CS 150 Quantum Computer Science

Lecture 4: Matrix formulation of quantum mechanics

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1 Logistics

- Extension: Problem set 1 is now due Wednesday night

2 Overview

Last time:

- Reversible computation

Today:

- Reversible $\rightarrow$ Unitary computation

3 Hadamard transform

In the previous section, we saw that by rotating the SG experiment 90 degrees, we change the basis of measurement from $\{|0\rangle, |1\rangle\}$ to $\{|+\rangle, |-\rangle\}$. Similarly, suppose I start with the quantum state $|0\rangle$. If I keep the direction of the experiment fixed and rotate the electron, I have mapped the state of the electron from $|+\rangle$. Similarly, if I start with $|1\rangle$ and rotate it 90 degrees, the state of the electron becomes $|-\rangle$ (up to an unobservable minus sign). We saw that classical computations have matrix representations. Is there a matrix representation for the operation that performs the map $|0\rangle \mapsto |+\rangle$ and $|1\rangle \mapsto |-\rangle$? The answer is yes, and this map is called the Hadamard transform. It is the matrix:

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

See Figure 1 for a geometric interpretation of the Hadamard operation. Furthermore, Hadamard operation is self-adjoint, meaning $H = H^\dagger$. (Recall that we define $(A^\dagger)_{ij} = A^*_{ji}$). In other words, $HH^\dagger = I$. In linear algebra, we call such matrices unitary. Hadamard also satisfies $H^{-1} = H$. That means it is the inverse of itself. Recall our discussion about reversible computations. We can see from this example that the Hadamard operation is reversible.

We can view Hadamard as a coin-flip operation. Because when we apply Hadamrard to $|0\rangle$, we obtain $|+\rangle$, which has $1/2$ probability of being in $|0\rangle$ or $|1\rangle$. How is this coin-flip different from

Figure 1: The Hadamard transform.

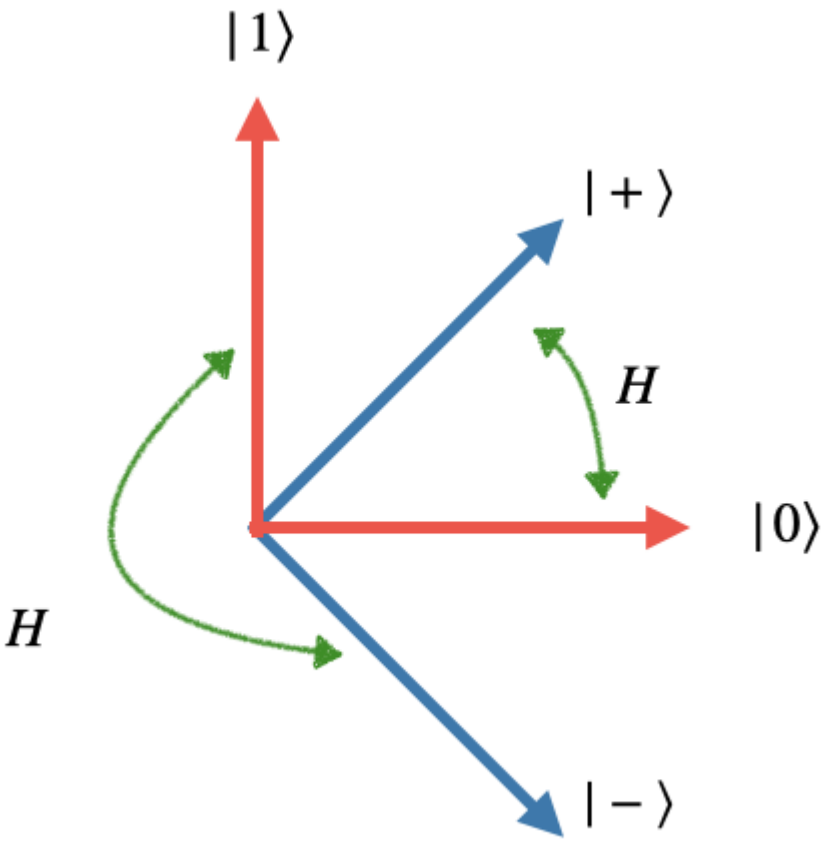
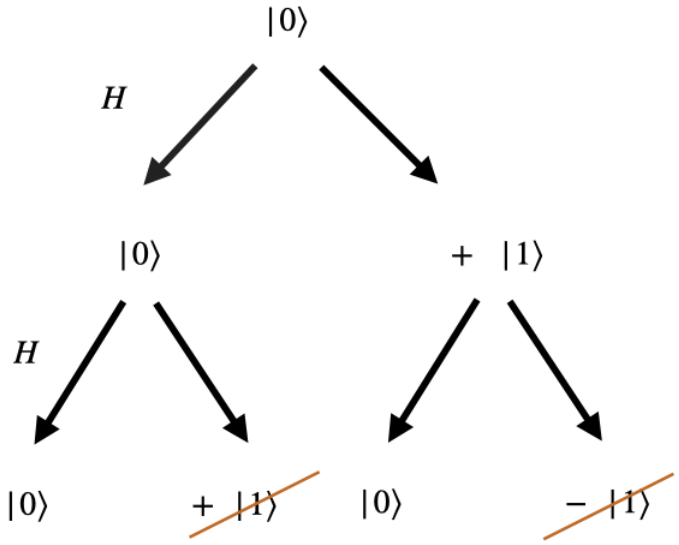


