^m \gamma^m}{m!}.$$

Expressing m even by $m = 2p$, and m odd by $m = 2p+1$, with $p = 0, 1, 2, \ldots$ this expression can be cast as

$$\begin{aligned}
e^{i\gamma \boldsymbol{n}\cdot\boldsymbol{\sigma}} &= I \sum_{p=0}^{\infty} \frac{i^{2p}\gamma^{2p}}{(2p)!} + (\boldsymbol{n}\cdot\boldsymbol{\sigma}) \sum_{p=0}^{\infty} \frac{i^{2p+1}\gamma^{2p+1}}{(2p+1)!} \\
&= I \sum_{p=0}^{\infty} \frac{\left(i^2\right)^p \gamma^{2p}}{(2p)!} + (\boldsymbol{n}\cdot\boldsymbol{\sigma}) \sum_{p=0}^{\infty} \frac{i\left(i^2\right)^p \gamma^{2p+1}}{(2p+1)!} \\
&= I \sum_{p=0}^{\infty} \frac{(-1)^p \gamma^{2p}}{(2p)!} + i\,(\boldsymbol{n}\cdot\boldsymbol{\sigma}) \sum_{p=0}^{\infty} \frac{(-1)^p \gamma^{2p+1}}{(2p+1)!}.
\end{aligned}$$

The last step is to recognize that the two sums left represent the Taylor series of $\cos\gamma$ and $\sin\gamma$, respectively. Therefore,

$$e^{i\gamma \boldsymbol{n}\cdot\boldsymbol{\sigma}} = I\, \cos\gamma + i\,(\boldsymbol{n}\cdot\boldsymbol{\sigma})\, \sin\gamma.$$

3. First, let us write $\boldsymbol{n}$ in polar coordinates:

$$\boldsymbol{n} = \sin\theta\cos\phi\,\boldsymbol{u}_x + \sin\theta\sin\phi\,\boldsymbol{u}_y + \cos\theta\,\boldsymbol{u}_z.$$

The matrix $\boldsymbol{n}\cdot\boldsymbol{\sigma}$ is then

$$\boldsymbol{n}\cdot\boldsymbol{\sigma} = \begin{pmatrix} \cos\theta & \sin\theta\cos\phi - i\sin\theta\sin\phi \\ \sin\theta\cos\phi + i\sin\theta\sin\phi & -\cos\theta \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix}$$

Let us calculate its eigenvalues:

$$\begin{vmatrix} \cos\theta - \lambda & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta - \lambda \end{vmatrix} = 0 \quad \Leftrightarrow \quad \lambda^2 = \sin^2\theta + \cos^2\theta = 1 \quad \Leftrightarrow \quad \lambda = \pm 1$$

And now its eigenvectors, which we designate

$$|\lambda\rangle_{\boldsymbol{n}} \mapsto \begin{bmatrix} u_\lambda \\ v_\lambda \end{bmatrix}$$

This notation means that for $\lambda = +1$ we have $|+\rangle_{\boldsymbol{n}}$ and for $\lambda = -1$ it becomes $|-\rangle_{\boldsymbol{n}}$. We can read $|\lambda\rangle_{\boldsymbol{n}}$ as *"the eigenvector of $\boldsymbol{\sigma} \cdot \boldsymbol{n}$ associated with the eigenvalue λ"*. From the eigenvector condition follows that

$$
\begin{aligned}
\boldsymbol{n} \cdot \boldsymbol{\sigma} |\lambda\rangle_{\boldsymbol{n}} = \lambda |\lambda\rangle_{\boldsymbol{n}} \quad &\Leftrightarrow \quad \begin{bmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{bmatrix} \begin{bmatrix} u_\lambda \\ v_\lambda \end{bmatrix} = \lambda \begin{bmatrix} u_\lambda \\ v_\lambda \end{bmatrix} \\
&\Leftrightarrow \quad \begin{cases} (\cos\theta - \lambda)\ u_\lambda + \sin\theta e^{-i\phi}\, v_\lambda & = 0 \\ \sin\theta e^{i\phi}\, u_\lambda - (\cos\theta + \lambda)\ v_\lambda & = 0 \end{cases} \\
&\Leftrightarrow \quad (\lambda - \cos\theta)\, u_\lambda = \sin\theta e^{-i\phi} v_\lambda
\end{aligned}
$$

