Quantum Computing — Homework 1

Bra-Ket Notation, Linear Algebra, and Quantum Subroutines

Work through all the problems, your abilities will be tested.

Prerequisites. Basic linear algebra (vector spaces, matrices, inner products). No prior quantum mechanics required.

Notation summary.

- $|\psi\rangle \in \mathcal{H}$: ket (column vector). $\langle\psi| = |\psi\rangle^\dagger$: bra (row vector).
- $\langle\phi|\psi\rangle$: inner product. $|\phi\rangle\langle\psi|$: outer product (rank-1 operator).
- $\mathbf{1}$: identity operator. $[A, B] = AB - BA$: commutator.
- $\delta_{ab} = \begin{cases} 1 & \text{if } a = b \\ 0 & \text{Otherwise} \end{cases}$ $\epsilon_{abc} = \begin{cases} +1 & \text{if } (a,b,c) \text{ is } (1,2,3),(2,3,1),(3,1,2) \\ -1 & \text{if } (a,b,c) \text{ is } (1,3,2),(2,1,3),(3,2,1) \\ 0 & \text{Otherwise} \end{cases}$

Part I Foundations of Bra-Ket Notation

Exercise 1 — Inner products, norms and projections

Let $\mathcal{H} = \mathbb{C}^n$ with the standard inner product $\langle\phi|\psi\rangle = \sum_{i=1}^n \phi_i^* \psi_i$.

(a) Show that $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^*$.

(b) The single-qubit states

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

are defined in the computational basis $\{|0\rangle, |1\rangle\}$. Compute $\langle+|-\rangle$, $\langle+|+\rangle$, and $\| |+\rangle + i\,|-\rangle \|$.

(c) Let $|\psi\rangle \in \mathcal{H}$ be normalised. Show that $P_\psi = |\psi\rangle\langle\psi|$ satisfies $P_\psi^2 = P_\psi$ (idempotent) and $P_\psi^\dagger = P_\psi$ (Hermitian). Why are these properties important? Which class of operators are characterized by these two properties?

Exercise 2 — Hermitian and unitary operators

(a) Show that eigenvalues of a Hermitian operator $H = H^\dagger$ are real, and that eigenvectors belonging to distinct eigenvalues are orthogonal.

(b) Let U be unitary ($U^\dagger U = \mathbf{1}$). Prove: (i) U preserves inner products: $\langle U\phi|U\psi\rangle = \langle\phi|\psi\rangle$; (ii) eigenvalues of U lie on the unit circle.

(c) The Pauli matrices are

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

Verify that each is both Hermitian and unitary. Show that $\sigma_x\sigma_y = i\sigma_z$ and deduce $\sigma_a\sigma_b = \delta_{ab}\mathbf{1} + i\varepsilon_{abc}\sigma_c$. Where δ_{ab} is the Kronecker delta function and ϵ_{abc} is the Levi-Civita tensor as defined above.

(d) For a Hermitian operator satisfying $H^2 = \mathbf{1}$, show that

$$e^{i\theta H} = \cos\theta\,\mathbf{1} + i\sin\theta\, H.$$

Hint: Expand the matrix exponential as a power series and split even/odd terms.

Exercise 3 — Change of basis

Let $\{|\delta_k\rangle\}$ and $\{|\tilde{\delta}_k\rangle\}$ be two orthonormal bases of $\mathcal{H}$, and define $U^j{}_k = \langle\tilde{\delta}^j|\delta_k\rangle$.

(a) Show that U is a unitary matrix.

(b) Show that ket components transform as $\tilde{\psi}^k = \sum_j U^k{}_j\psi^j$, and operator matrix elements as $\tilde{A}^j{}_m = \sum_{k,l} U^j{}_k\, A^k{}_l\, (U^\dagger)^l{}_m$.

(c) The **Hadamard matrix** $H = \frac{1}{\sqrt{2}}\left(\begin{smallmatrix}1 & 1\\ 1 & -1\end{smallmatrix}\right)$ changes between the computational basis $\{|0\rangle, |1\rangle\}$ and the Hadamard basis $\{|+\rangle, |-\rangle\}$. Express the Pauli Z operator in the Hadamard basis. What familiar operator do you recover?

