Crash Course in Quantum Mechanics for Quantum Computing
Qubits, Pauli Algebra, Bloch Sphere & Density Matrices

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1 Refresher: Schrödinger Equation & Observables

1.1 States and dynamics

A quantum state is a unit vector $|\psi(t)\rangle$ in a complex Hilbert space $\mathcal{H}$ (finite-dimensional here). The evolution is (for time-independent Hamiltonian $\hat{H}$)

$$i\hbar\,\partial_t\,|\psi(t)\rangle = \hat{H}\,|\psi(t)\rangle \quad \Longrightarrow \quad |\psi(t)\rangle = e^{-i\hat{H}t/\hbar}\,|\psi(0)\rangle\,, \tag{1}$$

where $U(t) = e^{-i\hat{H}t/\hbar}$ is unitary.

1.2 Observables and Born rule

Observables are represented by Hermitian operators $\hat{A} = \hat{A}^\dagger$. If $\hat{A}\,|a_k\rangle = a_k\,|a_k\rangle$, then measuring $\hat{A}$ in state $|\psi\rangle$ returns a_k with probability $|\langle a_k|\psi\rangle|^2$. Expectation values are $\langle \hat{A}\rangle_\psi = \langle\psi|\,\hat{A}\,|\psi\rangle$.

Proposition 1 (Reality of eigenvalues). *If $\hat{A} = \hat{A}^\dagger$, then its eigenvalues are real.*

Proof. $\hat{A}\,|v\rangle = \lambda\,|v\rangle \Rightarrow \langle v|\,\hat{A}\,|v\rangle = \lambda\,\langle v|v\rangle$. But $\langle v|\,\hat{A}\,|v\rangle$ is real since $\hat{A}$ is Hermitian. As $\langle v|v\rangle > 0$, $\lambda \in \mathbb{R}$. $\square$

QC connection. Because $U(t)$ is unitary, quantum gates are unitary matrices. Hamiltonians generate gates via exponentials.

2 Dirac Notation and Linear Algebra Basics

Fix an orthonormal basis $\{|i\rangle\}_{i=1}^d$ of $\mathcal{H} \simeq \mathbb{C}^d$. Every vector $|\psi\rangle = \sum_i c_i\,|i\rangle$ with $\sum_i |c_i|^2 = 1$. Operators act linearly, and in a basis are $d \times d$ matrices. The adjoint is the conjugate transpose.

Proposition 2 (Spectral theorem (finite-dim.)). *Every Hermitian $\hat{A}$ has an orthonormal eigenbasis and $\hat{A} = \sum_k a_k\,|a_k\rangle\,\langle a_k|$.*

Proposition 3 (Commuting observables). *If Hermitians $\hat{A}, \hat{B}$ commute and have nondegenerate spectra, they share an eigenbasis. In the degenerate case, each eigenspace of $\hat{A}$ can be chosen to diagonalize $\hat{B}$ simultaneously.*

QC connection. Simultaneous eigenbases underlie measurement in different registers and controlled gates.

3 Qubits and Tensor Products

3.1 Single qubit

The two-dimensional Hilbert space $\mathcal{H} \simeq \mathbb{C}^2$ with computational basis $|0\rangle = \left(\begin{smallmatrix}1\\0\end{smallmatrix}\right)$, $|1\rangle = \left(\begin{smallmatrix}0\\1\end{smallmatrix}\right)$. A pure state is $|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$, $|\alpha|^2 + |\beta|^2 = 1$.

3.2 Two qubits and tensor products

For systems A, B, the joint space is $\mathcal{H}_A \otimes \mathcal{H}_B$ (dimension multiplies). If $|\psi\rangle_A = \alpha\,|0\rangle + \beta\,|1\rangle$ and $|\phi\rangle_B = \gamma\,|0\rangle + \delta\,|1\rangle$ then

$$|\psi\rangle \otimes |\phi\rangle = \begin{pmatrix}\alpha\\ \beta\end{pmatrix} \otimes \begin{pmatrix}\gamma\\ \delta\end{pmatrix} = \begin{pmatrix}\alpha\gamma\\ \alpha\delta\\ \beta\gamma\\ \beta\delta\end{pmatrix} = \alpha\gamma\,|00\rangle + \alpha\delta\,|01\rangle + \beta\gamma\,|10\rangle + \beta\delta\,|11\rangle\,. \tag{2}$$

Operators combine via the Kronecker product: $(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$.