This tells us how the two components u_λ and v_λ of the eigenvector associated with eigenvalue λ are related. In particular

$$
\frac{u_\lambda}{v_\lambda} = \frac{\sin\theta e^{-i\phi}}{\lambda - \cos\theta}
$$

and so, replacing explicitly for the two cases $\lambda = +1$ and $\lambda = -1$, it becomes

$$
\begin{aligned}
\lambda = +1: \qquad & \frac{u_+}{v_+} = \frac{\sin\theta e^{-i\phi}}{1 - \cos\theta} = \frac{\cos\frac{\theta}{2} e^{-i\phi/2}}{\sin\frac{\theta}{2} e^{i\phi/2}} \\
\lambda = -1: \qquad & \frac{u_-}{v_-} = -\frac{\sin\theta e^{-i\phi}}{1 + \cos\theta} = -\frac{\sin\frac{\theta}{2} e^{-i\phi/2}}{\cos\frac{\theta}{2} e^{i\phi/2}}
\end{aligned}
$$

We can then choose, for $\lambda = +1$,

$$
u_+ = \mathcal{N}_+ \cos\frac{\theta}{2} e^{-i\phi/2} \qquad \text{and} \qquad v_+ = \mathcal{N}_+ \sin\frac{\theta}{2} e^{i\phi/2},
$$

and, for the case $\lambda = -1$,

$$
u_- = \mathcal{N}_- \sin\frac{\theta}{2} e^{i\phi/2} \qquad \text{and} \qquad v_- = -\mathcal{N}_- \cos\frac{\theta}{2} e^{-i\phi/2}.
$$

where $\mathcal{N}_\pm$ is a yet to be determined normalization constant. Hence the eigenvectors associated with $\lambda = \pm 1$ can be written as

$$
|+\rangle_{\boldsymbol{n}} \to \mathcal{N}_+ \begin{bmatrix} \cos\frac{\theta}{2} e^{-i\phi/2} \\ \sin\frac{\theta}{2} e^{i\phi/2} \end{bmatrix} \qquad \text{and} \qquad |-\rangle_{\boldsymbol{n}} \to \mathcal{N}_- \begin{bmatrix} \sin\frac{\theta}{2} e^{-i\phi/2} \\ -\cos\frac{\theta}{2} e^{i\phi/2} \end{bmatrix}.
$$

Finally, the factor $\mathcal{N}$ must be determined by normalization. This imposes the condition

$$
{}_{\boldsymbol{n}}\langle + | + \rangle_{\boldsymbol{n}} = |\mathcal{N}_+|^2 \left(\left| \cos\frac{\theta}{2} e^{-i\phi/2} \right|^2 + \left| \sin\frac{\theta}{2} e^{i\phi/2} \right|^2 \right) = 1 \quad \Rightarrow \quad |\mathcal{N}_+|^2 = 1.
$$

Since we can always choose the overall normalization factor to be real, the solution of the normalization condition above can be chosen as $\mathcal{N}_+ = 1$, and equivalently for $\mathcal{N}_-$. The final result is then that the *normalized* eigenvectors of $\boldsymbol{n} \cdot \boldsymbol{\sigma}$ can be written as

$$
|+\rangle_{\boldsymbol{n}} \to \begin{bmatrix} \cos\frac{\theta}{2} e^{-i\phi/2} \\ \sin\frac{\theta}{2} e^{i\phi/2} \end{bmatrix} \qquad \text{and} \qquad |-\rangle_{\boldsymbol{n}} \to \begin{bmatrix} \sin\frac{\theta}{2} e^{-i\phi/2} \\ -\cos\frac{\theta}{2} e^{i\phi/2} \end{bmatrix}.
$$

