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Lecture 2: Quantum computation review

"I think that a particle must have a separate reality independent of measurements. That is, an electron has spin, location and so forth even when it is not being measured. I like to think the moon is there even if I am not looking at it."
— Albert Einstein

"... experiments have now shown that what bothered Einstein is not a debatable point but the observed behaviour of the real world."
— N. David Mermin

Contents

Introduction. In Lecture 1, we reviewed the basics of classical complexity theory, including Turing machines, P, NP, reductions, and NP-completeness. We now move to the quantum realm and review the basics of quantum computation. Again, we shall move rather quickly, as a beginning background in quantum computation is assumed for this course.

1 Linear Algebra

In this course, we shall discuss quantum computation exclusively from a finite-dimensional linear algebraic perspective. For this, we begin with a quick review of linear algebraic terminology and definitions.

We denote d-dimensional complex column vectors $|\psi\rangle \in \mathbb{C}^d$ using Dirac notation, i.e. as

$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_d \end{pmatrix}, \tag{1}$$

for $\psi_i \in \mathbb{C}$. The term $|\psi\rangle$ is read "ket ψ". Recall also that a complex number $c \in \mathbb{C}$ can be written in two equivalent ways: Either as $c = a + bi$ for $a, b \in \mathbb{R}$ and $i = \sqrt{-1}$, or in its *polar form* as $c = re^{i\theta}$ for $r \in \mathbb{R}$ and $\theta \in [0, 2\pi)$. The *complex conjugate* of c is $c = a - bi$, or equivalently $c = re^{-i\theta}$.

Exercise. The *magnitude* or "length" of $c \in \mathbb{C}$ is given by $|c| = \sqrt{cc^*}$. What is the magnitude of $e^{i\theta}$ for any $\theta \in \mathbb{R}$? How about the magnitude of $re^{i\theta}$?

The *conjugate transpose* of $|\psi\rangle$ is given by

$$\langle\psi| = (\psi_1^*, \psi_2^*, \ldots, \psi_d^*)\,, \tag{2}$$

where note $\langle\psi|$ is a *row* vector. The term $\langle\psi|$ is pronounced "bra ψ". This allows us to define how much two vectors "overlap" via the *inner product* function, defined as $\langle\psi|\phi\rangle = \sum_{i=1}^d \psi_i^*\phi_i$, which satisfies $(\langle\psi|\phi\rangle)^* = \langle\phi|\psi\rangle$. The "length" of a vector $|\psi\rangle$ can then be quantified by measuring the overlap of $|\psi\rangle$ with itself, which yields the *Euclidean norm*, $\| \, |\psi\rangle \, \|_2 = \sqrt{\langle\psi|\psi\rangle}$.

Exercise. Let $|\psi\rangle = \frac{1}{\sqrt{2}}(1, i)^T \in \mathbb{C}^2$, where T denotes the transpose. What is $\langle\psi|$? How about $\| \, |\psi\rangle \, \|_2$?

Orthonormal bases. A set of vectors $\{|\psi\rangle_i\} \subseteq \mathbb{C}^d$ is *orthogonal* if for all $i \neq j$, $\langle\psi|_i|\psi\rangle_j = 0$, and *orthonormal* if $\langle\psi|_i|\psi\rangle_i = \delta_{ij}$. Here, δ_{ij} is the Kroenecker delta, whose value is 1 if $i = j$ and 0 otherwise. For the vector space $\mathbb{C}^d$, which has dimension d, it is necessary and sufficient to use d orthonormal vectors in order to form an orthonormal basis.

One of the most common bases we use is the *computational* or *standard* basis, defined for $\mathbb{C}^d$ as

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix} \qquad |1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix} \qquad \cdots \qquad |d-1\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix} \tag{3}$$

Since $\{|0\rangle, |1\rangle, \ldots, |d-1\rangle\}$ is an orthonormal basis, any unit vector $|\psi\rangle \in \mathbb{C}^d$ can be written as $|\psi\rangle = \sum_{i=0}^{d-1} \alpha_i|i\rangle$ for $\alpha_i \in \mathbb{C}$ satisfying the *normalization* condition $\| \, |\psi\rangle \, \|_2 = 1$.

Exercise. What does $\| \, |\psi\rangle \, \|_2 = 1$ mean in terms of a condition on the amplitudes α_i?

Linear maps and matrices. In this course, maps $\Phi : \mathbb{C}^d \mapsto \mathbb{C}^d$ will typically be *linear*, meaning they satify for any $\sum_i \alpha_i|\psi_i\rangle \in \mathbb{C}^d$ that $\Phi\left(\sum_i \alpha_i|\psi_i\rangle\right) = \sum_i \alpha_i\Phi(|\psi_i\rangle)$. The set of linear maps from vector space $\mathcal{X}$ to $\mathcal{Y}$ is denoted $\mathcal{L}(\mathcal{X}, \mathcal{Y})$. For brevity, we use shorthand $\mathcal{L}(\mathcal{X})$ to mean $\mathcal{L}(\mathcal{X}, \mathcal{X})$.

Recall that linear maps have a *matrix* representation. A $d \times d$ *matrix* A is a two-dimensional array of complex numbers whose (i, j)th entry is denoted $A(i, j) \in \mathbb{C}$ for $i, j \in [d]$. To represent a linear map $\Phi : \mathbb{C}^d \mapsto \mathbb{C}^d$ as a $d \times d$ matrix A_Φ, we use its action on a basis for $\mathbb{C}^d$. Specifically, define the ith column of A_Φ as $\Phi(|i\rangle)$ for $\{|i\rangle\}$ the standard basis for $\mathbb{C}^d$, or

$$A_\Phi = \left[\ \Phi(|0\rangle), \Phi(|1\rangle), \ldots, \Phi(|d-1\rangle)\ \right]. \tag{4}$$

In this course, we use both the matrix and linear map views interchangeably.