QC connection. Multi-qubit gates are built from tensor products (e.g. $X \otimes I$, CNOT, etc.).

4 Pauli Matrices, Algebra, and Unitaries

The Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3}$$

satisfy

$$\sigma_i^2 = \mathbb{1}, \qquad \{\sigma_i, \sigma_j\} = 2\delta_{ij}\mathbb{1}, \qquad [\sigma_i, \sigma_j] = 2i\,\epsilon_{ijk}\sigma_k. \tag{4}$$

Any Hermitian 2×2 matrix can be written as

$$\hat{A} = a_0\mathbb{1} + \boldsymbol{a} \cdot \boldsymbol{\sigma}, \qquad \boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z),\ \boldsymbol{a} \in \mathbb{R}^3. \tag{5}$$

Similarly any unitary in SU(2) can be written as

$$U = \exp\left(-\frac{i}{2}\,\alpha\,\boldsymbol{n} \cdot \boldsymbol{\sigma}\right), \qquad \|\boldsymbol{n}\| = 1, \tag{6}$$

which is a rotation of angle α about axis $\boldsymbol{n}$ on the Bloch sphere (see §6).

Proposition 4 (Exponentiation identity)**.** *For any unit vector $\boldsymbol{n} \in \mathbb{R}^3$ and real α,*

$$e^{-i\frac{\alpha}{2}\,\boldsymbol{n}\cdot\boldsymbol{\sigma}} = \cos\frac{\alpha}{2}\,\mathbb{1} - i\sin\frac{\alpha}{2}\,(\boldsymbol{n} \cdot \boldsymbol{\sigma}). \tag{7}$$

Proof. Use $(\boldsymbol{n} \cdot \boldsymbol{\sigma})^2 = \mathbb{1}$ from the Pauli anticommutation relation. Expand the exponential into even/odd power series: $e^{xM} = \sum_{k\geq 0} \frac{x^{2k}}{(2k)!}M^{2k} + \sum_{k\geq 0} \frac{x^{2k+1}}{(2k+1)!}M^{2k+1}$ with $M = \boldsymbol{n} \cdot \boldsymbol{\sigma}$, $M^2 = \mathbb{1}$ gives the result. □

QC connection. Single-qubit rotations $R_x(\theta) = e^{-i\theta\sigma_x/2}$, etc., are elementary gates.

5 Projective Measurements

A projective measurement in basis $\{|i\rangle\}$ is given by projectors $P_i = |i\rangle\langle i|$ with $\sum_i P_i = \mathbb{1}$. For state ρ (density matrix, §7), outcome i occurs with

$$p(i) = \mathrm{Tr}(P_i\rho), \qquad \rho \ \mapsto\ \rho_i = \frac{P_i\rho P_i}{\mathrm{Tr}(P_i\rho)}. \tag{8}$$

For pure $\rho = |\psi\rangle\langle\psi|$ this is the familiar $p(i) = |\langle i|\psi\rangle|^2$ and post-measurement state $|i\rangle$.

QC connection. Readout in computational basis uses $P_0 = |0\rangle\langle 0|$, $P_1 = |1\rangle\langle 1|$.

6 Bloch Sphere and the $\mathrm{SU}(2) \leftrightarrow \mathrm{SO}(3)$ Map

6.1 Coordinates and geometry

Any single-qubit *pure* state (up to global phase) can be written as

$$|\psi\rangle = \cos\frac{\theta}{2}\,|0\rangle + e^{i\phi}\sin\frac{\theta}{2}\,|1\rangle, \quad \theta \in [0, \pi],\ \phi \in [0, 2\pi). \tag{9}$$

The associated Bloch vector in $\mathbb{R}^3$ is

$$\boldsymbol{r} = (x, y, z) = (\sin\theta\cos\phi,\ \sin\theta\sin\phi,\ \cos\theta), \qquad \|\boldsymbol{r}\| = 1. \tag{10}$$

For a *mixed* state, $\|\boldsymbol{r}\| \le 1$ (see §7).