Problema 5 | Funções de matrizes

Considere duas matrizes quadradas A e B que são *diagonais*:

$$A = \begin{pmatrix} a_1 & 0 & \cdots & 0 \\ 0 & a_2 & \cdots & 0 \\ \vdots & & \ddots & 0 \\ 0 & 0 & \cdots & a_m \end{pmatrix}, \qquad B = \begin{pmatrix} b_1 & 0 & \cdots & 0 \\ 0 & b_2 & \cdots & 0 \\ \vdots & & \ddots & 0 \\ 0 & 0 & \cdots & b_m \end{pmatrix}$$

1. Mostre que $[A, B] = 0$, concluindo assim que matrizes diagonais comutam sempre entre si.

2. Mostre que a potência $A^n = \text{diag}\,(a_1^n,\, a_2^n,\, \ldots, a_m^n)$, onde $n \in \mathbb{N}$.

3. Mostre que $\det\,[f(A)] = f(a_1) \times f(a_2) \times \cdots \times f(a_m)$, onde $f(z)$ é uma função arbitrária de uma variável z, com série de Taylor convergente no domínio de interesse de z.

Solution

1. To do that we note that the product of any two diagonal matrices is another diagonal matrix, that contains in each diagonal element to product of the elements of the two matrices. More explicitly:

$$A = \begin{bmatrix} a_1 & 0 & 0 & \cdots \\ 0 & a_2 & 0 & \cdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & a_n \end{bmatrix}, B = \begin{bmatrix} b_1 & 0 & 0 & \cdots \\ 0 & b_2 & 0 & \cdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & b_n \end{bmatrix} \to AB = \begin{bmatrix} a_1b_1 & 0 & 0 & \cdots \\ 0 & a_2b_2 & 0 & \cdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & a_nb_n \end{bmatrix}$$

Therefore the products AB and BA correspond to the same diagonal matrix, and hence, for the two diagonal matrices A, B

$$[A, B] = AB - BA = 0$$

which means that any two diagonal matrices commute.

2. We just showed that the product of any two diagonal matrices is still diagonal. In particular, the product of A with itself will be diagonal as well:

$$AA = A^2 = \begin{bmatrix} a_1^2 & 0 & 0 & 0 \\ 0 & a_2^2 & 0 & 0 \\ 0 & 0 & a_3^2 & 0 \\ 0 & 0 & 0 & \ddots \end{bmatrix}$$

We can repeat this as many times as we want, and show that $AA^2 = A^3$ is still diagonal, and so on, so that, in the end

$$A^n = \underbrace{AAA\cdots A}_{n\text{ times}} = \begin{bmatrix} a_1 & 0 & 0 & 0 \\ 0 & a_2 & 0 & 0 \\ 0 & 0 & a_3 & 0 \\ 0 & 0 & 0 & \ddots \end{bmatrix}^n = \begin{bmatrix} a_1^n & 0 & 0 & 0 \\ 0 & a_2^n & 0 & 0 \\ 0 & 0 & a_3^n & 0 \\ 0 & 0 & 0 & \ddots \end{bmatrix}$$

3. Recall the definition of $f(A)$:

$$f(A) \equiv \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \, A^n$$

The matrix elements of $f(A)$ are then

$$[f(A)]_{ij} = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \, [A^n]_{ij}$$

But we concluded just above that $[A^n]_{ij} = a_i^n \delta_{ij}$ and thus

$$[f(A)]_{ij} = \delta_{ij} \left(\sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \, a_i^n \right)$$

The contents of $(\cdots)$ is just the Taylor expansion of the function $f(z)$ evaluated at $z = a_i$ and we then conclude that

$$[f(A)]_{ij} = \delta_{ij} f(a_i)$$

or, in explicit form

$$f(A) = \begin{bmatrix} f(a_1) & 0 & 0 & 0 \\ 0 & f(a_2) & 0 & 0 \\ 0 & 0 & f(a_3) & 0 \\ 0 & 0 & 0 & \ddots \end{bmatrix}$$

This means that to get the function of a diagonal matrix, we need only to apply that function to each diagonal element, and form the resulting diagonal matrix.