Figure 2: The interference phenomenon for two applications of Hadamard.



classical coin-flip? If we flip a coin and obtain heads, then there is no way we can get back to see if the initial state was heads or tails. However, if we use the Hadamard operation twice, we will get back to where we started! It is easy to check that $H^2 = I$.

Remark 3.1. We note that by rotating the Stern-Gerlach experiment, we obtain the change of basis according to the matrix $R = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$ which is different from Hadamard. It maps $|0\rangle$ to $|+\rangle$ but it maps $|1\rangle$ to $-|-\rangle$. We introduced Hadamard because of its fundamental role in the rest of this course.

Interference phenomenon: We discussed the strange phenomenon of two quantum bit flips being equivalent to having done nothing. We can explain this using the interference phenomenon. See Figure 2. After one application of Hadamard, we obtain a superposition of $|0\rangle$ and $|1\rangle$. If we apply H another time, we obtain four superposition terms $|0\rangle$, $|1\rangle$, another $|0\rangle$ and $-|1\rangle$. $|1\rangle$ and $-|1\rangle$ cancel each other out. This is the same interference phenomenon we observe in classical waves. In other words, one of the immediate differences between quantum and classical computation is the existence of negative signs in the matrix representation of computations.

4 Matrix formulation of quantum mechanics

Up to this point, we saw that arbitrary classical computations can be captured using a matrix formalism. In particular, we can use a vector $|x_0\rangle$ to encode the initial state of a computation. We then use a matrix A to represent the process of the computation: the final state of the computation

becomes $|x_1\rangle = A|x_0\rangle$. We then measure $|x_1\rangle$. For instance, recall the controlled-NOT operation is according to the matrix

$$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

we encode the two-bit states using vectors according to

$$|00\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |01\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad |10\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad |11\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

Suppose the initial state is $|11\rangle$. After the application of $CNOT$ we obtain:

$$CNOT|11\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = |10\rangle.$$

Fact 4.1. *Classical reversible matrices are permutation matrices.*

Matrix formulation of quantum computations–and quantum mechanics in general–is very similar: The initial state of a system, e.g., $|\psi_0\rangle$, is evolved according to a matrix evolution like U to obtain a final state $|\psi_1\rangle = U|\psi_0\rangle$. In what follows, we explain the three main postulates of quantum formalism

4.1 Quantum states:

One main feature of quantum formalism is that quantum states are unit vectors in a given Hilbert space. A Hilbert space is a vector space that is complete and normed. By normed, we mean that the space is equipped with an inner product. We consider the following inner product between vectors in $\mathbb{C}^N$: Let

$$|\psi\rangle = \begin{pmatrix} \alpha_1 \\ \ddots \\ \alpha_N \end{pmatrix}, \quad |\phi\rangle = \begin{pmatrix} \beta_1 \\ \ddots \\ \beta_N \end{pmatrix}$$

. Then, the inner product between the two vectors is according to:

$$\langle\psi|\phi\rangle = \begin{pmatrix} \alpha_1^* & \dots & \alpha_N^* \end{pmatrix} \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_N \end{pmatrix} = \alpha_1^*\beta_1 + \ldots + \alpha_N^*\beta_N.$$

We immediately observe two properties of the inner product:

- For any vectors $|\psi\rangle$ and $|\phi\rangle$, $\langle\phi,\psi\rangle = \langle\psi,\phi\rangle^*$.
- For any vector $|\psi\rangle \in \mathbb{C}^N$, $\langle\psi,\psi\rangle$ is real and furthermore $\langle\psi,\psi\rangle \geq 0$ with equality iff $|\psi\rangle = 0$.

I encourage you to use a simple Google search to learn complete metric spaces; for this course, we are not going to get into the details any further.

