QT207: Introduction to Quantum Computation

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Problem 1

Let $\{|\varphi_1\rangle, \dots, |\varphi_n\rangle\}$ and $\{|\psi_1\rangle, \dots, |\psi_n\rangle\}$ be orthonormal bases of a finite-dimensional vector space V. Define

$$U = \sum_{i=1}^{n} |\psi_i\rangle\langle\varphi_i|$$

1. **Show that U is unitary, i.e., $U^\dagger U = I$.**

$$\begin{aligned} U^\dagger U &= \left(\sum_{i=1}^{n} |\varphi_i\rangle\langle\psi_i|\right)\left(\sum_{j=1}^{n} |\psi_j\rangle\langle\varphi_j|\right) \\ &= \sum_{i,j=1}^{n} |\varphi_i\rangle\langle\psi_i|\psi_j\rangle\langle\varphi_j| \end{aligned}$$

   Since $\langle\psi_i|\psi_j\rangle = \delta_{ij}$ (orthonormality),

$$\begin{aligned} &= \sum_{i=1}^{n} |\varphi_i\rangle\langle\varphi_i| \\ &= I \end{aligned}$$

   Thus, U is unitary.

2. **Show that $U|\varphi_j\rangle = |\psi_j\rangle$ for all j.**

$$\begin{aligned} U|\varphi_j\rangle &= \sum_{i=1}^{n} |\psi_i\rangle\langle\varphi_i|\varphi_j\rangle \\ &= \sum_{i=1}^{n} |\psi_i\rangle\delta_{ij} \quad (\text{since } \langle\varphi_i|\varphi_j\rangle = \delta_{ij}) \\ &= |\psi_j\rangle \end{aligned}$$

   So U maps each $|\varphi_j\rangle$ to $|\psi_j\rangle$.

Problem 2

Let H be Hermitian and U be unitary.

1. **All eigenvalues of U have unit modulus.**

   $U|u\rangle = \lambda|u\rangle \implies \langle u|U^\dagger = \langle u|\lambda^*$ where λ & λ^* are the eigenvalues of U and $U^\dagger$ respectively.

$$\langle u|U^\dagger U|u\rangle = \langle u|U^\dagger \lambda|u\rangle = \langle u|\lambda^*\lambda|u\rangle$$
$$\langle u|I|u\rangle = \langle u||\lambda|^2|u\rangle = |\lambda|^2\langle u|u\rangle$$
$$\langle u|u\rangle = |\lambda|^2\langle u|u\rangle \implies |\lambda|^2 = 1$$

   Since λ is a complex number and the only condition is the magnitude = 1, we can write $\lambda = e^{i\phi}$ for some **real** ϕ.

   Each unitary U can be written as $U = \exp(iH)$ for some Hermitian H.

   We will be using the following properties to prove the above :

   - Unitary matrix U is diagonalizable and can be written as $U = V^{-1}DV$ for some diagonal matrix D and the Diagonal matrix contains all the eigen values of U.
   - Exponent of a diagonal matrix is the diagonal matrix of the exponents, i.e., if $D = \text{diag}(d_1, d_2, \ldots, d_n)$, then $\exp(D) = \text{diag}(e^{d_1}, e^{d_2}, \ldots, e^{d_n})$.
   - if $U = V^{-1}DV$, then $\exp(U) = V^{-1}\exp(D)V$.
   - For a Hermitian matrix $H^\dagger = H$ and eigenvalues of H are real, diagonalizable via unitary tranformation i.e $H = WD'W^{-1}$ where D' is diagonal matrix with real eigenvalues.

   Let U be a unitary matrix with eigen values $\lambda_j = e^{i\phi_j} \quad j = 1\ldots n$.

$$\textbf{Defining}: \; D' = \text{diag}(\phi_j) \quad \& \quad D = \text{diag}(e^{i\phi_j}) \implies exp(iD') = D$$

   Then:

$$U = V^{-1}DV = V^{-1}\exp(iD')V$$
$$\text{Let } H = V^{-1}D'V \implies exp(iH) = V^{-1}\exp(iD')V$$
$$\implies U = \exp(iH)$$

   The Above H is Hermitian as the matrix is a diagonalizable matrix with real eigen values ϕ_j.