Finally, since the determinant of a diagonal matrix is simply the product of its diagonal elements, we reach the final result

$$\det f(A) = f(a_1) \times f(a_2) \times \cdots \times f(a_m)$$

Problema 6

Considere uma matriz 2×2 genérica

$$C = \begin{bmatrix} a & b \\ c & d \end{bmatrix}, \qquad (a, b, c, d \in \mathbb{C})$$

1. Calcule explicitamente a matriz inversa C^{-1}.

2. Identifique que condições devem existir entre os elementos de matriz a, b, c, d de modo a que C seja uma matriz unitária.

3. Se U for uma matriz unitária 2×2 com $\det U = 1$ e tiver a primeira linha como

$$U = \begin{bmatrix} a & b \\ ? & ? \end{bmatrix}, \qquad (a, b \in \mathbb{C}),$$

quais deverão ser os elementos da segunda linha, expressos em termos de a e b?

Solution

1. The inverse matrix is

$$C^{-1} = \frac{1}{\det C} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}.$$

2. The Hermitian conjugate is

$$C^{\dagger} = \begin{bmatrix} a^* & c^* \\ b^* & d^* \end{bmatrix}$$

In order for C to be a unitary matrix we must have $C^{-1} = C^{\dagger}$. Expanding this equality element-by-element we get 4 equations

$$\begin{cases} \frac{d}{ad-bc} & = a^* \\ \frac{-b}{ad-bc} & = c^* \\ \frac{-c}{ad-bc} & = b^* \\ \frac{a}{ad-bc} & = d^* \end{cases},$$

which must be simultaneously fulfilled. From here follows that

$$a^* d^* - b^* c^* = (ad - bc)^* = \frac{ad - bc}{(ad - bc)^2} \quad \Leftrightarrow \quad |ad - bc|^2 = 1 \quad \Leftrightarrow \quad |\det C| = 1$$

This means that **one condition** is that the determinant have unitary modulus

$$|\det C| = 1$$

or, in other words, that it is of the form

$$\det C = e^{i\theta} \qquad \theta \in \mathbb{R}.$$

If that must be the case, then substituting in the equations above leads to the **additional condition**:

$$a = e^{i\theta} d^* \qquad \text{and} \qquad b = -e^{i\theta} c^*$$

Now notice that combining these two conditions leads also to the **requirement**

$$|a|^2 + |b|^2 = 1.$$

3. In order to fulfill the three conditions above, any unitary matrix will have the following structure:

$$U = \begin{bmatrix} a & b \\ -e^{i\theta} b^* & e^{i\theta} a^* \end{bmatrix}, \qquad \text{with } |a|^2 + |b|^2 = 1.$$

The condition $\det U = 1$ implies that $e^{i\theta} = 1$ and therefore we arrive at

$$U = \begin{bmatrix} a & b \\ b^* & a^* \end{bmatrix}, \qquad \text{with } |a|^2 + |b|^2 = 1.$$

We can double check this by verifying that any matrix of this form indeed satisfies the unitarity condition $UU^\dagger = \mathbf{1}$:

$$UU^\dagger = \begin{bmatrix} a & b \\ -b^* & a^* \end{bmatrix} \begin{bmatrix} a^* & -b \\ b^* & a \end{bmatrix} = \begin{bmatrix} |a|^2 + |b|^2 & 0 \\ 0 & |a|^2 + |b|^2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Problema 7 | Operações com matrizes e funções de matrizes

Nas questões seguintes, A, B e C são matrizes *quadradas* arbitrárias.

1. Mostre que o produto AB se pode escrever

$$AB = \frac{1}{2}\left[A,B\right] + \frac{1}{2}\left\{A,B\right\},$$

onde $[A,B]$ é o comutador e $\{A,B\} \equiv AB + BA$ é o anti-comutador das duas matrizes.

2. Mostre que, qualquer que seja a forma de A e B,

$$\{A,B\} = \{B,A\} \qquad \text{e} \qquad [A,B] = -\left[B,A\right].$$

3. Quando $[A,B] = 0$, dizemos que *A e B comutam*; quando $\{A,B\} = 0$, dizemos que anti-comutam. Tendo presente estas designações:

   a) Expanda $(A+B)^2$. Em que circunstâncias se pode dizer que $(A+B)^2 = A^2 + B^2 + 2AB$?

   b) Expanda $(A+BC)^2$. Em que circunstâncias se pode dizer que $(A+BC)^2 = A^2 + B^2C^2 + 2ABC$?