Part II Multi-Qubit Systems and Tensor Products

Exercise 4 — Tensor products and Bell states

(a) The two-qubit computational basis is $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ where $|ij\rangle \equiv |i\rangle \otimes |j\rangle$. Express the four **Bell states**

$$|\Phi^\pm\rangle = \frac{1}{\sqrt{2}}\big(|00\rangle \pm |11\rangle\big), \quad |\Psi^\pm\rangle = \frac{1}{\sqrt{2}}\big(|01\rangle \pm |10\rangle\big)$$

as column vectors in $\mathbb{C}^4$. Verify they form an orthonormal basis.

(b) Show $(A \otimes B)^\dagger = A^\dagger \otimes B^\dagger$ and $(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$.

(c) A state $|\Psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ is *separable* if $|\Psi\rangle = |\phi\rangle \otimes |\chi\rangle$. Show that none of the four Bell states is separable.

(d) Compute $(X \otimes Z)|\Phi^+\rangle$ and express the result as a linear combination of Bell states.

Part III Quantum Gates as Unitary Operators

Exercise 5 — Single-qubit gates

(a) The rotation about the z-axis is $R_z(\theta) = e^{-i\theta Z/2} = \mathrm{diag}(e^{-i\theta/2}, e^{i\theta/2})$. Derive explicit matrix forms for $R_x(\theta) = e^{-i\theta X/2}$ and $R_y(\theta) = e^{-i\theta Y/2}$.

(b) Show $H^2 = \mathbf{1}$ and prove $HXH = Z$, $HZH = X$, $HYH = -Y$.

(c) The **phase gate** is $S = \left(\begin{smallmatrix} 1 & 0 \\ 0 & i \end{smallmatrix}\right)$. Show $S = R_z(\pi/2)$ up to global phase, compute HSH, and identify the result.

(d) Show that every single-qubit unitary can be written as $U = e^{i\alpha} R_z(\beta) R_y(\gamma) R_z(\delta)$ for real $\alpha, \beta, \gamma, \delta$.

Hint: Every $U \in SU(2)$ *has the form* $\left(\begin{smallmatrix} a & -b^* \\ b & a^* \end{smallmatrix}\right)$ *with* $|a|^2 + |b|^2 = 1$; *parametrise using polar form.*

Exercise 6 — Two-qubit gates

The controlled-NOT gate acts on two qubits $|\psi_1\rangle \otimes |\psi_2\rangle$. The qubit $|\psi_1\rangle$ is known as the control and the the qubit $|\psi_2\rangle$ is the target. If the control qubit is in the state $|0\rangle$ then the Identity is applied to the target and if the control is in state $|1\rangle$ then the X gate is applied to the target qubit

(a) The **CNOT** gate is $\mathrm{CNOT} = |0\rangle\langle 0| \otimes \mathbf{1} + |1\rangle\langle 1| \otimes X$. Write it as a 4×4 matrix and verify unitarity.

(b) Show $\mathrm{CNOT}\,(|+\rangle \otimes |0\rangle) = |\Phi^+\rangle$. Describe a two-gate circuit that prepares $|\Phi^+\rangle$ from $|00\rangle$.

(c) Prove

$$(H \otimes H)\,\mathrm{CNOT}_{1\to 2}\,(H \otimes H) = \mathrm{CNOT}_{2\to 1}.$$

(d) The **Toffoli** gate flips the target iff both controls are $|1\rangle$. Write it in bra-ket notation analogous to part (a) and as an 8×8 matrix.

Part V Bonus Problems

Exercise 7 — Commutators and uncertainty ⋆

(a) Let $[A, B] = iC$ with C Hermitian. Prove $\Delta A\, \Delta B \geq \dfrac{1}{2}\big|\langle C\rangle\big|$, where $\Delta A = \sqrt{\langle A^2\rangle - \langle A\rangle^2}$.

(b) Using $[X_j, Z_j] = 2iY_j$, find the minimum of $\Delta X_1\, \Delta Z_1$ for the state $|+\rangle \otimes |0\rangle$.

(c) The Heisenberg equation is $\frac{d}{dt}A(t) = \frac{i}{\hbar}[H, A(t)]$. For $H = \frac{\hbar\omega}{2}Z$, solve this ODE with $A(0) = X$.

Exercise 8 — Trace and distinguishability ⋆⋆

(a) Show $\mathrm{Tr}(A)$ is basis-independent. Deduce that $UAU^\dagger$ and A have the same eigenvalues.

(b) The **trace distance** is $T(\rho, \sigma) = \frac{1}{2}\,\mathrm{Tr}\,|\rho - \sigma|$, where $|M| = \sqrt{M^\dagger M}$. Compute $T(|0\rangle\langle 0|\,, |+\rangle\langle +|)$ explicitly.