Quiz Solutions (Numericals)

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1. Any arbitrary unitary operator can be written as $U = e^{i\alpha} R_{\hat{n}}(\theta)$ where $R_{\hat{n}}$ is the rotation operator around a unit vector $\hat{n}$. Find the value of α, θ, $\hat{n}$ for the following matrices:

   (a) $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$

   (b) $\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$

   (c) $\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$

   Solution

   If $\hat{n} = (n_x, n_y, n_z)$ is a real unit vector in three dimensions then we can define a rotation about the $\hat{n}$ axis as:

$$R_{\hat{n}}(\theta) \equiv e^{-i\theta \hat{n}\cdot\vec{\sigma}/2} = \cos\frac{\theta}{2} I - i \sin\frac{\theta}{2}(n_x X + n_y Y + n_z Z)$$

   Here, $\vec{\sigma}$ denotes the three components vector (X, Y, Z) of Pauli matrices. Now the best strategy to solve is to either try breaking down the given matrix into sum of Pauli matrices, else try guessing a global phase factor which turns the matrix into a *rotation operator*, $R_k(\theta)$ for any $k \in \{X, Y, Z\}$.

   (a)

$$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \Rightarrow \frac{1}{\sqrt{2}} \left[\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \right] = \frac{1}{\sqrt{2}}(X + Z)$$

$$\therefore \quad \theta = \pi \quad \alpha = \pi/2 \quad n_x = 1, n_y = 0, n_z = 1$$

   (b)

$$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix} \Rightarrow e^{i\frac{\pi}{4}} \begin{bmatrix} e^{-i\frac{\pi}{4}} & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{bmatrix} = e^{i\frac{\pi}{4}} R_z\left(\frac{\pi}{2}\right)$$

$$\therefore \quad \theta = \pi/2 \quad \alpha = \pi/4 \quad n_x = 0, n_y = 0, n_z = 1$$

   (c)

$$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix} \Rightarrow e^{i\frac{\pi}{8}} \begin{bmatrix} e^{-i\frac{\pi}{8}} & 0 \\ 0 & e^{i\frac{\pi}{8}} \end{bmatrix} = e^{i\frac{\pi}{8}} R_z\left(\frac{\pi}{4}\right)$$

$$\therefore \quad \theta = \pi/4 \quad \alpha = \pi/8 \quad n_x = 0, n_y = 0, n_z = 1$$

2. For an O_2^- ion the Hamiltonian position representation (assume computational basis) is of the form

$$\begin{bmatrix} E_0 & -A \\ -A & E_0 \end{bmatrix}$$

Suppose we prepare the ion in the state:

(a)

$$\psi = \frac{1}{5}\begin{pmatrix} 3 \\ 4 \end{pmatrix}$$

(b)

$$\psi = \frac{1}{13}\begin{pmatrix} 5 \\ 12 \end{pmatrix}$$

Then find:

(a) Probability of finding the ion in its energy state E_1

(b) Probability of finding the ion in its energy state E_2

(c) Probability of finding electron at first oxygen atom.

(d) Probability of finding electron at second oxygen atom.

Solution

Given the Hamiltonian $\hat{H}$, the first step would to find its eigenvalues using the characteristic equation for a $|E\rangle = \alpha |0\rangle + \beta |1\rangle$:

$$\hat{H}|E\rangle = E|E\rangle \Rightarrow \begin{bmatrix} E_0 - E & -A \\ -A & E_0 - E \end{bmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0 \Rightarrow \begin{vmatrix} E_0 - E & -A \\ -A & E_0 - E \end{vmatrix} = 0$$

This yields the eigenvalues:

$$E_1 = E_0 + A \qquad E_2 = E_0 - A$$

Substituting these two back into the original eigenvalue equation then gives the equations for their eigenstates:

$$|E_1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = |-\rangle \qquad |E_2\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = |+\rangle$$

Now, for an O_2^- ion prepared in $|\psi\rangle$, the probability of being in state E_1 and E_2 will be just $|\langle E_1|\psi\rangle|^2$ and $|\langle E_2|\psi\rangle|^2$ respectively. Similarly, the probability of being on first and second oxygen atom will be $|\langle 0|\psi\rangle|^2$ and $|\langle 1|\psi\rangle|^2$ respectively. (Marks have been given manually for all the permutations.)

(a)
   i. Probability of finding the ion in its energy state E_1: $\Rightarrow 0.02$
   ii. Probability of finding the ion in its energy state E_2: $\Rightarrow 0.98$
   iii. Probability of finding electron at first oxygen atom: $\Rightarrow 0.36$
   iv. Probability of finding electron at second oxygen atom: $\Rightarrow 0.64$

(b)
   i. Probability of finding the ion in its energy state E_1: $\Rightarrow 0.145$
   ii. Probability of finding the ion in its energy state E_2: $\Rightarrow 0.855$
   iii. Probability of finding electron at first oxygen atom: $\Rightarrow 0.148$
   iv. Probability of finding electron at second oxygen atom: $\Rightarrow 0.852$