Física Quântica I / Mecânica Quântica (2021/22)

Folha de Problemas 3 (postulados em prática)

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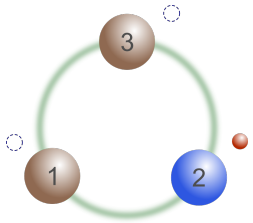
— Soluções —

Problema 1 | Prática com os postulados da mecânica quântica



Consideremos uma variação da descrição de um eletrão numa molécula tri-atómica discutida nas aulas teóricas, em que o eletrão pode transitar entre três átomos equivalentes.

Denotemos os estados que representam o eletrão em cada um dos átomos por $|x_1\rangle$, $|x_2\rangle$, $|x_3\rangle$, e usemos este conjunto para definir uma base ortonormal do espaço de estados. O operador Hamiltoniano (energia) para este eletrão é definido pelas relações seguintes:

$$\hat{\mathrm{H}}\,|x_1\rangle = |x_2\rangle - |x_3\rangle, \quad \hat{\mathrm{H}}\,|x_2\rangle = |x_1\rangle - |x_3\rangle, \quad \mathrm{Tr}\,\hat{\mathrm{H}} = 0.$$

Uma segunda observável $\hat{\mathrm{A}}$ de interesse neste sistema é definida por

$$\hat{\mathrm{A}}\,|x_1\rangle = -|x_3\rangle, \quad \hat{\mathrm{A}}\,|x_2\rangle = |x_2\rangle, \quad \hat{\mathrm{A}}\,|x_3\rangle = -|x_1\rangle.$$

Nas questões que se seguem, assumiremos que o eletrão foi preparado no estado

$$|\psi\rangle = |x_2\rangle.$$

1. Determine a representação matricial de $\hat{\mathrm{H}}$ e $\hat{\mathrm{A}}$ nesta base.

2. Calcule os valores esperados de $\hat{\mathrm{H}}$ e $\hat{\mathrm{A}}$ no estado ψ.

3. Os dois kets seguintes são auto-estados de energia:

$$|\varepsilon_1\rangle = \frac{1}{\sqrt{2}}|x_1\rangle + \frac{1}{\sqrt{2}}|x_3\rangle, \qquad |\varepsilon_2\rangle = -\frac{1}{\sqrt{6}}|x_1\rangle + \frac{2}{\sqrt{6}}|x_2\rangle + \frac{1}{\sqrt{6}}|x_3\rangle.$$

   Quais são os valores próprios, ε_1 e ε_2, associados a cada um destes auto-estados?

4. Determine o terceiro valor próprio de $\hat{\mathrm{H}}$ (ε_3) e o auto-estado normalizado correspondente. (*Este cálculo fica mais simples se recordar que o traço de uma matriz é igual à soma dos seus valores próprios.*)

5. Quais são os resultados possíveis numa medição da energia deste eletrão quando ele se encontra no estado ψ? Calcule as probabilidades associadas a cada um desses resultados.

6. Mostre que
$$\langle\psi|\hat{\mathrm{H}}|\psi\rangle = \sum_n \mathcal{P}_n\, \varepsilon_n,$$
onde $\mathcal{P}_n$ são as probabilidades determinadas na questão anterior.

7. Suponha que foi feita uma medição da energia do eletrão, na qual se obteve o menor dos valores possíveis:

   a) Qual é o vetor de estado (normalizado) do eletrão imediatamente após essa medida? Expresse-o na base $\{|x_i\rangle\}$.

   b) Em qual dos átomos é mais provável encontrar o eletrão imediatamente após essa medida, e qual é essa probabilidade?

   c) Quais são os valores esperados de $\hat{\mathrm{H}}$ e $\hat{\mathrm{A}}$ imediatamente após esta medida de energia?

8. As observáveis $\hat{\mathrm{H}}$ e $\hat{\mathrm{A}}$ são compatíveis ou incompatíveis? Explique porquê.

9. Deixando o sistema evoluir no tempo sem efetuar qualquer medição desde que ele foi preparado no estado ψ, o valor esperado de $\hat{\mathrm{H}}$ manter-se-á constante ou irá variar no tempo? E quanto ao valor esperado de $\hat{\mathrm{A}}$? Justifique.