2. **Two eigenvectors of U with different eigenvalues are orthogonal.** Let $U|u_1\rangle = \lambda_1|u_1\rangle$ and $U|u_2\rangle = \lambda_2|u_2\rangle$ with $\lambda_1 \neq \lambda_2$. Consider

$$\langle u_1|U|u_2\rangle = \lambda_2\langle u_1|u_2\rangle$$
$$\langle Uu_1|u_2\rangle = \lambda_1\langle u_1|u_2\rangle$$
$$\text{But } \langle Uu_1|u_2\rangle = \langle u_1|U^\dagger|u_2\rangle = \lambda_2^*\langle u_1|u_2\rangle$$

Since U is unitary, $\lambda_1^* = \lambda_1^{-1}$ and $|\lambda_1| = |\lambda_2| = 1$. Equating both expressions:

$$\lambda_1\langle u_1|u_2\rangle = \lambda_2^*\langle u_1|u_2\rangle \implies (\lambda_1 - \lambda_2^*)\langle u_1|u_2\rangle = 0$$

Since $\lambda_1 \neq \lambda_2$, $\langle u_1|u_2\rangle = 0$. Thus, eigenvectors with distinct eigenvalues are orthogonal.

Same for Hermitian H: If $H|v_1\rangle = \mu_1|v_1\rangle$, $H|v_2\rangle = \mu_2|v_2\rangle$, $\mu_1 \neq \mu_2$, then

$$\begin{aligned}\langle v_1|H|v_2\rangle &= \mu_2\langle v_1|v_2\rangle \\ \langle Hv_1|v_2\rangle &= \mu_1\langle v_1|v_2\rangle \\ \text{But } \langle Hv_1|v_2\rangle &= \langle v_1|H|v_2\rangle \text{ (since } H \text{ is Hermitian)}\end{aligned}$$

So $(\mu_1 - \mu_2)\langle v_1|v_2\rangle = 0$. If $\mu_1 \neq \mu_2$, $\langle v_1|v_2\rangle = 0$.

3. **All columns of U are orthonormal.** Write U in the basis $\{|\varphi_j\rangle\}$: $U|\varphi_j\rangle = |\psi_j\rangle$. The columns of U are $\{|\psi_j\rangle\}$.

$$\begin{aligned}\langle\psi_i|\psi_j\rangle &= \langle\varphi_i|U^\dagger U|\varphi_j\rangle \\ &= \langle\varphi_i|I|\varphi_j\rangle = \delta_{ij}\end{aligned}$$

Thus, the columns of U form an orthonormal set. Similarly, since U is unitary, its rows are also orthonormal.

Problem 3

Let P be a linear operator on a finite-dimensional complex inner-product space V with $P^2 = P$.

1. **All eigenvalues of P are 0 or 1.**

$$\begin{aligned}P|v\rangle &= \lambda|v\rangle \\ P^2|v\rangle = P(P|v\rangle) = P(\lambda|v\rangle) = \lambda P|v\rangle &= \lambda^2|v\rangle \\ \text{But } P^2|v\rangle = P|v\rangle &= \lambda|v\rangle \\ \implies \lambda^2 = \lambda \implies \lambda &= 0 \text{ or } 1\end{aligned}$$

Thus, P is diagonalizable.