Exercise. Consider the linear map $\Phi : \mathbb{C}^2 \mapsto \mathbb{C}^2$ with action $\Phi(|0\rangle) = |1\rangle$ and $\Phi(|1\rangle) = |0\rangle$. What is the 2×2 complex matrix representing Φ?

Exercise. Given any $d \times d$ matrix A, what is $A|i\rangle$ for $|i\rangle \in \mathbb{C}^d$ a standard basis state?

The product AB of two $d \times d$ matrices A and B is also a $d \times d$ matrix with entries $AB(i, j) = \sum_{k=1}^d A(i, k)B(k, j)$. Note that unlike for scalars, for matrices it is *not* always true that $AB = BA$. In the special case where $AB = BA$, we say A and B *commute*.

Exercise. Do the following Pauli X and Z matrices commute:

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \text{and} \qquad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}? \tag{5}$$

The *image* of a matrix A is the set of all possible output vectors under the action of A, i.e. $\mathrm{Im}(A) := \left\{|\psi\rangle \in \mathbb{C}^d \mid |\psi\rangle = A|\phi\rangle \text{ for some } |\phi\rangle \in \mathbb{C}^d\right\}$. The *rank* of A is the dimension of its image, i.e. $\dim(\mathrm{Im}(A))$. The set of all vectors sent to zero by A is called its *null space*, i.e. $\mathrm{Null}(A) := \left\{|\psi\rangle \in \mathbb{C}^d \mid A|\psi\rangle = 0\right\}$. The *Rank-Nullity Theorem* says that these two spaces are related via $\dim(\mathrm{Null}(A)) + \dim(\mathrm{Im}(A)) = d$.

Exercise. Is the null space of matrix Z from Equation (5) non-empty? What is $\mathrm{rank}(Z)$?

Matrix operations. We will frequently apply the *complex conjugate*, *transpose* and *adjoint* operations to matrices in this course; they are defined, respectively, as

$$A^*(i,j) = (A(i,j))^* \qquad A^T(i,j) = A(j,i) \qquad A^\dagger = (A^*)^T. \tag{6}$$

Note that $(AB)^\dagger = B^\dagger A^\dagger$, and similarly for the transpose.

The *trace* is a linear map $\mathrm{Tr} : \mathcal{L}(\mathbb{C}^d) \mapsto \mathbb{C}$ summing the entries on the diagonal of A, i.e. $\mathrm{Tr}(A) = \sum_{i=1}^d A(i,i)$. A wonderful property of the trace is that it is *cyclic*, i.e. $\mathrm{Tr}(ABC) = \mathrm{Tr}(CAB)$.

Exercise. In a previous exercise, you showed that X and Z do not commute. What is nevertheless true about $\mathrm{Tr}(XZ)$ versus $\mathrm{Tr}(ZX)$?

Outer products. Whereas the inner product mapped a pair of vectors $|\psi\rangle, |\phi\rangle \in \mathbb{C}^d$ to a scalar, the *outer product* produces a $d \times d$ matrix $|\psi\rangle\langle\phi| \in \mathcal{L}(\mathbb{C}^d)$. For example,

$$|0\rangle\langle 0| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad |1\rangle\langle 0| = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \tag{7}$$

More generally, the matrix $|i\rangle\langle j| \in \mathcal{L}(\mathbb{C}^d)$ has a 1 at position (i,j) and zeroes elsewhere. Thus, any matrix $A \in \mathcal{L}(\mathbb{C}^d)$ written in the computational basis can written $\sum_{ij} A(i,j)|i\rangle\langle j|$. We hence see that

$$\langle i|A|j\rangle = \langle i| \left(\sum_{i'j'} A(i',j')|i'\rangle\langle j'|\right) |j\rangle = \sum_{i'j'} A(i',j')\langle i|i'\rangle\langle j|j'\rangle = \sum_{i'j'} A(i',j')\delta_{ii'}\delta_{jj'} = A(i,j), \tag{8}$$

where the third equality follows since $\{|i\rangle\}$ forms an orthonormal basis for $\mathbb{C}^d$. In other words, $\langle i|A|j\rangle$ simply rips out entry $A(i,j)$.

Exercise. Observe that X from Equation 5 can be written $X = |0\rangle\langle 1| + |1\rangle\langle 0|$. What is $\langle 0|X|0\rangle$? How about $\langle 0|X|1\rangle$? How can you rewrite $\mathrm{Tr}(X)$ in terms of expressions of the form $\langle i|X|j\rangle$?

Eigenvalues and eigenvectors. Given any matrix $A \in \mathcal{L}(\mathbb{C}^d)$, an *eigenvector* is any non-zero vector $|\psi\rangle \in \mathbb{C}^d$ satisfying the equation

$$A|\psi\rangle = \lambda|\psi\rangle, \tag{9}$$

for some $\lambda \in \mathbb{C}$ which is the corresponding *eigenvalue*.

Exercise. Show that $|+\rangle := \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ and $|-\rangle := \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$ are eigenvectors of X from Equation (5). What are their respective eigenvalues?