Solution

1. Since the matrix elements are, by definition, given by $H_{ij} = \langle x_i|\hat{\mathrm{H}}|x_j\rangle$, the relations given lead to
$$\hat{\mathrm{H}} \mapsto H = \begin{bmatrix} 0 & 1 & -1 \\ 1 & 0 & -1 \\ -1 & -1 & 0 \end{bmatrix}, \qquad \text{and} \qquad \hat{\mathrm{A}} \mapsto A = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix}.$$
To obtain the last column of H above we used the fact that this matrix must be Hermitian, hence $H_{ij} = H^*_{ji}$. To obtain the last diagonal element we used the fact that $\mathrm{Tr}\, H = H_{11} + H_{22} + H_{33}$.

2. Since we are told that $|\psi\rangle = |x_2\rangle$, we have
$$\langle\psi|\hat{\mathrm{A}}|\psi\rangle = \langle x_2|\hat{\mathrm{A}}|x_2\rangle = A_{22} = 1, \qquad \text{and} \qquad \langle\psi|\hat{\mathrm{H}}|\psi\rangle = \langle x_2|\hat{\mathrm{H}}|x_2\rangle = H_{22} = 0.$$
Note: these results could, of course, have been obtained by applying the general procedure of converting the expectation value into the matrix product
$$\langle\psi|\hat{\mathrm{A}}|\psi\rangle \quad \mapsto \quad \begin{bmatrix} 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = 1,$$
and analogously for $\langle\psi|\hat{\mathrm{H}}|\psi\rangle$. But, since in this particular case the state is very simple and coincides with one of the basis vectors, $|\psi\rangle = |x_2\rangle$, it is more expedite and direct to use the first procedure.

3. Since it is already known that the given kets are eigenstates of $\hat{\mathrm{H}}$, they must obey the eigenstate/eigenvector conditions

$$\hat{\mathrm{H}}|\varepsilon_1\rangle = \varepsilon_1\,|\varepsilon_1\rangle, \quad \hat{\mathrm{H}}|\varepsilon_2\rangle = \varepsilon_2|\varepsilon_2\rangle.$$

They are also normalized, which means that we can obtain the corresponding eigenvalues, for example, by computing

$$\varepsilon_1 = \langle\varepsilon_1|\hat{\mathrm{H}}|\varepsilon_1\rangle = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 0 & 1 & -1 \\ 1 & 0 & -1 \\ -1 & -1 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{bmatrix} = -1,$$

$$\varepsilon_2 = \langle\varepsilon_2|\hat{\mathrm{H}}|\varepsilon_2\rangle = \begin{bmatrix} -\frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{bmatrix} \begin{bmatrix} 0 & 1 & -1 \\ 1 & 0 & -1 \\ -1 & -1 & 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \end{bmatrix} = -1.$$

We see that these two eigenstates belong to the same eigenvalue. Hence -1 is a doubly degenerate eigenvalue.

4. Let us denote the remaining eigenvalue by ε_3, and the corresponding eigenstate by $|\varepsilon_3\rangle$. Following the hint given in the question, and recalling that we know from the text of the problem that $\mathrm{Tr}\,\hat{\mathrm{H}} = 0$, we can conclude that

$$\mathrm{Tr}\,\hat{\mathrm{H}} = 0 \quad \Leftrightarrow \quad \varepsilon_1 + \varepsilon_2 + \varepsilon_3 = 0 \quad \Rightarrow \quad \varepsilon_3 = 2,$$

which tells us that the third eigenvalue is non-degenerate. To find the associated normalized eigenstate we can simply follow the general procedure based on the matrix H:

$$(\hat{\mathrm{H}} - \varepsilon_3\mathbf{1})|\varepsilon_3\rangle = 0 \xrightarrow{\varepsilon_3=2} \begin{bmatrix} -2 & 1 & -1 \\ 1 & -2 & -1 \\ -1 & -1 & -2 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix} = 0 \quad \Leftrightarrow \quad |\varepsilon_3\rangle \mapsto \frac{1}{\sqrt{3}} \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix}.$$

As a verification, we note that

$$|\varepsilon_3\rangle = \frac{1}{\sqrt{3}}|x_1\rangle + \frac{1}{\sqrt{3}}|x_2\rangle - \frac{1}{\sqrt{3}}|x_3\rangle$$

is the correct result because it is simultaneously orthogonal to the other two eigenstates $|\varepsilon_1\rangle$ and $|\varepsilon_2\rangle$, as it should be, because these two belong to a different eigenvalue of an Hermitian operator.