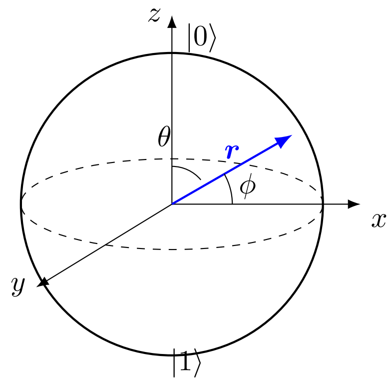

Figure 1: Bloch sphere with state $\boldsymbol{r}$ and Pauli axes.

6.2 Rotations from unitaries

For $U = \exp\left(-\frac{i}{2}\alpha\, \boldsymbol{n}\cdot\boldsymbol{\sigma}\right) \in \mathrm{SU}(2)$ and density ρ, the transformed state is $\rho' = U\rho U^\dagger$. In Bloch-vector form (§7), this induces a real-space rotation:

$$\rho = \tfrac{1}{2}(\mathbb{1} + \boldsymbol{r}\cdot\boldsymbol{\sigma}) \quad\Longrightarrow\quad \rho' = \tfrac{1}{2}(\mathbb{1} + (R_{\boldsymbol{n}}(\alpha)\boldsymbol{r})\cdot\boldsymbol{\sigma}), \tag{11}$$

where $R_{\boldsymbol{n}}(\alpha) \in \mathrm{SO}(3)$ is the 3D rotation by angle α about $\boldsymbol{n}$. Thus SU(2) double-covers SO(3).

QC connection. Any single-qubit unitary is a (possibly global-phase–lifted) rotation of the Bloch vector.

7 Density Matrices, Mixed States, and Partial Trace

7.1 Density matrices

An ensemble $\{(p_k, |\psi_k\rangle)\}$ is represented by

$$\rho = \sum_k p_k \,|\psi_k\rangle\langle\psi_k|\,, \qquad p_k \ge 0, \quad \sum_k p_k = 1. \tag{12}$$

Properties: ρ is Hermitian, positive semidefinite, and $\operatorname{Tr}\rho = 1$. A state is *pure* iff $\rho = |\psi\rangle\langle\psi|$; equivalently $\operatorname{Tr}(\rho^2) = 1$.

Proposition 5 (Purity bound)**.** *For qubits, writing $\rho = \frac{1}{2}(\mathbb{1} + \boldsymbol{r}\cdot\boldsymbol{\sigma})$ with $\boldsymbol{r} \in \mathbb{R}^3$,*

$$\operatorname{Tr}\left(\rho^2\right) = \tfrac{1}{2}(1 + \|\boldsymbol{r}\|^2) \le 1 \quad\Longleftrightarrow\quad \|\boldsymbol{r}\| \le 1, \tag{13}$$

with equality iff ρ is pure.

Proof. Compute $\rho^2 = \frac{1}{4}(\mathbb{1} + 2\,\boldsymbol{r}\cdot\boldsymbol{\sigma} + (\boldsymbol{r}\cdot\boldsymbol{\sigma})^2)$ and use $(\boldsymbol{r}\cdot\boldsymbol{\sigma})^2 = \|\boldsymbol{r}\|^2\mathbb{1}$. Then $\operatorname{Tr}(\rho^2) = \frac{1}{4}\operatorname{Tr}((1 + \|\boldsymbol{r}\|^2)\mathbb{1}) = \frac{1}{2}(1 + \|\boldsymbol{r}\|^2)$. □

7.2 Reduced density matrix and partial trace

For a bipartite system AB with joint state ρ_{AB}, the reduced state of A is

$$\rho_A = \mathrm{Tr}_B(\rho_{AB}) = \sum_j (\mathbb{1}_A \otimes \langle j|)\, \rho_{AB}\, (\mathbb{1}_A \otimes |j\rangle), \tag{14}$$

for any orthonormal basis $\{|j\rangle\}$ of B.