A matrix $A \in \left\{\mathcal{L}(\mathbb{C}^d)\right\}$ is *normal* (i.e. satisfies $AA^\dagger = A^\dagger A$) if and only if it is unitarily diagonalizable, meaning it has *spectral decomposition*

$$A = \sum_{i=1}^{d} \lambda_i |\lambda_i\rangle\langle\lambda_i|, \tag{10}$$

where λ_i and $|\lambda_i\rangle$ are the eigenvalues and corresponding eigenvectors of A, respectively. Equivalently, there exists a unitary matrix (defined shortly) U such that $UAU^\dagger$ is diagonal. Note that if the eigenvalues λ_i are all distinct, then the eigenvectors $|\lambda_i\rangle$ are uniquely determined (and hence the spectral decomposition is unique). For normal operators, the eigenvectors form an orthonormal set. (Aside: It is worth noting that some non-normal matrices A may also be diagonalized, albeit with a similarity transformation more general than a unitary, i.e. by some invertible S such that SAS^{-1} is diagonal. In this case, the eigenvectors of A are no longer guaranteed to be orthonormal, but they are linearly independent. In this course, we will typically take "diagonalizable" to mean "unitarily diagonalizable".)

Exercise. Suppose A is unitarily diagonalizable and has two matching eigenvalues, e.g. $\lambda_1 = \lambda_2$. (We then say A is *degenerate*.) Prove that there are infinitely many eigenvectors $|\psi\rangle$ such that $A|\psi\rangle = \lambda_1|\psi\rangle$.

Using the spectral decomposition, we see that $\mathrm{Tr}(A)$ has a simple expression in terms of A's eigenvalues for diagonalizable A, namely $\mathrm{Tr}(A) = \sum_i \lambda_i$. Let us quickly prove this claim:

$$\mathrm{Tr}(A) = \mathrm{Tr}\left(\sum_i \lambda_i |\lambda_i\rangle\langle\lambda_i|\right) = \sum_i \lambda_i \mathrm{Tr}(|\lambda_i\rangle\langle\lambda_i|) = \sum_i \lambda_i \mathrm{Tr}(\langle\lambda_i|\lambda_i\rangle) = \sum_i \lambda_i. \tag{11}$$

Here, the second equality follows since the trace is linear, the third by the cyclic property of the trace, and the last since the eigenvectors $|\lambda_i\rangle$ are unit vectors.

Exercise. Prove that for diagonalizable A, $\mathrm{rank}(A)$ equals the number of non-zero eigenvalues of A.

Important classes of matrices. The following classes of matrices are ubiquitous in quantum information.

1. *Unitary matrices*: A matrix $U \in \mathcal{L}(\mathbb{C}^d)$ is *unitary* if $UU^\dagger = I$ (equivalently, $U^\dagger U = I$). Thus, all unitary matrices are invertible. The set of unitary matrices acting on space $\mathcal{X}$ is denoted $\mathcal{U}((X))$.

   Exercise. Prove that any eigenvalue of a unitary matrix U is of form $e^{i\theta}$ for some $\theta \in \mathbb{R}$. Thus, unitaries are high-dimensional generalizations of unit complex numbers.

2. *Hermitian matrices*: A matrix $M \in \mathcal{L}(\mathbb{C}^d)$ is *Hermitian* if $M = M^\dagger$. The eigenvectors of Hermitian matrices can always be taken to form an orthonormal basis (rather than just being linearly independent). The set of Hermitian matrices acting on space $\mathcal{X}$ is denoted $\mathrm{Herm}(\mathcal{X})$.

   Exercise. Prove that any eigenvalue of a Hermitian matrix M is in $\mathbb{R}$. Thus, Hermitian matrices are high-dimensional generalizations of real numbers.

3. *Positive (semi-)definite matrices*: A Hermitian matrix with only positive (resp., non-negative) eigenvalues is called *positive definite* (resp., positive semidefinite). Thus, positive matrices generalize the positive (resp., non-negative) real numbers. We use $M \succ 0$ (resp., $M \succeq 0$) to specify that M is positive definite (resp. positive semidefinite). The set of positive semi-definite matrices acting on space $\mathcal{X}$ is denoted $\mathrm{Pos}(\mathcal{X})$.

Exercise. Prove that the X and Z matrices are not positive semi-definite.

4. *Orthogonal projections:* A Hermitian matrix $\Pi \in \mathcal{L}(\mathbb{C}^d)$ is an *orthogonal projection* (or projector for short) if $\Pi^2 = \Pi$.

   Exercise. Prove a Hermitian matrix $\Pi \in \mathcal{L}(\mathbb{C}^d)$ is a projector if and only if all its eigenvalues are from set $\{0, 1\}$. Thus, projectors are high-dimensional generalizations of bits.

   Since a projector Π's eigenvalues are 0's and 1's, its spectral decomposition must take the form $\Pi = \sum_i |\psi_i\rangle\langle\psi_i|$, where $\{|\psi_i\rangle\}$ are an orthonormal set. Conversely, summing any set of orthonormal $\{|\psi_i\rangle\}$ in this fashion yields a projector. A projector Π has rank 1 if and only if $\Pi = |\psi\rangle\langle\psi|$ for some $|\psi\rangle \in \mathbb{C}^d$.

   Exercise. Let $\{|\psi_i\rangle\} \subseteq \mathbb{C}^d$ be an orthonormal set. Prove that $\Pi = \sum_i |\psi_i\rangle\langle\psi_i|$ is a projector.