5. According to one of the postulates of quantum mechanics, the outcome of a measurement of the energy in this system can only yield one of the eigenvalues of $\hat{\mathrm{H}}$, because this is the operator associated with the electron's energy. Therefore, there are only two possible outcomes in any such single measurement: -1 or 2.

The probabilities associated with these outcomes are given, according to the probability postulate, by

$$\mathcal{P}\left(\mathcal{E} \to 2\right) = \mathcal{P}(\varepsilon_3) = |\langle\varepsilon_3|\psi\rangle|^2 = |\langle\varepsilon_3|x_2\rangle|^2 = \frac{1}{3}$$

and

$$\mathcal{P}\left(\mathcal{E}\to -1\right)=\mathcal{P}\left(\varepsilon_1\vee\varepsilon_2\right)=\left|\langle\varepsilon_1|\psi\rangle\right|^2+\left|\langle\varepsilon_2|\psi\rangle\right|^2=1-\mathcal{P}\left(\varepsilon_3\right)=\frac{2}{3}.$$

Note that we used here the fact that there are only two outcomes (because one of the eigenvalues is doubly degenerate). Hence, since the sum of the two must be one, we can shortcut the calculation by computing only the probability associated with the non-degenerate eigenvalue (which is faster to calculate in general).

Note: We could have derived these probabilities in a completely equivalent way by recalling that if the state of the system is written in the eigenbasis of $\hat{\mathrm{H}}$, it will be a linear combination of the type

$$|\psi\rangle=\chi_1|\varepsilon_1\rangle+\chi_2|\varepsilon_2\rangle+\chi_3|\varepsilon_3\rangle,$$

where the coefficients (components) χ_n correspond directly to the probability amplitudes of obtaining each of the values ε_n in a measurement of the energy:

$$\mathcal{P}(\varepsilon_n)=\left|\chi_n\right|^2.$$

But, if the three $|\varepsilon_n\rangle$ are mutually orthogonal and normalized, we have

$$\langle\varepsilon_1|\psi\rangle=\chi_1,\qquad\langle\varepsilon_2|\psi\rangle=\chi_2,\qquad\langle\varepsilon_3|\psi\rangle=\chi_3,$$

and we see that we immediately obtain the same as the above results for $\mathcal{P}(\varepsilon_n)$:

$$\begin{aligned}\mathcal{P}(\mathcal{E}\to -1)&=\left|\chi_1\right|^2+\left|\chi_2\right|^2=\frac{2}{3},\\ \mathcal{P}(\mathcal{E}\to 2)&=\left|\chi_3\right|^2=\frac{1}{3}.\end{aligned}$$

6. If we express the state vector in the energy eigenbasis,

$$|\psi\rangle=\chi_1|\varepsilon_1\rangle+\chi_2|\varepsilon_2\rangle+\chi_3|\varepsilon_3\rangle,$$

then, since $\hat{\mathrm{H}}|\varepsilon_n\rangle=\varepsilon_n|\varepsilon_n\rangle$, we see immediately that

$$\begin{aligned}\langle\psi|\hat{\mathrm{H}}|\psi\rangle&=\langle\psi|\left(\chi_1\varepsilon_1|\varepsilon_1\rangle+\chi_2\varepsilon_2|\varepsilon_2\rangle+\varepsilon_3\chi_3|\varepsilon_3\rangle\right)\\&=\left(\chi_1^*\langle\varepsilon_1|+\chi_2^*\langle\varepsilon_2|+\chi_3^*\langle\varepsilon_3|\right)\left(\chi_1\varepsilon_1|\varepsilon_1\rangle+\chi_2\varepsilon_2|\varepsilon_2\rangle+\varepsilon_3\chi_3|\varepsilon_3\rangle\right)\\&=\left|\chi_1\right|^2\varepsilon_1+\left|\chi_2\right|^2\varepsilon_2+\varepsilon_3\left|\chi_3\right|^2\\&=\sum_n\mathcal{P}_n\,\varepsilon_n,\end{aligned}$$

