QT207: Introduction to Quantum Computation

Assignment #1 | Due: 4 Sep. 2025, Thursday | Maximum Marks: 30

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August 26, 2025

Note:

- Show all steps and justify answers clearly; unreadable work may not receive credit.
- All vector spaces are finite-dimensional.
- For any doubts in the questions, please ask the TAs.
- Submit the assignment at the end of class to the TAs.

Problem 1 (4 marks)**.** Let $\{|\varphi_1\rangle, \dots, |\varphi_n\rangle\}$ be an orthonormal (ON) basis of a vector space V, and let $\{|\psi_1\rangle, \dots, |\psi_n\rangle\}$ be a possibly different ON basis of V. Define

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

1. Show that U is unitary, i.e., $U^\dagger U = I$. *(2 marks)*
2. Show that $U|\varphi_j\rangle = |\psi_j\rangle$ for all j. *(2 marks)*

Thus, U is a change-of-basis operator that transforms one ON basis into another.

Problem 2 (5 marks)**.** Let H and U be Hermitian and unitary respectively. Prove the following.

1. All eigenvalues of U have unit modulus (of the form $e^{i\phi}$ for $\phi \in \mathbb{R}$). Use this to show that each unitary U can be written as $U = \exp(iH)$ for some Hermitian H. *(2 marks)*
2. Two eigenvectors of U with different eigenvalues are orthogonal. Prove the same for H. *(2 marks)*
3. All the columns of U are orthonormal. Prove the same for the rows. *(1 mark)*

Problem 3 (5 marks)**.** Let P be a linear operator on a finite-dimensional complex inner-product space V satisfying $P^2 = P$. Prove:

1. All eigenvalues of P are either 0 or 1. Hence, conclude that P is diagonalizable. *(2 marks)*
2. The complementary operator $Q := I - P$ is also a projector, i.e., $Q^2 = Q$. *(1 mark)*
3. If $\{|u_i\rangle\}_{i=1}^{r}$ is an orthonormal set (not necessarily complete), then

$$P = \sum_{i=1}^{r} |u_i\rangle\langle u_i|$$

is a projector. *(2 marks)*

Problem 4 (6 marks)**.** 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 $\sigma_k^{-1} = \sigma_k$. As $\mathrm{tr}(\sigma_k) = 0$ and eigenvalues are ± 1. *(1 mark)*
2. Commutators and anticommutators: $[\sigma_i, \sigma_j] = 2i\,\varepsilon_{ijk}\sigma_k$ and $\{\sigma_i, \sigma_j\} = 2\delta_{ij}I$. *(2 marks)*
3. Product identity: $\sigma_i\sigma_j = \delta_{ij}I + i\,\varepsilon_{ijk}\sigma_k$. *(1 mark)*
4. Vector identities for $\mathbf{a}, \mathbf{b} \in \mathbb{R}^3$: $(\mathbf{a}\cdot\boldsymbol{\sigma})^2 = \|\mathbf{a}\|^2 I$ and $(\mathbf{a}\cdot\boldsymbol{\sigma})(\mathbf{b}\cdot\boldsymbol{\sigma}) = (\mathbf{a}\cdot\mathbf{b})I + i(\mathbf{a}\times\mathbf{b})\cdot\boldsymbol{\sigma}$. *(2 marks)*

Problem 5 (6 marks)**.** A density operator (density matrix) ρ on a finite-dimensional Hilbert space $\mathcal{H}$ for an ensemble $\{p_i, |\psi_i\rangle\}$ ($p_i \geq 0$, $\sum_i p_i = 1$) is $\rho = \sum_i p_i\, |\psi_i\rangle\langle\psi_i|$. Prove:

1. ρ is Hermitian, positive semidefinite, and $\mathrm{Tr}(\rho) = 1$. *(2 marks)*
2. $0 \leq \mathrm{Tr}\big(\rho^2\big) \leq 1$ and that

   $$\rho \text{ represents a pure state } \iff \rho^2 = \rho \iff \mathrm{Tr}\big(\rho^2\big) = 1.$$

   Conclude that for mixed states $\mathrm{Tr}\big(\rho^2\big) < 1$.. *(2 marks)*
3. Spectral form: Using the spectral theorem for Hermitian operators, write $\rho = \sum_k \lambda_k\, |\phi_k\rangle\langle\phi_k|$, where $\{|\phi_k\rangle\}$ is an orthonormal eigenbasis and $\lambda_k \geq 0$, $\sum_k \lambda_k = 1$. Interpret λ_k as probabilities and relate $\mathrm{Tr}\big(\rho^2\big)$ to the purity $\sum_k \lambda_k^2$. *(1 mark)*
4. Expectation values: for any observable A, $\langle A\rangle = \mathrm{Tr}(\rho A) = \sum_i p_i\, \langle\psi_i|\, A\, |\psi_i\rangle$.. *(1 mark)*

Problem 6 (2 marks)**.** In finite dimensions, positivity of X means $\langle\psi|\, X\, |\psi\rangle \geq 0$ for all $|\psi\rangle$. Using this, prove:

1. A positive operator is Hermitian: if $\langle\psi|\, A\, |\psi\rangle \geq 0$ for all $|\psi\rangle$ then $A = A^\dagger$. *(1 mark)*

   Hint. Any operator A can be decomposed as $A = B + iC$, where both B and C are hermitian.
2. For any linear operator A, the operator $A^\dagger A$ is positive; hence $A^\dagger A$ is Hermitian with nonnegative eigenvalues. *(1 mark)*

Problem 7 (2 marks)**.** For matrices $A \in \mathbb{C}^{m\times n}$ and $B \in \mathbb{C}^{k\times\ell}$, the Kronecker product $A\otimes B$ is the $mk \times n\ell$ block matrix

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & \cdots & a_{1n}B \\ \vdots & \ddots & & \vdots \\ a_{m1}B & a_{m2}B & \cdots & a_{mn}B \end{bmatrix}.$$

Prove the mixed-product property for conformable matrices:

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

(2 marks)