Problem 3.25

The Hamiltonian for a certain two-level system is

$$\hat{H} = \epsilon(|1\rangle\langle 1| - |2\rangle\langle 2| + |1\rangle\langle 2| + |2\rangle\langle 1|),$$

where $|1\rangle$, $|2\rangle$ is an orthonormal basis and ϵ is a number with the dimensions of energy. Find its eigenvalues and eigenvectors (as linear combinations of $|1\rangle$ and $|2\rangle$. What is the matrix H representing $\hat{H}$ with respect to this basis?

Solution

As shown at the top of page 469,

$$\hat{H}|1\rangle = H_{11}|1\rangle + H_{21}|2\rangle$$

$$\hat{H}|2\rangle = H_{12}|1\rangle + H_{22}|2\rangle$$

apply the Hamiltonian operator $\hat{H}$ to each of the basis vectors to determine the elements of the Hamiltonian matrix H.

$$\begin{aligned}\hat{H}|1\rangle &= \epsilon(|1\rangle\langle 1| - |2\rangle\langle 2| + |1\rangle\langle 2| + |2\rangle\langle 1|)|1\rangle \\ &= \epsilon|1\rangle\langle 1\,|\,1\rangle - \epsilon|2\rangle\langle 2\,|\,1\rangle + \epsilon|1\rangle\langle 2\,|\,1\rangle + \epsilon|2\rangle\langle 1\,|\,1\rangle \\ &= \epsilon|1\rangle(1) - \epsilon|2\rangle(0) + \epsilon|1\rangle(0) + \epsilon|2\rangle(1) \\ &= \epsilon|1\rangle + \epsilon|2\rangle\end{aligned}$$

Note that since the basis is orthonormal, $\langle 1\,|\,1\rangle = \langle 2\,|\,2\rangle = 1$ and $\langle 1\,|\,2\rangle = \langle 2\,|\,1\rangle = 0$.

$$\begin{aligned}\hat{H}|2\rangle &= \epsilon(|1\rangle\langle 1| - |2\rangle\langle 2| + |1\rangle\langle 2| + |2\rangle\langle 1|)|2\rangle \\ &= \epsilon|1\rangle\langle 1\,|\,2\rangle - \epsilon|2\rangle\langle 2\,|\,2\rangle + \epsilon|1\rangle\langle 2\,|\,2\rangle + \epsilon|2\rangle\langle 1\,|\,2\rangle \\ &= \epsilon|1\rangle(0) - \epsilon|2\rangle(1) + \epsilon|1\rangle(1) + \epsilon|2\rangle(0) \\ &= \epsilon|1\rangle - \epsilon|2\rangle\end{aligned}$$

Therefore, the Hamiltonian matrix is

$$\mathsf{H} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} = \begin{pmatrix} \epsilon & \epsilon \\ \epsilon & -\epsilon \end{pmatrix}.$$

Now consider the eigenvalue problem for the Hamiltonian operator, the TISE.

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

With respect to the $|1\rangle, |2\rangle$ basis, it becomes

$$\mathsf{H}|\psi\rangle = E|\psi\rangle$$

$$\mathsf{H}|\psi\rangle - E|\psi\rangle = \mathsf{0}$$

$$(\mathsf{H} - E\mathsf{I})|\psi\rangle = \mathsf{0}. \tag{1}$$

Since $|\psi\rangle$ can't be the zero vector, the matrix in parentheses is singular.

$$\det(\mathsf{H} - E\mathsf{I}) = 0$$

$$\begin{vmatrix} \epsilon - E & \epsilon \\ \epsilon & -\epsilon - E \end{vmatrix} = 0$$

$$(\epsilon - E)(-\epsilon - E) - \epsilon^2 = 0$$

$$E^2 - 2\epsilon^2 = 0$$

$$E = \pm\sqrt{2}\epsilon$$

Therefore, the eigenvalues of H are $E_- = -\sqrt{2}\epsilon$ and $E_+ = \sqrt{2}\epsilon$. Plug them into equation (1) to determine the corresponding eigenvectors.

$$(\mathsf{H} - E_-\mathsf{I})|\psi_-\rangle = 0 \qquad\qquad (\mathsf{H} - E_+\mathsf{I})|\psi_+\rangle = 0$$

$$\begin{pmatrix} \epsilon(\sqrt{2}+1) & \epsilon \\ \epsilon & \epsilon(\sqrt{2}-1) \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \qquad\qquad \begin{pmatrix} -\epsilon(\sqrt{2}-1) & \epsilon \\ \epsilon & -\epsilon(\sqrt{2}+1) \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\left.\begin{aligned} \epsilon(\sqrt{2}+1)\psi_1 + \epsilon\psi_2 = 0 \\ \epsilon\psi_1 + \epsilon(\sqrt{2}-1)\psi_2 = 0 \end{aligned}\right\} \qquad\qquad \left.\begin{aligned} -\epsilon(\sqrt{2}-1)\psi_1 + \epsilon\psi_2 = 0 \\ \epsilon\psi_1 - \epsilon(\sqrt{2}+1)\psi_2 = 0 \end{aligned}\right\}$$

Solve either equation for either ψ_1 or ψ_2.

$$\psi_2 = -(\sqrt{2}+1)\psi_1 \qquad\qquad \psi_2 = (\sqrt{2}-1)\psi_1$$

As a result,

$$|\psi_-\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} \psi_1 \\ -(\sqrt{2}+1)\psi_1 \end{pmatrix} = \psi_1 \begin{pmatrix} 1 \\ -\sqrt{2}-1 \end{pmatrix} \qquad |\psi_+\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} \psi_1 \\ (\sqrt{2}-1)\psi_1 \end{pmatrix} = \psi_1 \begin{pmatrix} 1 \\ \sqrt{2}-1 \end{pmatrix},$$

where ψ_1 is an arbitrary constant. For the eigenvectors to be physically relevant, ψ_1 has to be chosen so that

$$\psi_1^2\left[1^2 + (-\sqrt{2}-1)^2\right] = 1 \qquad\qquad \psi_1^2\left[1^2 + (\sqrt{2}-1)^2\right] = 1$$

$$\psi_1 = \pm\frac{1}{\sqrt{2(2+\sqrt{2})}} \qquad\qquad \psi_1 = \pm\frac{1}{\sqrt{2(2-\sqrt{2})}}.$$

Therefore, the normalized eigenvectors associated with $E_- = -\sqrt{2}\epsilon$ and $E_+ = \sqrt{2}\epsilon$ are

$$|\psi_-\rangle = \frac{1}{\sqrt{2(2+\sqrt{2})}} \begin{pmatrix} 1 \\ -\sqrt{2}-1 \end{pmatrix} = \frac{1}{\sqrt{2(2+\sqrt{2})}} \left[|1\rangle + (-\sqrt{2}-1)|2\rangle\right]$$

and

$$|\psi_+\rangle = \frac{1}{\sqrt{2(2-\sqrt{2})}} \begin{pmatrix} 1 \\ \sqrt{2}-1 \end{pmatrix} = \frac{1}{\sqrt{2(2-\sqrt{2})}} \left[|1\rangle + (\sqrt{2}-1)|2\rangle\right],$$

respectively.