Example 1 (Bell state reduction)**.** *Let* $|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ *and* $\rho_{AB} = |\Phi^+\rangle\langle\Phi^+|$. *Then* $\rho_A = \mathrm{Tr}_B(\rho_{AB}) = \frac{1}{2}\mathbb{1}$ *(the maximally mixed state). Hence each qubit alone is mixed although* ρ_{AB} *is pure.*

7.3 Thermal states (Gibbs states)

For Hamiltonian H at inverse temperature $\beta = 1/(k_B T)$, the equilibrium state is

$$\rho_\beta = \frac{e^{-\beta H}}{Z}, \qquad Z = \mathrm{Tr}\Big(e^{-\beta H}\Big). \tag{15}$$

For a qubit with $H = E\sigma_z$, $Z = 2\cosh(\beta E)$ and

$$\rho_\beta = \frac{1}{2}\Big(\mathbb{1} - \tanh(\beta E)\,\sigma_z\Big) \quad\Longrightarrow\quad \boldsymbol{r} = (0, 0, -\tanh(\beta E)). \tag{16}$$

Low-T limit $\beta E \to \infty$: $\boldsymbol{r} \to (0, 0, -1)$ (ground state $|1\rangle$ for this convention). High-T limit $\beta E \to 0$: $\boldsymbol{r} \to \boldsymbol{0}$ (maximally mixed).

QC connection. Noise and thermalization push Bloch vectors toward the origin (depolarization).

8 Worked Mini-Examples

Example 2 (Basis change of a qubit operator)**.** *Let* $A = \left(\begin{smallmatrix} a & t \\ t & b \end{smallmatrix}\right)$ *in basis* $\{|\psi_1\rangle, |\psi_2\rangle\}$. *Define new basis* $|\phi_1\rangle = \frac{1}{\sqrt{2}}(|\psi_1\rangle + |\psi_2\rangle)$, $|\phi_2\rangle = \frac{1}{\sqrt{2}}(|\psi_1\rangle - |\psi_2\rangle)$ *with change-of-basis* $S = \frac{1}{\sqrt{2}}\left(\begin{smallmatrix} 1 & 1 \\ 1 & -1 \end{smallmatrix}\right)$. *Then* $A' = S^\dagger A S$. *Compute explicitly to get* $A' = \begin{pmatrix} \frac{a+b}{2}+t & \frac{a-b}{2} \\ \frac{a-b}{2} & \frac{a+b}{2}-t \end{pmatrix}$.

Example 3 (Projective measurement on a two-qubit state)**.** *Let* $|\chi\rangle = \frac{1}{6}(2|00\rangle - 5|01\rangle + 2|10\rangle + \sqrt{3}|11\rangle)$. *The probability to measure the* second *qubit in* $|1\rangle$ *is* $p = \|-5/6\|^2 + \|\sqrt{3}/6\|^2 = \frac{25}{36} + \frac{3}{36} = \frac{28}{36} = \frac{7}{9}$. *The post-measurement (normalized) state is proportional to* $(-5)|01\rangle + \sqrt{3}|11\rangle$, *i.e.* $|\chi'\rangle = \frac{-5|01\rangle + \sqrt{3}|11\rangle}{\sqrt{28}}$.

Example 4 (Tensor-product operators)**.** $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix}$, $\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & -i & 0 \\ 0 & -1 & 0 & i \\ i & 0 & 1 & 0 \\ 0 & -i & 0 & -1 \end{pmatrix}$.

9 Exercises

E1. Normalization. Let $|\psi\rangle = (2 + i)|0\rangle + (1 - 2i)|1\rangle$. Normalize it and write in the form $\cos(\theta/2)|0\rangle + e^{i\phi}\sin(\theta/2)|1\rangle$ (give θ, ϕ).

E2. Pauli algebra. Prove $\{\sigma_i, \sigma_j\} = 2\delta_{ij}\mathbb{1}$ and $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$ directly.