   As for what a projector intuitively *does* — for any projector $\Pi = \sum_i |\psi_i\rangle\langle\psi_i|$ and vector $|\phi\rangle$,

$$\Pi|\phi\rangle = \left(\sum_i |\psi_i\rangle\langle\psi_i|\right)|\phi\rangle = \sum_i |\psi_i\rangle(\langle\psi_i|\phi\rangle) = \sum_i (\langle\psi_i|\phi\rangle)|\psi_i\rangle \in \text{Span}(\{|\psi_i\rangle\}),$$

   where note $\langle\psi_i|\phi\rangle \in \mathbb{C}$. Thus, Π projects us down onto the span of the vectors $\{|\psi_i\rangle\}$.

   Exercise. Consider three-dimensional vector $|\phi\rangle = \alpha|0\rangle + \beta|1\rangle + \gamma|2\rangle \in \mathbb{C}^3$ and $\Pi = |0\rangle\langle 0| + |1\rangle\langle 1|$. Compute $\Pi|\phi\rangle$, and observe that the latter indeed lies in the two-dimensional space $\text{Span}(\{|0\rangle, |1\rangle\})$.

Operator functions. A key idea used repeatedly in quantum information is that of an *operator function*, or in English, "how to apply real-valued functions to matrices". To apply function $f : \mathbb{R} \mapsto \mathbb{R}$ to a Hermitian matrix $H \in \text{Herm}\left(\mathbb{C}^d\right)$, we take the spectral decomposition $H = \sum_i \lambda_i |\lambda_i\rangle\langle\lambda_i|$, and define $f(H)$ as

$$H = \sum_i f(\lambda_i)|\lambda_i\rangle\langle\lambda_i|,$$

i.e. we apply f to the eigenvalues of H. Why does this "work"? Let us look at the Taylor series expansion of f, which for e.g. $f = e^x$ is (the series converges for all x)

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots . \tag{12}$$

The naive idea for defining e^H would be to substitute H in the right hand side of the Taylor series expansion of e^x:

$$e^H := I + H + \frac{H^2}{2!} + \frac{H^3}{3!} + \cdots . \tag{13}$$

Indeed, this leads to our desired definition; that to generalize the function $f(x) = e^x$ to Hermitian matrices, we apply f to the eigenvalues of H, as you will now show.

Exercise. Let H have spectral decomposition $H = \sum_i \lambda_i |\lambda_i\rangle\langle\lambda_i|$. Show that in Equation (13),

$$e^H = \sum_i e^{\lambda_i} |\lambda_i\rangle\langle\lambda_i|.$$

Exercise. Let $f(x) = x^2$. What is $f(X)$, for X the Pauli X operator? Why does this yield the same results as multiplying X by itself via matrix multiplication?

Exercise. Let $f(x) = \sqrt{x}$. For any pure state $|\psi\rangle \in \mathbb{C}^d$, define rank one density operator $\rho = |\psi\rangle\langle\psi|$. What is $\sqrt{\rho}$?

Exercise. What is $\sqrt{Z}$ for Z the Pauli Z operator? Is it uniquely defined?

2 Basic quantum computation

We now review the basics of quantum computation. Recall here there are two successively more general notions of quantum states we utilize. The first, *pure* states, are the quantum analogue of "perfect knowledge" about our state; in the classical world, a "pure state" means your computer's state is described by a fixed string $x \in \{0,1\}^n$. The second, and more general notion, is that of *mixed* states, which model the notion of "uncertainty" about our state. The classical analogue here would be a computer whose state is described by some *distribution* over n-bit strings x.

2.1 Pure state quantum computation

We begin by discussing pure state quantum computation.

2.1.1 Individual systems

Recall that an arbitrary d-dimensional pure quantum state is represented by a unit vector

$$|\psi\rangle = \sum_{i=0}^{d-1} \alpha_i |i\rangle \in \mathbb{C}^d.$$

If we interpret quantum mechanics *literally* (i.e. adopt the "Copenhagen interpretation" of quantum mechanics), we take $|\psi\rangle$ to mean that our quantum system is in all d basis states $|i\rangle$ *simultaneously*, with some appropriate *amplitudes* $\alpha_i \in \mathbb{C}$. Typically, in this course we will work with $d = 2$, i.e. qubit systems.

2.1.2 Quantum gates

In the pure state setting, the set of allowable operations or *gates* on $|\psi\rangle \in \mathbb{C}^d$ is the set of $d \times d$ unitary matrices $U \in \mathcal{L}(\mathbb{C}^d)$ (i.e. $UU^\dagger = U^\dagger U = I$). In particular, this means pure-state quantum computation is fully reversible, since all gates have inverses.

You have already seen two of the three single-qubit Pauli matrices below, which are unitary. The fourth gate, H, is the Hadamard.

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

Exercise. What classical gate does Pauli X simulate? (Hint: Look at the action of X on $|0\rangle$ and $|1\rangle$.)

Exercise. What is the action of Pauli Z on the standard basis? Give the spectral decomposition of Z.

Recall the Z gate allows us to inject a *relative phase* into a quantum state. For example,

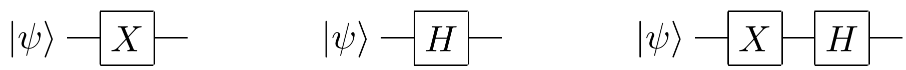
$$Z|+\rangle = Z\left(\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle\right) = \frac{1}{\sqrt{2}}Z|0\rangle + \frac{1}{\sqrt{2}}Z|1\rangle = \frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle = |-\rangle.$$

By relative phase, we mean that only the amplitude on $|1\rangle$ was multiplied by phase $e^{i\pi} = -1$. If *all* the amplitudes in the state were instead multiplied by $e^{i\pi}$, we could simply factor out the $e^{i\pi}$ from the entire state — in this case, $e^{i\pi}$ is a *global* phase, which cannot be detected via experiment, and hence is ignored.