4. Mostre que a operação de comutação é distributiva obedecendo à seguinte ordem de fatores:

$$[A,BC] = [A,B]\,C + B\,[A,C],$$
$$[AB,C] = A\,[B,C] + [A,C]\,B.$$

5. Mostre que

$$[AB,C] = A\,\{B,C\} - \{A,C\}\,B.$$

6. Mostre que

$$[A,B^n] = \left[A,B^{n-1}\right]B + B^{n-1}\,[A,B],$$

onde B^n é a n-ésima potência da matriz B ($n \in \mathbb{N}$).

7. Considere $f(A)$, uma função arbitrária de uma matriz quadrada A:

   a) Mostre que $[A, f(A)] = 0$.

   b) Mostre que $f(A)^\top = f(A^\top)$.

   c) Mostre que $f(A)^* = f^*(A^*)$.

   d) Mostre que $f(A)^\dagger = f^*(A^\dagger)$.

   e) Se A for simétrica, será $f(A)$ simétrica em geral?

   f) Se A for Hermítica, será $f(A)$ Hermítica em geral?

8. (*) Mostre que:

   a) se u e v forem dois números arbitrários

   $$e^{uA+vA} = e^{uA}e^{vA};$$

   b) se S for uma matriz anti-simétrica, então

   $$O = e^{S}$$

   é uma matriz ortogonal.

   c) se H for uma matriz Hermítica, então

   $$U = e^{iH}$$

   é uma matriz unitária.

   d) se duas matrizes A e B não comutam, então

   $$e^{uA+vB} \neq e^{uA}e^{vB}, \qquad \text{se } [A,B] \neq 0.$$

   (*sugestão: expanda cada um dos lados até segunda ordem em* u *e* v.)

Solution

1. Add and subtract

$$\begin{aligned} AB &= AB + (AB - AB) + (BA - BA) \\ &= AB - BA + AB + BA - AB \\ &= (AB - BA) + (AB + BA) - AB \end{aligned}$$

$$AB + AB = (AB - BA) + (AB + BA)$$

$$AB = \frac{1}{2}[A,B] + \frac{1}{2}\{A,B\}$$

2. Simply using the definitions

$$\{B,A\} = BA + AB = AB + BA = \{A,B\}$$

$$[B,A] = BA - AB = -(AB - BA) = -[A,B]$$

3.

   a) Expanding the square

   $$(A+B)^2 = (A+B)(A+B) = A^2 + AB + BA + B^2$$

   so if we want to obtain the stated result we need

   $$AB + BA = 2AB \quad \Leftrightarrow \quad AB = BA \quad \Leftrightarrow \quad [A,B] = 0$$

   Only if A and B commute can we expand the square as stated.

b) Expanding again

$$(A + BC)^2 = (A + BC)(A + BC) = A^2 + ABC + BCA + BCBC$$

to get the stated result we need

$$ABC + BCA + BCBC = B^2C^2 + 2ABC = BBCC + 2ABC$$

which requires, first, that $BC = CB$. In addition, we need

$$2ABC = ABC + BCA \qquad \Leftrightarrow \qquad ABC = BCA$$

We can try to bring the RHS to coincide with the LHS by doing the following:

$$\begin{aligned} BCA &= B\left(AC - [A, C]\right) = BAC - B\,[A, C] = \left(AB - [A, B]\right) C - B\,[A, C] \\ &= ABC - [A, B]\,C - B\,[A, C] \end{aligned}$$

Consequently, in order to have $ABC = BCA$ we need that Acommutes with B and C.

So, in summary, $(A + BC)^2 = A^2 + B^2C^2 + 2ABC$ only if

$$[A, B] = [A, C] = [B, C] = 0$$

which means that all three matrices have to commute with each other.