where

$$|\chi_n|=|\langle\varepsilon_n|\psi\rangle|^2=\mathcal{P}_n.$$

Note 1: This result shows that $\langle\psi|\hat{\mathrm{H}}|\psi\rangle$ is a sum over all possible outcomes ε_n weighted by the probability of each one. That is precisely the definition of "statistical average", or "mean", or "expectation value" (these three words are all synonyms) of the random quantity ε_n. The physical meaning of the quantity $\langle\psi|\hat{\mathrm{H}}|\psi\rangle$ is thus the following. Suppose one takes a large number of identical systems all prepared in the same quantum state $|\psi\rangle$ (we call that an *ensemble*). Next, we perform a measurement of energy on each system: each measurement will yield one of the eigenvalues ε_n with a certain probability. If one is interested in the average outcome, we would compute the simple

mean of all the results registered in each individual experiment (that would be what is called an *ensemble average*). The quantity $\langle\psi|\hat{\mathrm{H}}|\psi\rangle$ tells you what such an ensemble average would be.

Note 2: As discussed in Lecture 6 (see the discussion of the probability postulate in the lecture notes), this result holds for any Hermitian operator, say $\hat{\mathrm{G}}$, because, when we express the state vector in the eigenbasis of $\hat{\mathrm{G}}$, we have a linear combination of the type

$$|\psi\rangle = \sum_n \beta_n |g_n\rangle, \qquad \text{where} \qquad \hat{\mathrm{G}}|g_n\rangle = g_n|g_n\rangle,$$

and thus

$$\langle\psi|\hat{\mathrm{G}}|\psi\rangle = \sum_{nm} \beta_m^* \beta_n \langle g_m|\hat{\mathrm{G}}|g_n\rangle = \sum_{nm} g_n \beta_m^* \beta_n \langle g_m|g_n\rangle = \sum_n g_n \,|\beta_n|^2 = \sum_n g_n \,\mathcal{P}(g_n).$$

Therefore $\langle\psi|\hat{\mathrm{G}}|\psi\rangle$ *always* represents the ensemble average of the physical quantity that the operator $\hat{\mathrm{G}}$ describes.

7. Recall that, if an energy measurement yields the lowest possible eigenvalue of $\hat{\mathrm{H}}$, the state of the system immediately afterwards is reduced to its projection on the eigen-subspace associated with that eigenvalue. In this case, note that the lowest energy eigenvalue of $\hat{\mathrm{H}}$ is -1, and it is *doubly* degenerate, as we found in question 3 above.

   a) If we call $\hat{\mathrm{P}}_{\{\varepsilon_1,\varepsilon_2\}}$ the projector on the eigen-subspace associated with this degenerate eigenvalue, we know that the state reduction postulate means that, after the measurement,

   $$|\psi\rangle \;\longrightarrow\; |\psi'\rangle = \hat{\mathrm{P}}_{\{\varepsilon_1,\varepsilon_2\}}|\psi\rangle,$$

   where

   $$\hat{\mathrm{P}}_{\{\varepsilon_1,\varepsilon_2\}} = |\varepsilon_1\rangle\langle\varepsilon_1| + |\varepsilon_2\rangle\langle\varepsilon_2|.$$

   Performing the projection explicitly on the state vector before the measurement:

   $$\begin{aligned} |\psi'\rangle = \hat{\mathrm{P}}_{\{\varepsilon_1,\varepsilon_2\}}|\psi\rangle &= \left(|\varepsilon_1\rangle\langle\varepsilon_1| + |\varepsilon_2\rangle\langle\varepsilon_2|\right)|\psi\rangle \\ &= \langle\varepsilon_1|\psi\rangle\,|\varepsilon_1\rangle + \langle\varepsilon_2|\psi\rangle\,|\varepsilon_2\rangle \\ &= 0\,|\varepsilon_1\rangle + \frac{2}{\sqrt{6}}\,|\varepsilon_2\rangle \\ &= \frac{2}{\sqrt{6}}\,|\varepsilon_2\rangle. \end{aligned}$$

   Hence, the normalized state after this measurement will be

   $$|\psi'\rangle = |\varepsilon_2\rangle = -\frac{1}{\sqrt{6}}|x_1\rangle + \frac{2}{\sqrt{6}}|x_2\rangle + \frac{1}{\sqrt{6}}|x_3\rangle.$$

   b) The previous result allows us to read immediately the probabilities of finding the electron in either of the 3 atoms because the coefficients of the expansion of $|\psi'\rangle$ in the basis $\{|x_n\rangle\}$ are precisely those probability amplitudes. They are, in order, $1/6$, $2/3$, and $1/6$. Therefore, immediately after the measurement of the energy that yielded this outcome, the atom is more likely to be found in atom 2, with a probability of $2/3$.