The Hadamard, on the other hand, allows us to create or destroy certain superpositions. Namely, $H|0\rangle = |+\rangle$ and $H|1\rangle = |-\rangle$, and $H|+\rangle = |0\rangle$ and $H|-\rangle = |1\rangle$. In other words, H is self-inverse.

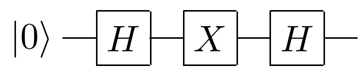
Exercise. Verify that X, Y, Z, H are all self-inverse, e.g. the inverse of X is just X. What does this mean about the eigenvalues of X? (Hint: Use the fact that the eigenvalues of any unitary must lie on the unit circle.)

In this course, we work with the *quantum circuit model*, which allows us to graphically depict gates:



These correspond to evolutions $X|\psi\rangle$, $H|\psi\rangle$, and $HX|\psi\rangle$, respectively. Each wire in such a diagram denotes a quantum system, and a box labelled by gate U depicts the action of unitary U. We think of time going from left to right; for the last circuit above, note that the X appears on the "left" in the circuit diagram but on the "right" in the expression $HX|\psi\rangle$; this is because X should be applied first to $|\psi\rangle$, then H.

Exercise. Which Pauli matrix does the following circuit simulate? (Hint: Use the spectral decomposition of X.)



2.1.3 Composite quantum systems

Thus far we have described single qudit systems. The mathematical formalism for describing the joint state for *multiple* qudits is the *tensor product*, $\otimes : \mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2} \mapsto \mathbb{C}^{d_1 \times d_2}$. For input vectors $|\psi\rangle \in \mathbb{C}^{d_1}, |\phi\rangle \in \mathbb{C}^{d_2}$, the (i,j)-th entry of their tensor product is $(|\psi\rangle \otimes |\phi\rangle)(i,j) := \psi_i \phi_j$, where recall ψ_i and ϕ_j are the ith and jth entries of $|\psi\rangle$ and $|\phi\rangle$, respectively. For example,

$$\begin{pmatrix} a \\ b \end{pmatrix} \otimes \begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} ac \\ ad \\ bc \\ bd \end{pmatrix}.$$

It is crucial to note that the tensor product *multiplies* the dimensions of its input spaces. This is why classical simulations of quantum mechanics appear to require an exponential overhead.

Exercise. What is $|+\rangle \otimes |0\rangle$ (expressed in the standard basis)?

Exercise. What dimension do n-qubit states live in, i.e. what is the dimension of space $(\mathbb{C}^2)^{\otimes n}$?

The tensor product has the following properties for any $|a\rangle, |b\rangle \in \mathbb{C}^{d_1}$ and $|c\rangle, |d\rangle \in \mathbb{C}^{d_2}$:

$$\begin{aligned}
(|a\rangle + |b\rangle) \otimes |c\rangle &= |a\rangle \otimes |c\rangle + |b\rangle \otimes |c\rangle && (14)\\
|a\rangle \otimes (|c\rangle + |d\rangle) &= |a\rangle \otimes |c\rangle + |a\rangle \otimes |d\rangle && (15)\\
c(|a\rangle \otimes |c\rangle) &= (c|a\rangle) \otimes |c\rangle = |a\rangle \otimes (c|c\rangle) && (16)\\
(|a\rangle \otimes |c\rangle)^\dagger &= |a\rangle^\dagger \otimes |c\rangle^\dagger = \langle a| \otimes \langle c| && (17)\\
(\langle a| \otimes \langle c|)(|b\rangle \otimes |d\rangle) &= \langle a|b\rangle\langle c|d\rangle. && (18)
\end{aligned}$$

For brevity, we shall often drop the notation $\otimes$ and simply write $|\psi\rangle \otimes |\phi\rangle = |\psi\rangle|\phi\rangle$.

Exercise. Using the properties above, prove that for orthonormal bases $B_1 = \{|\psi_0\rangle, |\psi_1\rangle\}$ and $B_2 = \{|\phi_0\rangle, |\phi_1\rangle\}$ for $\mathbb{C}^2$, the set $\{|\psi_0\rangle \otimes |\phi_0\rangle, |\psi_0\rangle \otimes |\phi_1\rangle, |\psi_1\rangle \otimes |\phi_0\rangle, |\psi_1\rangle \otimes |\phi_1\rangle\}$ is an orthonormal basis for $\mathbb{C}^4$.

Quantum entanglement. Recall that while any pair of states $|\psi\rangle, |\phi\rangle \in \mathbb{C}^d$ can be stitched together via the tensor product to obtain a d^2-dimensional state $|\psi\rangle \otimes |\phi\rangle \in \mathbb{C}^{d^2}$, the converse is not always true: Given any d^2-dimensional state $|\eta\rangle \in \mathbb{C}^{d^2}$, it is not always true that there exist $|\psi\rangle, |\phi\rangle \in \mathbb{C}^d$ satisfying $|\eta\rangle = |\psi\rangle \otimes |\phi\rangle$. Such $|\eta\rangle$ are called *entangled.*