4. One can, of course, just expand each side and compare them directly, which is immediate. An alternative is to try to derive the RHS starting from the LHS only:

$$\begin{aligned} [A, BC] &= ABC - BCA = ABC - B\left(AC - [A, C]\right) = ABC - BAC + B\,[A, C] \\ &= \left(AB - BA\right) C + B\,[A, C] = [A, B]\,C + B\,[A, C] \end{aligned}$$

To demonstrate the second identity, we can use the result just derived, because:

$$[AB, C] = -\,[C, AB] = -A\,[C, B] - [C, A]\,B = A\,[B, C] + [A, C]\,B$$

5. We can do similarly to what we did above but using the anti-commutators to derive the RHS from the LHS. This time, however, I'll just expand each side and compare:

$$\begin{aligned} & [AB, C] \stackrel{?}{=} A\,\{B, C\} - \{A, C\}\,B \\ \Leftrightarrow \quad & ABC - CAB \stackrel{?}{=} A\left(BC + CB\right) - \left(AC + CA\right) B \\ \Leftrightarrow \quad & ABC - CAB \stackrel{?}{=} ABC + ACB - ACB - CAB \\ \Leftrightarrow \quad & ABC - CAB = ABC - CAB \end{aligned}$$

The two sides are equal, so the result is proven.

6. This is a simple application of the distributive property

$$[A, B^n] = \left[A, B^{n-1}B\right] = B^{n-1}\,[A, B] + \left[A, B^{n-1}\right] B$$

7. The function $f(A)$ is defined by the Taylor expansion

$$f(A) \equiv \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!}\, A^n$$

a) Replacing explicitly, and recalling that $[A, B + C + \dots] = [A, B] + [A, C] + \dots$

$$[A, f(A)] = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!}\, [A, A^n] = 0 \qquad \text{because } [A, A^n] = 0$$

b) We use the fact that $(A + B + \dots)^\top = A^\top + B^\top + \dots$ and see that

$$f(A)^\top = \left[\sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!}\, A^n\right]^\top = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!}\, (A^n)^\top$$

but $(A^n)^\top = (AAA\dots)^\top = A^\top A^\top A^\top \dots = \left(A^\top\right)^n$, and hence

$$f(A)^\top = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!}\, \left(A^\top\right)^n = f(A^\top)$$

c) Since the complex conjugate of a sum is the sum of the complex conjugates, and equivalently for the product,

$$f(A)^* = \sum_{n=0}^{\infty} \frac{\left[f^{(n)}(0)\right]^*}{n!}\, (A^n)^* = \sum_{n=0}^{\infty} \frac{\left[f^{(n)}(0)\right]^*}{n!}\, (A^*)^n = f^*(A^*)$$

d) Since the Hermitian conjugate is simply the conjugate transpose, the two results above can be combined

$$f(A)^\dagger = \left[f(A)^\top\right]^* = \left[f(A^\top)\right]^* = f^*\left(\left(A^\top\right)^*\right) = f^*\left(A^\dagger\right)$$

e) If A is symmetric, then $A^\top = A$. Therefore, using the result above

$$f(A)^\top = f(A^\top) = f(A)$$

Since $f(A)^\top = f(A)$, $f(A)$ is itself symmetric.

f) If A is Hermitian, then $A^\dagger = A$. Therefore, using the result above

$$f(A)^\dagger = f^*\left(A^\dagger\right) = f^*\left(A\right)$$

In this case, $f(A)$ is not Hermitian, unless f is a real function.

8.

a) For complex numbers z_1 and z_2 the exponential function has the property

$$e^{z_1+z_2} = e^{z_1}e^{z_2}$$

This means that, in terms of the respective Taylor series on each side it must be true that

$$\sum_{n=0}^{\infty}\frac{(z_1+z_2)^n}{n!} = \left[\sum_{n=0}^{\infty}\frac{z_1^n}{n!}\right] \times \left[\sum_{n=0}^{\infty}\frac{z_2^n}{n!}\right]$$