c) Immediately after the energy measurement discussed in the previous question, the expectation value of $\hat{\mathrm{H}}$ must be exactly -1 (you can calculate it explicitly to check, but you can also think about why we can answer straught away that it *must* be that without any computation...). The other requested expectation value is

$$\langle\psi'|\hat{\mathrm{A}}|\psi'\rangle = \begin{bmatrix} -\frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{bmatrix} \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \end{bmatrix} = 1.$$

8. By definition, compatible observables commute. Since we have the matrix representations of both operators, we can calculate their commutator explicitly:

$$[A,H] = \begin{bmatrix} 0 & 1 & -1 \\ 1 & 0 & -1 \\ -1 & -1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix} - \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & -1 \\ 1 & 0 & -1 \\ -1 & -1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} = \mathbf{0}.$$

The two observables are, therefore, compatible.

9. In the absence of any measurement, the time evolution of the state vector is governed only by Schrödinger's equation. One consequence of that is Ehrenfest's theorem (derived in the lectures) for the time-dependence of expectation values of any observable $\hat{\mathrm{O}}$. Since in this problem there is no explicit time dependence in either $\hat{\mathrm{H}}$ or $\hat{\mathrm{A}}$, the statement of this theorem reduces to

$$i\hbar\frac{d}{dt}\langle\psi(t)|\hat{\mathrm{O}}|\psi(t)\rangle = \langle\psi(t)|\big[\hat{\mathrm{O}},\hat{\mathrm{H}}\big]|\psi(t)\rangle.$$

Consequently, since any operator always commutes with itself, the expectation value of $\hat{\mathrm{H}}$ will remain unchanged. In addition, in the last question we showed that $[A,H] = 0$, which implies

$$i\hbar\frac{d}{dt}\langle\psi(t)|\hat{\mathrm{A}}|\psi(t)\rangle = 0 \qquad \Rightarrow \qquad \langle\psi(t)|\hat{\mathrm{A}}|\psi(t)\rangle = \text{constant}.$$

Problema 2

Neste problema continuamos a considerar os operadores $\hat{\mathrm{H}}$ e $\hat{\mathrm{A}}$ definidos no Problema 1 acima. Podemos facilmente confirmar que os valores próprios de $\hat{\mathrm{A}}$ são $a_1 = -1$ e $a_2 = +1$ (duplamente degenerado). Nas questões abaixo, use o conjunto seguinte de vetores próprios e ortonormados *do Hamiltoniano* $\hat{\mathrm{H}}$:

$$|\varepsilon_1^{(1)}\rangle \mapsto \frac{1}{\sqrt{2}}\begin{bmatrix}0\\1\\1\end{bmatrix}, \qquad |\varepsilon_1^{(2)}\rangle \mapsto \frac{1}{\sqrt{6}}\begin{bmatrix}2\\-1\\1\end{bmatrix}, \qquad |\varepsilon_2\rangle \mapsto \frac{1}{\sqrt{3}}\begin{bmatrix}1\\1\\-1\end{bmatrix},$$

associados respetivamente aos valores próprios $\varepsilon_1 = -1$ e $\varepsilon_2 = 2$. Estamos agora interessados nos vetores próprios de $\hat{\mathrm{A}}$, que designaremos por $|a_1\rangle$, $|a_2^{(1)}\rangle$, $|a_2^{(2)}\rangle$, respetivamente associados aos valores próprios $a_1 = -1$ e $a_2 = +1$ (degenerado).

1. Mostre que $|\varepsilon_2\rangle$ é também um vetor próprio de $\hat{\mathrm{A}}$, e que o podemos identificar com $|a_2^{(1)}\rangle$.

2. Mostre que nem $|\varepsilon_1^{(1)}\rangle$ nem $|\varepsilon_1^{(2)}\rangle$ é vetor próprio de $\hat{\mathrm{A}}$.

3. Mostre que, todavia, é possível determinar constantes $\alpha, \beta, \gamma, \delta \in \mathbb{C}$, tais que as combinações lineares

$$|a_1\rangle \equiv \alpha|\varepsilon_1^{(1)}\rangle + \beta|\varepsilon_1^{(2)}\rangle, \qquad |a_2^{(2)}\rangle \equiv \gamma|\varepsilon_1^{(1)}\rangle + \delta|\varepsilon_1^{(2)}\rangle,$$

   são vetores próprios de $\hat{\mathrm{A}}$ associados aos valores próprios -1 e 1, respetivamente. (*Basta substituir cada um na definição do que é um vetor próprio de* $\hat{\mathrm{A}}$ *e resolver para obter as constantes*).