2. **The complementary operator $Q = I - P$ is also a projector.**

$$\begin{aligned}Q^2 &= (I-P)^2 = I - 2P + P^2 \\ &= I - 2P + P = I - P = Q\end{aligned}$$

3. **If $\{|u_i\rangle\}_{i=1}^r$ is an orthonormal set, then $P = \sum_{i=1}^r |u_i\rangle\langle u_i|$ is a projector.**

$$\begin{aligned} P^2 &= \left(\sum_{i=1}^r |u_i\rangle\langle u_i|\right)^2 \\ &= \sum_{i,j=1}^r |u_i\rangle\langle u_i|u_j\rangle\langle u_j| \\ &= \sum_{i=1}^r |u_i\rangle\langle u_i| = P \end{aligned}$$

Problem 4

The Pauli matrices are:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

They are Hermitian, unitary, and traceless. Prove:

1. **Squares and inverses: $\sigma_k^2 = I$ and $\sigma_k^{-1} = \sigma_k$.**

$$\begin{aligned} \sigma_x^2 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I \\ \sigma_y^2 &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I \\ \sigma_z^2 &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I \end{aligned}$$

   Since $\sigma_k^2 = I$, $\sigma_k^{-1} = \sigma_k$.

2. **Commutators and anticommutators: $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$ and $\{\sigma_i, \sigma_j\} = 2\delta_{ij}I$.**

$$\begin{aligned} [\sigma_x, \sigma_y] &= \sigma_x\sigma_y - \sigma_y\sigma_x = i\sigma_z - (-i\sigma_z) = 2i\sigma_z \\ [\sigma_y, \sigma_z] &= 2i\sigma_x, \quad [\sigma_z, \sigma_x] = 2i\sigma_y \\ \{\sigma_i, \sigma_j\} &= \sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij}I \end{aligned}$$

3. **Product identity: $\sigma_i\sigma_j = \delta_{ij}I + i\epsilon_{ijk}\sigma_k$.**

$$\begin{aligned} \sigma_x\sigma_y &= i\sigma_z, \quad \sigma_y\sigma_x = -i\sigma_z \\ \sigma_i\sigma_j &= \delta_{ij}I + i\epsilon_{ijk}\sigma_k \end{aligned}$$

4. **Vector identities for $\mathbf{a}, \mathbf{b} \in \mathbb{R}^3$:**

$$\begin{aligned} (\mathbf{a} \cdot \boldsymbol{\sigma})^2 &= |\mathbf{a}|^2 I \\ (\mathbf{a} \cdot \boldsymbol{\sigma})(\mathbf{b} \cdot \boldsymbol{\sigma}) &= (\mathbf{a} \cdot \mathbf{b})I + i(\mathbf{a} \times \mathbf{b}) \cdot \boldsymbol{\sigma} \end{aligned}$$

Problem 5

A density operator ρ on a finite-dimensional Hilbert space $\mathcal{H}$ for an ensemble $\{p_i, |\psi_i\rangle\}$ is $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$. Prove:

1. ρ is Hermitian, positive semidefinite, and $\mathrm{Tr}(\rho) = 1$.

$$\begin{aligned} \rho^\dagger &= \sum_i p_i (|\psi_i\rangle\langle\psi_i|)^\dagger = \sum_i p_i |\psi_i\rangle\langle\psi_i| = \rho \\ \langle\phi|\rho|\phi\rangle &= \sum_i p_i |\langle\psi_i|\phi\rangle|^2 \geq 0 \\ \mathrm{Tr}(\rho) &= \sum_i p_i \langle\psi_i|\psi_i\rangle = \sum_i p_i = 1 \end{aligned}$$

2. $0 \leq \mathrm{Tr}(\rho^2) \leq 1$ and ρ represents a pure state $\iff \rho^2 = \rho \implies \mathrm{Tr}(\rho^2) = 1$.

$$\begin{aligned} \mathrm{Tr}(\rho^2) &= \mathrm{Tr}\left(\sum_{i,j} p_i p_j |\psi_i\rangle\langle\psi_i|\psi_j\rangle\langle\psi_j|\right) \\ &= \sum_{i,j} p_i p_j |\langle\psi_i|\psi_j\rangle|^2 \leq \sum_{i,j} p_i p_j = (\sum_i p_i)^2 = 1 \end{aligned}$$

   For pure states, $\rho = |\psi\rangle\langle\psi|$, $\rho^2 = \rho$, $\mathrm{Tr}(\rho^2) = 1$. For mixed states, $\mathrm{Tr}(\rho^2) < 1$.