E3. Matrix exponential with Pauli. Using Prop. 4, compute explicitly $U = e^{-i\frac{\pi}{3}\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma}}$ for $\hat{\boldsymbol{n}} = \frac{1}{\sqrt{3}}(1,1,1)$.

E4. Basis change. With $A = \left(\begin{smallmatrix} a & t \\ t & b \end{smallmatrix}\right)$ and $|\phi_\pm\rangle = \frac{1}{\sqrt{2}}(|\psi_1\rangle \pm |\psi_2\rangle)$, find A' in the $\{|\phi_+\rangle, |\phi_-\rangle\}$ basis (verify the worked example).

E5. Measurement & post-state. For $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ in computational basis, compute $p(0)$ and post-measurement state conditioned on outcome 0. Repeat in the X-basis $\{|\pm\rangle\}$.

E6. Tensor products. Expand $(\sigma_z \otimes \sigma_x)|\Phi^+\rangle$ where $|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$.

E7. Bloch coordinates. For $|\psi\rangle = \frac{1}{\sqrt{5}}(2|0\rangle + i|1\rangle)$, compute (x,y,z) and plot it on the Bloch sphere. Which Pauli measurement is most biased?

E8. Unitary $\Rightarrow$ rotation. Show that $R_x(\theta) = e^{-i\theta\sigma_x/2}$ rotates the Bloch vector by angle θ about the x-axis. (Hint: conjugate $\sigma_{y,z}$ by $R_x(\theta)$ and use Pauli algebra.)

E9. Purity and Bloch length. Given $\rho = \frac{1}{2}(\mathbb{1} + \boldsymbol{r}\cdot\boldsymbol{\sigma})$, compute $\mathrm{Tr}(\rho^2)$ and show $\mathrm{Tr}(\rho^2) = 1 \iff \|\boldsymbol{r}\| = 1$.

E10. Partial trace. Let $\rho_{AB} = |\Psi\rangle\langle\Psi|$ with $|\Psi\rangle = \sqrt{p}\,|00\rangle + \sqrt{1-p}\,|11\rangle$. Find $\rho_A = \mathrm{Tr}_B(\rho_{AB})$ and its eigenvalues. For which p is ρ_A maximally mixed?

E11. Non-separability of Bell state. Prove that $|\Phi^+\rangle$ cannot be written as $|a\rangle \otimes |b\rangle$ for any single-qubit states $|a\rangle, |b\rangle$.

E12. Thermal qubit. For $H = E\sigma_z$, compute ρ_β and its Bloch vector $(0,0,-\tanh\beta E)$. Give the $T \to 0$ and $T \to \infty$ limits.

E13. Sudden quench (Gibbs $\to$ new basis). Start from the thermal state for $H_z = E\sigma_z$ at temperature T. At $t = 0$ switch to $H_x = E\sigma_x$. Express $\rho(0)$ in the eigenbasis of H_x and write the Liouville–von Neumann equation $\dot{\rho}(t) = -\frac{i}{\hbar}[H_x, \rho(t)]$. Solve for $\rho(t)$ and give $\boldsymbol{r}(t)$.

E14. Commuting observables. Let $A, B \in \mathrm{Herm}(2)$ commute and have nondegenerate spectra. Prove they are diagonal in the same basis.

E15. Two-qubit operator matrices. Expand $\left(\left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right) \otimes \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)\right)$ and $\left(\left(\begin{smallmatrix} 1 & -i \\ i & 1 \end{smallmatrix}\right) \otimes \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)\right)$ into 4×4 matrices.

E16. Expectation from ρ. For $\rho = \frac{1}{2}(\mathbb{1} + \boldsymbol{r}\cdot\boldsymbol{\sigma})$ and observable $A = a_0\mathbb{1} + \boldsymbol{a}\cdot\boldsymbol{\sigma}$, show $\mathrm{Tr}(\rho A) = a_0 + \boldsymbol{a}\cdot\boldsymbol{r}$.

Tip for study. When in doubt, rewrite everything in Pauli/Bloch form: operators $\leftrightarrow (a_0, \boldsymbol{a})$ and states $\leftrightarrow \boldsymbol{r}$. Many identities become dot/cross products.