To analyse the case of the matrices e^{uA} and e^{vA}, we likewise write

$$e^{uA+vA} \equiv \sum_{n=0}^{\infty}\frac{(uA+vA)^n}{n!}$$

Now, since we have only one matrix A everywhere, and since $[A, A] = 0$, this means that $(uA + vA)^n$ has the same binomial expansion as if uA and vA were simple numbers, rather than matrices. Consequently, it must be true that

$$\sum_{n=0}^{\infty}\frac{(uA+vA)^n}{n!} = \left[\sum_{n=0}^{\infty}\frac{u^nA^n}{n!}\right] \times \left[\sum_{n=0}^{\infty}\frac{v^nA^n}{n!}\right]$$

as well, which is exactly the same as saying

$$e^{uA+vA} = e^{uA}e^{vA}$$

b) We use the fact that $f(A)^\top = f(A^\top)$ in general, that $S^\top = -S$, and the last result derived above:

$$OO^\top = e^S\left(e^S\right)^\top = e^Se^{S^\top} = e^Se^{-S} = e^{S-S} = \mathbf{1}$$

and thus O is orthogonal.

c) Basically the same as above, but recalling that $f(A)^\dagger = f^*(A^\dagger)$:

$$UU^\dagger = e^{iH}\left(e^{iH}\right)^\dagger = e^{iH}e^{-iH^\dagger} = e^{iH}e^{-iH} = e^{iH-iH} = \mathbf{1}$$

and hence U is unitary.

d) Expanding the exponentials o second order we have, for the left-hand side:

$$\begin{aligned} e^{uA+vB} &\simeq I + (uA+vB) + \frac{(uA+vB)^2}{2} \\ &= I + uA + vB + \frac{u^2A^2 + v^2B^2 + uv\,(AB+BA)}{2} \end{aligned}$$

For the right-hand side:

$$\begin{aligned} e^{uA}e^{vB} &\simeq \left(I + uA + \frac{1}{2}u^2A^2\right)\left(I + vB + \frac{1}{2}v^2B^2\right) \\ &= I + uA + vB + \frac{u^2A^2 + v^2B^2 + 2uvAB}{2} + \text{higher order} \end{aligned}$$

As a result, we see already in second order that for $e^{uA+vB} = e^{uA}e^{vB}$ to be true, $[A, B]$ should be zero. Consequently, if the matrices A and B do not commute

$$e^{uA+vB} \neq e^{uA}e^{vB}.$$

Problema 8

Considere um conjunto de 4 matrizes *gama* γ_1, γ_2, γ_3, γ_4 que obedece à relação seguinte:

$$\gamma_i\gamma_j + \gamma_j\gamma_i = 2\delta_{ij}I.$$

1. A que é igual a matriz γ_i^2 (o quadrado de γ_i, qualquer que seja $i \in \{1, 2, 3, 4\}$)?

2. Mostre que cada γ_i tem traço nulo ($\mathrm{Tr}\,\gamma_i = 0$). (*sugestão: comece por multiplicar ambos os lados da relação acima por* γ_i).

Solution

1. When $i = j$ the given relation reduces to

$$\gamma_i^2 = I,$$

and thus γ_i^2 is the identity.

2. Consider the cases where $i \neq j$, where the given relation (which, if you look at it, is simply the anti-commutation relation for the matrices γ_i) becomes

$$\gamma_i\gamma_j + \gamma_j\gamma_i = 0.$$

Let us follow the suggestion by multiplying both sides by γ_i from the left, and taking the trace of the result:

$$\begin{aligned}
& \gamma_i^2\gamma_j + \gamma_i\gamma_j\gamma_i = 0 \\
& \qquad\downarrow \\
\Leftrightarrow \quad & \text{Tr}\,(I\gamma_j + \gamma_i\gamma_j\gamma_i) = 0 \\
\Leftrightarrow \quad & \text{Tr}\,(\gamma_j) + \text{Tr}\,(\gamma_i\gamma_j\gamma_i) = 0 \\
\Leftrightarrow \quad & \text{Tr}\,(\gamma_j) + \text{Tr}\,(\gamma_j\gamma_i\gamma_i) = 0 \\
\Leftrightarrow \quad & \text{Tr}\,(\gamma_j) + \text{Tr}\,\left(\gamma_j\gamma_i^2\right) = 0 \\
\Leftrightarrow \quad & \text{Tr}\,(\gamma_j) + \text{Tr}\,(\gamma_j) = 0 \\
\Leftrightarrow \quad & \text{Tr}\,(\gamma_j) = 0
\end{aligned}$$

where we used the cyclic property of the trace. The above shows that Tr $(\gamma_j) = 0$.