For pure bipartite (i.e. two-party) states, entanglement is easy to characterize fully via the *Schmidt decomposition*, which says that any bipartite state $|\eta\rangle \in \mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2}$ can be written

$$|\eta\rangle = \sum_{i=0}^{\min(d_1,d_2)-1} s_i |a_i\rangle|b_i\rangle,$$

for non-negative *Schmidt coefficients* s_i and orthonormal bases $\{|a_i\rangle\}_{i=0}^{d_1}$ and $\{|b_i\rangle\}_{i=0}^{d_2}$ for $\mathbb{C}^{d_1}$ and $\mathbb{C}^{d_2}$, respectively. The *Schmidt rank* of $|\eta\rangle$ is its number of non-zero Schmidt coefficients. The canonical entangled two-qubit states are the Bell states

$$\begin{aligned}
|\Phi^+\rangle &= \frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle \\
|\Phi^-\rangle &= \frac{1}{\sqrt{2}}|00\rangle - \frac{1}{\sqrt{2}}|11\rangle \\
|\Psi^+\rangle &= \frac{1}{\sqrt{2}}|01\rangle + \frac{1}{\sqrt{2}}|10\rangle \\
|\Psi^-\rangle &= \frac{1}{\sqrt{2}}|01\rangle - \frac{1}{\sqrt{2}}|10\rangle,
\end{aligned}$$

where we simplified notation by letting (e.g.) $|0\rangle|0\rangle = |00\rangle$.

Exercise. Prove the Bell states are an orthonormal basis for $\mathbb{C}^4$.

It is worth mentioning that while the Schmidt rank of a bipartite pure state $|\psi\rangle \in \mathbb{C}^d \otimes \mathbb{C}^d$ yields an efficient[1] test for entanglement in pure states, it is highly unlikely for there to be an efficient test for entanglement in mixed states. This is because determining whether a *mixed* state $\rho \in \mathcal{L}(\mathbb{C}^d \otimes \mathbb{C}^d)$ is separable is (strongly) NP-hard. (Mixed states are reviewed in Section 2.2.)

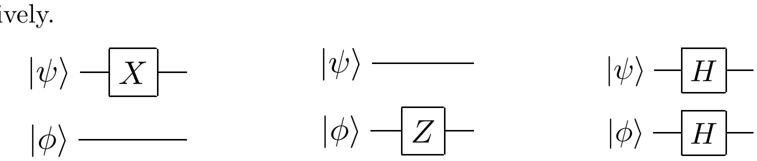
Two-qubit quantum gates. Two qubit gates are either a tensor product of one-qubit gates, such as $X \otimes Z$ or $H \otimes I$, or a genuinely two-qubit gate. For the former, recall the tensor product acts on matrices as

$$A = \begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix}, \qquad B = \begin{pmatrix} b_1 & b_2 \\ b_3 & b_4 \end{pmatrix}, \qquad A \otimes B = \begin{pmatrix} a_1 \cdot \begin{pmatrix} b_1 & b_2 \\ b_3 & b_4 \end{pmatrix} & a_2 \cdot \begin{pmatrix} b_1 & b_2 \\ b_3 & b_4 \end{pmatrix} \\ a_3 \cdot \begin{pmatrix} b_1 & b_2 \\ b_3 & b_4 \end{pmatrix} & a_4 \cdot \begin{pmatrix} b_1 & b_2 \\ b_3 & b_4 \end{pmatrix} \end{pmatrix}.$$

The tensor product for matrices shares the properties of the tensor product for vectors, with the addition of two rules: $(A \otimes B)(C \otimes D) = AC \otimes BD$ and $\mathrm{Tr}(A \otimes B) = \mathrm{Tr}(A)\mathrm{Tr}(B)$.

Exercise. What is $\mathrm{Tr}((X \otimes X)(X \otimes X))$?

Circuit diagrams for tensor products of unitaries are depicted below: We consider the cases of $X \otimes I$, $I \otimes Z$, and $H \otimes H$, respectively.



[1] "Efficient" here means the test can be computed in time polynomial in the *dimension*, d, of the system.

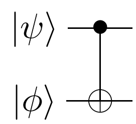
Exercise. What is the circuit diagram for $Z \otimes Z$? What is $(X \otimes X)|0\rangle \otimes |1\rangle$? How about $(Z \otimes Z)|1\rangle \otimes |1\rangle$?

An important genuinely two-qubit gate is the *controlled-NOT* gate, denoted CNOT. The CNOT treats one qubit as the *control* qubit, and the other as the target *qubit*. It then applies the Pauli X gate to the target qubit only if the control qubit is set to $|1\rangle$. More precisely, the action of the CNOT on a two-qubit basis is given as follows, where qubit 1 is the control and qubit 2 is the target:

$$\mathrm{CNOT}\,|00\rangle = |00\rangle \quad \mathrm{CNOT}\,|01\rangle = |01\rangle \quad \mathrm{CNOT}\,|10\rangle = |11\rangle \quad \mathrm{CNOT}\,|11\rangle = |10\rangle.$$

Exercise. What is the matrix representation for CNOT?

The circuit diagram for the CNOT is given by



Exercise. What is $\mathrm{CNOT}\,|\Phi^+\rangle$ for $|\Phi^+\rangle$ the Bell state? Based on this, give a circuit diagram mapping $|00\rangle$ to the Bell state $|\Phi^+\rangle$.

2.1.4 Measurement

Recall that measuring or *observing* a quantum system allows us to extract classical information from the system.

The most basic type of measurement is a *projective measurement*, given by a set of projectors $B = \{\Pi_i\}_{i=0}^m$ such that $\sum_{i=0}^m \Pi_i = I$, where the latter condition is the *completeness* relation. If each Π_i is rank one, i.e. $\Pi_i = |\psi_i\rangle\langle\psi_i|$, then we say B models a *measurement in basis* $\{|\psi_i\rangle\}$. Often, we shall measure in the computational basis for $\mathbb{C}^d$, which is specified by $B = \{|i\rangle\langle i|\}_{i=0}^{d-1}$ for standard basis vectors $|i\rangle \in \mathbb{C}^d$.