4. Escreva as matrizes que representam $\hat{\mathrm{H}}$ e $\hat{\mathrm{A}}$ na base $\{|a_1\rangle, |a_2^{(1)}\rangle, |a_2^{(2)}\rangle\}$, mostrando assim que estes dois operadores são diagonais nesta base.

Solution

1. Computing explicitly,

$$\hat{\mathrm{A}}|\varepsilon_2\rangle \mapsto \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix} = (+1) \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix}.$$

   This establishes that

$$\hat{\mathrm{A}}|\varepsilon_2\rangle = (+1)|\varepsilon_2\rangle,$$

   which means $|\varepsilon_2\rangle$ is an eigenvector of the operator $\hat{\mathrm{A}}$ belonging to the eigenvalue 1. According the the initial text of the problem, this is the eigenvalue labeled as a_2. Therefore, we can say that $|a_2^{(1)}\rangle = |\varepsilon_2\rangle$.

2. Proceeding analogously for $|\varepsilon_1^{(1)}\rangle$ and $|\varepsilon_1^{(2)}\rangle$:

$$\hat{\mathrm{A}}|\varepsilon_1^{(1)}\rangle \mapsto \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix} \neq \text{constant} \times \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix},$$

   so that $|\varepsilon_1^{(1)}\rangle$ is not an eigenvector of $\hat{\mathrm{A}}$. Likewise,

$$\hat{\mathrm{A}}|\varepsilon_1^{(2)}\rangle \mapsto \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 2 \\ -1 \\ 1 \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \\ -2 \end{bmatrix} \neq \text{constant} \times \begin{bmatrix} 2 \\ -1 \\ 1 \end{bmatrix},$$

   is also not an eigenvector of $\hat{\mathrm{A}}$.

3. We just need to find out which values of α and β make the ket $|a_1\rangle$ an eigenstate of $\hat{A}$ belonging to the eigenvalue $a_1 = -1$:

$$\hat{\mathrm{A}}|a_1\rangle = (-1)\,|a_1\rangle = -|a_1\rangle$$

$$\Leftrightarrow \quad \alpha\hat{\mathrm{A}}|\varepsilon_1^{(1)}\rangle + \beta\hat{\mathrm{A}}|\varepsilon_1^{(2)}\rangle = -\big(\alpha|\varepsilon_1^{(1)}\rangle + \beta|\varepsilon_1^{(2)}\rangle\big)$$

$$\Leftrightarrow \quad \frac{\alpha}{\sqrt{2}}\begin{bmatrix}-1\\1\\0\end{bmatrix} + \frac{\beta}{\sqrt{6}}\begin{bmatrix}-1\\-1\\-2\end{bmatrix} = -\frac{\alpha}{\sqrt{2}}\begin{bmatrix}0\\1\\1\end{bmatrix} - \frac{\beta}{\sqrt{6}}\begin{bmatrix}2\\-1\\1\end{bmatrix}$$

$$\Leftrightarrow \quad \beta = \sqrt{3}\,\alpha.$$

From here we conclude that

$$|a_1\rangle = \alpha\,|\varepsilon_1^{(1)}\rangle + \sqrt{3}\alpha\,|\varepsilon_1^{(2)}\rangle,$$

or, after normalization,

$$|a_1\rangle = \frac{1}{2}|\varepsilon_1^{(1)}\rangle + \frac{\sqrt{3}}{2}|\varepsilon_1^{(2)}\rangle$$

In exactly the same way, we can determine the linear combination that makes $|a_2^{(2)}\rangle$ an eigenvector of $\hat{\mathrm{A}}$ belonging to the eigenvalue $a_2 = +1$, obtaining

$$|a_2^{(2)}\rangle = \frac{\sqrt{3}}{2}|\varepsilon_1^{(1)}\rangle - \frac{1}{2}|\varepsilon_1^{(2)}\rangle.$$

a) From the work done in the previous questions, it follows that $\{|a_1\rangle,\, |a_2^{(1)}\rangle,\, |a_2^{(2)}\rangle\}$ are, by explicit construction, eigenvectors of $\hat{\mathrm{A}}$:

$$\hat{\mathrm{A}}\,|a_1\rangle = a_1|a_1\rangle, \qquad \hat{\mathrm{A}}\,|a_2^{(1)}\rangle = a_2|a_2^{(1)}\rangle, \qquad \hat{\mathrm{A}}\,|a_2^{(2)}\rangle = a_2|a_2^{(2)}\rangle.$$

