Basics of Quantum Mechanics

Quantum computing and Complex geometry, Enjoying math Jeongwoo Jae, September 4, 2024

I. ALGEBRAIC PROPERTIES OF PAULI MATRICES

Definition.—Hermitian operators \mathbf{I} , $\hat{\sigma}_x$, $\hat{\sigma}_y$, and $\hat{\sigma}_z$ are given by

$$\mathbf{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{1}$$

where **I** is called identity operator, and $\hat{\sigma}_x$, $\hat{\sigma}_y$, and $\hat{\sigma}_z$ are called Pauli operators (or matrices). Pauli matrices form a basis for the real vector space of 2×2 Hermitian matrices.

- 1. Show that the identity and Pauli operators are Hermitian.
- 2. Show that the identity and Pauli operators are unitary.
- 3. Show that $I|\psi\rangle = |\psi\rangle$
- 4. Calculate $\hat{\sigma}_x |+\rangle$ and $\hat{\sigma}_x |-\rangle$.
- 5. Calculate $\hat{\sigma}_y \mid +i \rangle$ and $\hat{\sigma}_y \mid -i \rangle$.
- 6. Calculate $\hat{\sigma}_z |0\rangle$ and $\hat{\sigma}_z |1\rangle$.
- 7. Show that an exponential of anti-Hermitian operator $i\hat{G}$, $e^{i\hat{G}}$, is a unitary operator. Use $(\hat{A}^n)^{\dagger} = (\hat{A}^{\dagger})^n$ and $e^{\hat{A}} := \mathbf{I} + \hat{A} + \frac{1}{2!}\hat{A}^2 + \frac{1}{3!}\hat{A}^3 \cdot \cdot \cdot \cdot \cdot \hat{G}$ is called *generator*.

Definition (Bloch representation).—An arbitrary Hermitian operator can be written by a linear combination of the identity and Pauli operators with real-valued coefficients. In other words, a given Hermitian operator \hat{H} can be read

$$\hat{H} = c_0 \mathbf{I} + c_x \hat{\sigma}_x + c_y \hat{\sigma}_y + c_z \hat{\sigma}_z. \tag{2}$$

- 1. Show that Pauli operators are traceless, i.e., $\operatorname{Tr} \hat{\sigma}_i = 0$ for all $i \in \{x, y, z\}$.
- 2. Calculate $\text{Tr}\hat{\sigma}_i\hat{\sigma}_j$ for $i,j\in\{x,y,z\}$. Note that $\text{Tr}\hat{A}\hat{B}=\text{Tr}\hat{B}\hat{A}$.
- 3. Calculate $\text{Tr}\hat{H}\mathbf{I}$, $\text{Tr}\hat{H}\hat{\sigma}_x$, $\text{Tr}\hat{H}\hat{\sigma}_y$, and $\text{Tr}\hat{H}\hat{\sigma}_z$.

II. DENSITY MATRIX

A density matrix $\hat{\varrho}$ of a quantum state $|\psi\rangle=\alpha\,|0\rangle+\beta\,|1\rangle$ is defined by

$$\hat{\varrho} := |\psi\rangle\langle\psi| = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \begin{pmatrix} \alpha^* & \beta^* \end{pmatrix} = \begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \alpha^*\beta & |\beta|^2 \end{pmatrix}$$
 (3)

- 1. Show that the density matrix $\hat{\varrho}$ is a Hermitian operator.
- 2. Show that

$$|0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad |1\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$
 (4)

3. Show that the Bloch representation of $|0\rangle\langle 0|$ and $|1\rangle\langle 1|$ is given by

$$|0\rangle\langle 0| = \frac{1}{2} \left(\mathbf{I} + \hat{\sigma}_x \right) \quad \text{and} \quad |1\rangle\langle 1| = \frac{1}{2} \left(\mathbf{I} - \hat{\sigma}_x \right).$$
 (5)

Remark.—A density matrix of qubit state $|\psi\rangle = \sin\frac{\theta}{2}|0\rangle + e^{i\phi}\cos\frac{\theta}{2}|1\rangle$ is given by

$$|\psi\rangle\langle\psi| = \frac{1}{2} \left(\mathbf{I} + \sin\theta\cos\phi\hat{\sigma}_x + \sin\theta\sin\phi\hat{\sigma}_y + \cos\theta\hat{\sigma}_z \right)$$
$$= \frac{1}{2} \left(\mathbf{I} + \vec{r} \cdot \vec{\sigma} \right), \tag{6}$$

where $\vec{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$ and the vector $\vec{r} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$ is called *Bloch vector*. It is worth to note that $|\psi\rangle\langle\psi| \geq 0$ if and only if $|\vec{r}| \leq 1$.