Exercise. Verify that $B = \{|0\rangle\langle 0|, |1\rangle\langle 1|\}$ is a projective measurement on $\mathbb{C}^2$.

Given a projective measurement $B = \{\Pi_i\}_{i=0}^m \subseteq \mathbb{C}^d$ and quantum state $|\psi\rangle \in \mathbb{C}^d$, recall the probability of obtaining outcome $i \in \{0, \ldots, m\}$ when measuring $|\psi\rangle$ with B is given by

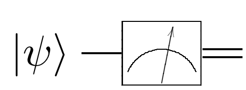
$$\Pr(\text{outcome } i) = \mathrm{Tr}(\Pi_i|\psi\rangle\langle\psi|\Pi_i) = \mathrm{Tr}(\Pi_i^2|\psi\rangle\langle\psi|) = \mathrm{Tr}(\Pi_i|\psi\rangle\langle\psi|),$$

where the second equality follows by the cyclic property of the trace and the third since Π_i is a projector. Upon obtaining outcome i, our state $|\psi\rangle$ *collapses* to a state $|\psi'\rangle$ consistent with this outcome, i.e.

$$|\psi'\rangle = \frac{\Pi_i|\psi\rangle}{\parallel \Pi_i|\psi\rangle \parallel_2} = \frac{\Pi_i|\psi\rangle}{\sqrt{\langle\psi|\Pi_i\Pi_i|\psi\rangle}} = \frac{\Pi_i|\psi\rangle}{\sqrt{\langle\psi|\Pi_i|\psi\rangle}}.$$

Exercise. Let $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \in \mathbb{C}^2$. Show that if we measure in the computational basis, i.e. using $B = \{|0\rangle\langle 0|, |1\rangle\langle 1|\}$, then the probabilities of obtaining outcomes 0 and 1 are $|\alpha|^2$ and $|\beta|^2$, respectively. What is the postmeasurement state $|\psi'\rangle$ if outcome 0 is obtained?

The circuit symbol denoting a measurement of state $|\psi\rangle \in \mathbb{C}^2$ in the *computational* basis is:



2.2 Mixed state quantum computation

Thus far, we have discussed pure state computation, where we know precisely the quantum state in which our system is throughout the computation. We now review *mixed state* computation, for which we recall the notion of density operators.

Recall that a *density operator* ρ acting on $\mathbb{C}^d$ is a $d \times d$ Hermitian matrix satisfying two properties: $\rho \succeq 0$ (ρ is positive-semidefinite) and $\text{Tr}(\rho) = 1$. By the former, ρ has spectral decomposition

$$\rho = \sum_{i=1}^{m} p_i |\psi_i\rangle\langle\psi_i|,$$

with eigenvalues p_i and orthonormal basis $\{|\psi_i\rangle\}$. One way to interpret ρ is via the following experiment: With probability p_i, we prepare pure state $|\psi_i\rangle$. This, in particular, means that any pure state $|\psi\rangle$ has density matrix $|\psi\rangle\langle\psi|$. Conversely, any rank one density operator by definition must be of form $\rho = |\psi\rangle\langle\psi|$ (why?), and hence represents a pure state $|\psi\rangle$. The set of density operators acting on $\mathbb{C}^d$ is denoted $\mathcal{D}(\mathbb{C}^d)$.

Exercise. Prove that the eigenvalues $\{p_i\}$ of a density operator form a probability distribution.

Exercise. Write down the density operator $\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|$ and state vector $|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$. How do they differ?

Exercise. What is the density matrix for pure state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$?

The maximally mixed state. A special density matrix in $\mathcal{L}(\mathbb{C}^d)$ is the *maximally mixed* state $\rho = I/d$, which is the state of "maximum uncertainty". To see why, use the fact that for any orthonormal basis $\{|\psi_i\rangle\}_{i=1}^d$ for $\mathbb{C}^d$, $\sum_{i=1}^d |\psi_i\rangle\langle\psi_i| = I$. In other words, for *any* orthonormal basis $\{|\psi_i\rangle\}_{i=1}^d$, ρ represents the following experiment: Pick state $|\psi_i\rangle$ with probability $1/d$, and prepare $|\psi_i\rangle$. Since this holds for any basis, ρ gives us absolutely no information about which state $|\psi\rangle$ we actually have.

The partial trace operation. Density operators arise naturally in answering the question: For any entangled state $|\psi\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2$, how do we describe the marginal state of $|\psi\rangle$ on (say) qubit 1? There is no way to answer this via pure states, since $|\psi\rangle$ is not a product state, and hence does not factorize. Instead, we require a density matrix to describe the state of qubit 1, and the correct procedure for obtaining it is the *partial trace* operation, which we now discuss.

For a bipartite density operator ρ system on parties A and B, the partial trace over B "discards" system B, and hence has signature $\text{Tr}_B : \mathcal{L}(\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2}) \mapsto \mathcal{L}(\mathbb{C}^{d_1})$. To formally define Tr_B, recall that we may write the (usual) trace of $\rho \in \mathcal{L}(\mathbb{C}^d)$ as $\text{Tr}(\rho) = \sum_i \rho(i,i) = \sum_{i=1}^d \langle i|\rho|i\rangle$. The *partial* trace over B applies this formula only to system B, i.e. for $\rho \in \mathcal{L}(\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2})$,

$$\text{Tr}_B(\rho) = \sum_{i=1}^{d_2} (I_A \otimes \langle i|)\rho(I_A \otimes |i\rangle).$$

Exercise. What should $\text{Tr}_B(I/4)$ intuitively be? Compute $\text{Tr}_B(I/4)$ to check your guess.