Therefore, in this basis, the operator $\hat{\mathrm{A}}$ is represented by the diagonal matrix

$$\hat{\mathrm{A}} \quad \mapsto \quad \begin{bmatrix}a_1 & 0 & 0\\0 & a_2 & 0\\0 & 0 & a_2\end{bmatrix} = \begin{bmatrix}-1 & 0 & 0\\0 & 1 & 0\\0 & 0 & 1\end{bmatrix}.$$

From question 1, we know that $|a_1\rangle = |\varepsilon_2\rangle$ is an eigenvector of $\hat{\mathrm{H}}$ belonging to the eigenvalue $\varepsilon_2 = 2$. From question 3, it follows that $|a_1\rangle$ and $|a_2^{(2)}\rangle$ are also eigenvectors of $\hat{\mathrm{H}}$ because each of these is given by a linear combination of $|\varepsilon_1^{(1)}\rangle$ and $|\varepsilon_1^{(2)}\rangle$, which are eigenvectors belonging to the same eigenvalue of $\hat{\mathrm{H}}$:

$$\hat{\mathrm{H}}|a_1\rangle = \alpha\,\hat{\mathrm{H}}\,|\varepsilon_1^{(1)}\rangle + \beta\,\hat{\mathrm{H}}\,|\varepsilon_1^{(2)}\rangle = \varepsilon_1\Big[\alpha\,|\varepsilon_1^{(1)}\rangle + \beta\,|\varepsilon_1^{(2)}\rangle\Big] = \varepsilon_1|a_1\rangle,$$

$$\hat{\mathrm{H}}|a_2^{(2)}\rangle = \gamma\,\hat{\mathrm{H}}\,|\varepsilon_1^{(1)}\rangle + \delta\,\hat{\mathrm{H}}\,|\varepsilon_1^{(2)}\rangle = \varepsilon_1|a_2^{(2)}\rangle.$$

This means that $\hat{\mathrm{H}}$ is also diagonal in this basis, with the matrix representation

$$\hat{\mathrm{H}} \quad \mapsto \quad \begin{bmatrix}\varepsilon_1 & 0 & 0\\0 & \varepsilon_2 & 0\\0 & 0 & \varepsilon_1\end{bmatrix} = \begin{bmatrix}-1 & 0 & 0\\0 & 2 & 0\\0 & 0 & -1\end{bmatrix}.$$

So, in conclusion, both matrices are diagonal in this particular basis:

$$\hat{\mathrm{H}} \mapsto \begin{bmatrix} -1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \qquad \hat{\mathrm{A}} \mapsto \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad \text{in basis } \{|a_1\rangle, |a_2^{(1)}\rangle, |a_2^{(2)}\rangle\}.$$

Note 1: Instead of using the arguments/reasoning above, we could of course just directly compute all the matrix elements

$$\langle a_1|\hat{\mathrm{H}}|a_1\rangle, \quad \langle a_1|\hat{\mathrm{H}}|a_2^{(1)}\rangle, \quad \langle a_1|\hat{\mathrm{H}}|a_2^{(2)}\rangle, \quad \text{etc.}$$

and the same for $\hat{\mathrm{A}}$; the end result is the same.

Note 2: The fact that both $\hat{\mathrm{A}}$ and $\hat{\mathrm{H}}$ are diagonal is not accidental because, as we have seen in Problem 1, $\left[\hat{\mathrm{A}}, \hat{\mathrm{H}}\right] = 0$. From a theorem of matrix algebra, any pair of commuting matrices can be simultaneously diagonalized. What we have done in this problem was to obtain the complete set of orthonormal vectors $\{|a_1\rangle, |a_2^{(1)}\rangle, |a_2^{(2)}\rangle\}$ that are common eigenvectors of both $\hat{\mathrm{A}}$ and $\hat{\mathrm{H}}$. This illustrates the validity of that general theorem in this specific example. In this basis, the two operators are, necessarily, represented by diagonal matrices.