3. Spectral form: $\rho = \sum_k \lambda_k |\phi_k\rangle\langle\phi_k|$, $\lambda_k \geq 0$, $\sum_k \lambda_k = 1$. Probabilities λ_k, purity $\mathrm{Tr}(\rho^2) = \sum_k \lambda_k^2$.

4. Expectation values: For observable A, $\langle A\rangle = \mathrm{Tr}(\rho A) = \sum_i p_i \langle\psi_i|A|\psi_i\rangle$.

Problem 6

In finite dimensions, positivity of an operator X means $\langle\psi|X|\psi\rangle \geq 0$ for all $|\psi\rangle$. Prove:

1. A positive operator is Hermitian.

   Proof. Write A as $A = B + iC$ where $B = (A + A^\dagger)/2$ and $C = (A - A^\dagger)/(2i)$ are Hermitian. For any vector $|\psi\rangle$,

$$\langle\psi|A|\psi\rangle = \langle\psi|B|\psi\rangle + i\langle\psi|C|\psi\rangle.$$

   By hypothesis the left-hand side is real and nonnegative for every $|\psi\rangle$, so its imaginary part must vanish for all $|\psi\rangle$, i.e.

$$\langle\psi|C|\psi\rangle = 0 \qquad \text{for all } |\psi\rangle.$$

   Since C is Hermitian it has a spectral decomposition $C = \sum_k c_k |\phi_k\rangle\langle\phi_k|$ with real eigenvalues c_k. Plugging $|\psi\rangle = |\phi_k\rangle$ gives $c_k = 0$ for every k. Hence $C = 0$ and $A = B$ is Hermitian. □

2. For any linear operator A, the operator $A^\dagger A$ is positive and Hermitian.

   Proof. For any $|\psi\rangle$,

   $$\langle\psi|A^\dagger A|\psi\rangle = \langle A\psi|A\psi\rangle = \||A|\psi\rangle\|^2 \geq 0,$$

   so $A^\dagger A$ is positive. Moreover $(A^\dagger A)^\dagger = A^\dagger(A^\dagger)^\dagger = A^\dagger A$, so it is Hermitian. Consequently all eigenvalues of $A^\dagger A$ are real and nonnegative. $\square$

Problem 7

For matrices $A \in \mathbb{C}^{m\times n}$, $C \in \mathbb{C}^{n\times p}$, $B \in \mathbb{C}^{k\times \ell}$ and $D \in \mathbb{C}^{\ell\times q}$ (so the products below are conformable), prove the mixed-product property

$$(A \otimes B)(C \otimes D) = (AC) \otimes (BD).$$

Proof. We prove the identity by comparing matrix entries using the standard row/column ordering for Kronecker products. Index the rows/columns of $A \otimes B$ by the pair (i, α) with $i = 1, \ldots, m$ and $\alpha = 1, \ldots, k$, similarly for columns by (j, β). The $((i, \alpha), (j, \delta))$ entry of the product is

$$\begin{aligned}
&\big[(A \otimes B)(C \otimes D)\big]_{(i,\alpha),(j,\delta)} \\
&= \sum_{(r,\beta)} (A \otimes B)_{(i,\alpha),(r,\beta)}\,(C \otimes D)_{(r,\beta),(j,\delta)} \\
&= \sum_{r=1}^{n}\sum_{\beta=1}^{\ell} \big(A_{ir}B_{\alpha\beta}\big)\big(C_{rj}D_{\beta\delta}\big) \\
&= \Big(\sum_{r=1}^{n} A_{ir}C_{rj}\Big)\Big(\sum_{\beta=1}^{\ell} B_{\alpha\beta}D_{\beta\delta}\Big) \\
&= (AC)_{ij}\,(BD)_{\alpha\delta}.
\end{aligned}$$

The right-hand side is exactly the $((i, \alpha), (j, \delta))$ entry of $(AC) \otimes (BD)$. Since all matrix entries agree, the two matrices are equal. $\square$