Exercise. More generally, prove that $\text{Tr}_B(\rho_A \otimes \rho_B) = \rho_A \cdot \text{Tr}(\rho_B) = \rho_A$ for density matrices ρ_A, ρ_B.

Example 1: Separable states. We have said that a pure state $|\psi\rangle \in \mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2}$ is not entangled, or *separable*, if and only if $|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$ for some $|\psi_1\rangle \in \mathbb{C}^{d_1}$ and $|\psi_2\rangle \in \mathbb{C}^{d_2}$. This idea extends to the setting of mixed states as follows: A bipartite density matrix $\rho \in \mathcal{L}(\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2})$ is unentangled or *separable* if

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \otimes |\phi_i\rangle\langle\phi_i|,$$

for some (possibly non-orthogonal) sets of vectors $\{|\psi_i\rangle\} \subseteq \mathbb{C}^{d_1}$ and $\{|\phi_i\rangle\} \subseteq \mathbb{C}^{d_2}$, and where the $\{p_i\}$ form a probability distribution. In other words, ρ is a probabilistic mixture of pure product states. An example of a separable state is

$$\rho = \frac{1}{2}|0\rangle\langle 0| \otimes |0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| \otimes |1\rangle\langle 1|. \tag{19}$$

Since the partial trace is a linear map, and since we know that $\mathrm{Tr}_B(\rho_1 \otimes \rho_2) = \rho_1 \cdot \mathrm{Tr}(\rho_2) = \rho_1$ for density matrices ρ_1, ρ_2, computing the partial trace of ρ for separable states is simple:

$$\mathrm{Tr}_B\left(\sum_i p_i|\psi_i\rangle\langle\psi_i| \otimes |\phi_i\rangle\langle\phi_i|\right) = \sum_i p_i \mathrm{Tr}_B\left(|\psi_i\rangle\langle\psi_i| \otimes |\phi_i\rangle\langle\phi_i|\right) = \sum_i p_i|\psi_i\rangle\langle\psi_i| \cdot \mathrm{Tr}(|\phi_i\rangle\langle\phi_i|) = \sum_i p_i|\psi_i\rangle\langle\psi_i|.$$

Exercise. What is $\mathrm{Tr}_B(\rho)$ for ρ from Equation (19)?

Example 2: Pure entangled states. We compute the single-qubit state of the Bell state $|\Phi^+\rangle$ on qubit 1:

$$\begin{aligned}
\mathrm{Tr}_B(|\Phi^+\rangle\langle\Phi^+|) &= \frac{1}{2}\mathrm{Tr}_B(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|) \\
&= \frac{1}{2}|0\rangle\langle 0|\mathrm{Tr}(|0\rangle\langle 0|) + \frac{1}{2}|0\rangle\langle 1|\mathrm{Tr}(|0\rangle\langle 1|) + \frac{1}{2}|1\rangle\langle 0|\mathrm{Tr}(|1\rangle\langle 0|) + \frac{1}{2}|1\rangle\langle 1|\mathrm{Tr}(|1\rangle\langle 1|) \\
&= \frac{1}{2}I,
\end{aligned}$$

where we have used the linearity of the partial trace. Thus, the reduced state on qubit 1 for the Bell state is *maximally mixed*, i.e. it is a completely random state about which we have zero information.

Exercise. Show that $\mathrm{Tr}_A(|\Phi^+\rangle\langle\Phi^+|) = I/2$.

2.2.1 Operations and measurements on mixed states

We close this lecture by generalizing our discussion on gates and measurements from the pure state setting to mixed states.

Composite systems. If ρ_A and ρ_B are density operators, then $\rho_A \otimes \rho_B$ is a density operator.

Exercise. Prove the claim above. (Hint: The slightly trickier part is to show that the tensor product preserves positivity — use the spectral decomposition for this.)

Unitary operations. For density operator $\rho \in \mathcal{D}(\mathbb{C}^d)$ and unitary $U \in \mathcal{U}(\mathbb{C}^d)$, the action of U on ρ is given by $U\rho U^\dagger$.

Exercise. What is the action of any unitary $U \in \mathcal{U}(\mathbb{C}^d)$ on the maximally mixed state, $\rho = I/d$?

Measurements. For projective measurement $B = \{\Pi_i\}_{i=0}^m \subseteq \mathcal{L}(\mathbb{C}^d)$ applied to density operator $\rho \in \mathcal{D}(\mathbb{C}^d)$, the probability of outcome i and postmeasurement state $\rho' \in \mathcal{D}(\mathbb{C}^d)$ upon obtaining outcome i are

$$\Pr(\text{outcome } i) = \mathrm{Tr}(\Pi_i\rho) \qquad \text{and} \qquad \rho' = \frac{\Pi\rho\Pi}{\mathrm{Tr}(\Pi_i\rho)}.$$

Exercise. Show that the following important identity holds: For any bipartite state ρ_{AB} and matrix M_B acting on B, it holds that

$$\mathrm{Tr}(\rho_{AB} I_A \otimes M_B) = \mathrm{Tr}(\mathrm{Tr}_A(\rho_{AB}) M_B).$$

In other words, measuring just system B of a joint state ρ_{AB} is equivalent to first discarding system A of ρ_{AB}, followed a measurement on the reduced state on system B. Does this agree with your intuition of how a local measurement should behave?