Example of quantum states:

- Our first example is 0, 1 quantum states: $|0\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, $|1\rangle = \begin{pmatrix}0\\1\end{pmatrix}$. We previously interpreted $|0\rangle$ as spin up and $|1\rangle$ as spin down.
- **Superposition:** $|\psi\rangle = \begin{pmatrix}\alpha\\\beta\end{pmatrix} = \alpha\begin{pmatrix}1\\0\end{pmatrix} + \beta\begin{pmatrix}0\\1\end{pmatrix}$ satisfying $|\alpha|^2 + |\beta|^2 = 1$. We say $|\psi\rangle$ is the superposition of $|0\rangle$ with amplitude α and $|1\rangle$ with amplitude β.
- We discussed the left-right spins, $|+\rangle := \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$ and $|-\rangle := \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$
- Normalization $|\psi\rangle = \begin{pmatrix}\alpha_0\\\alpha_1\\\cdots\\\alpha_{N-1}\end{pmatrix}$ then $\sum_i |\alpha_i|^2 = 1$
- $\langle 0,1\rangle = 0, \langle +,-\rangle = 0$ and $\langle 0,0\rangle = \langle 1,1\rangle = \langle -,-\rangle = \langle +,+\rangle = 1$. More specifically, they form orthonormal basis $\langle i,j\rangle = \delta_{i,j}$.

4.2 Unitary evolution:

Quantum operations are linear maps that map quantum states to quantum states, i.e., they map unit vectors into unit vectors. The family of matrices that preserve the norm of a vector is called "unitary" matrices. In particular, a matrix U is called unitary if for any pair of vectors $|\psi\rangle$ and $|\phi\rangle$, $\langle\phi,\psi\rangle = \langle U\phi, U\psi\rangle$. We can show that this criterion is satisfied if $U^\dagger U = I$. For a complex matrix $A \in \mathbb{C}^{M\times N}$ with entries $A_{i,j}, 1 \leq i \leq M, 1 \leq j \leq N$, $A^\dagger \in \mathbb{C}^{N\times M}$ with entries $A^\dagger_{i,j} = A^*_{j,i}$.

To see this, we need to define some notation that will be useful throughout this course. For a vector $|\psi\rangle = \begin{pmatrix}\alpha_1\\\vdots\\\alpha_N\end{pmatrix} \in \mathbb{C}^N$ the dual vector is denoted by $\langle\psi| = \begin{pmatrix}\alpha_1^* & \ldots & \alpha_N^*\end{pmatrix}$. One useful aspect of this notation is that the inner product of two vectors

$$|\psi\rangle = \begin{pmatrix}\alpha_1\\\vdots\\\alpha_N\end{pmatrix} \quad \text{and} \quad |\phi\rangle = \begin{pmatrix}\beta_1\\\vdots\\\beta_N\end{pmatrix}$$

is given by

$$\langle \psi, \phi \rangle = \begin{pmatrix} \alpha_1^* & \dots & \alpha_N^* \end{pmatrix} \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_N \end{pmatrix} = \langle \psi | \cdot | \phi \rangle.$$

We can show that for any matrix $A \in \mathbb{C}^{M \times N}$ and vector $|v\rangle \in \mathbb{C}^N$, $(A|v\rangle)^\dagger = \langle v|A^\dagger$. To see, let $|y\rangle = A|v\rangle$. Then we can expand $y_i = \sum_{j=1}^N A_{i,j} v_j$. Therefore, $y_i^* = \sum_{j=1}^N v_j^* A_{i,j}^* = \sum_{j=1}^N v_j^* A_{j,i}^\dagger$. Therefore $\langle y| = \langle v|A^\dagger$.

Now, using this observation, we want to reason to see what unitarity means. In particular, $\langle U\phi, U\psi \rangle = \langle \phi | U^\dagger U | \psi \rangle$. If $\langle U\phi, U\psi \rangle = \langle \phi, \psi \rangle$ for all ϕ and ψ, then we have no choice other than to choose $U^\dagger U = I$. We can easily see that this is equivalent to $U^\dagger = U^{-1}$. So, this immediately implies that quantum operations are reversible.

Examples of Unitary operations: Let's go over some examples of unitary matrices.

- Pauli gates

  $$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

  Hadamard gate

  $$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

  An operator with phases

  $$A = \begin{pmatrix} e^{i\frac{2\pi}{3}} & 0 & 0 & 0 \\ 0 & e^{i\frac{\pi}{3}} & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

  The following is known as the phase gate

  $$S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$$

  Other examples include CNOT, SWAP, Toffoli, Fredkin and any other reversible gates which we saw before:

  $$SWAP = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

4.3 Measurement of quantum states:

As we discussed, a quantum state is represented by a vector, like

$$|\psi\rangle = \sum_{1 \le i \le N} \alpha_i |i\rangle = \begin{pmatrix} \alpha_1 \\ \ddots \\ \alpha_N \end{pmatrix}.$$

The measurement rule, known as the Borne rule, says that upon measuring this quantum state, the probability of obtaining outcome i is $|\alpha_i|^2$. Using the Dirac notation, this rule is according to:

$$Pr(i) = |\langle i, \psi \rangle|^2.$$

For example, if we measure the state $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ we obtain 0 wp $|\frac{1}{\sqrt{2}}|^2 = 1/2$. If we measure the state $|-i\rangle = \frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle)$, the probability of obtaining 1 is $|\frac{-i}{\sqrt{2}}|^2 = \frac{1}{2}$. In other words, these two states are not distinguishable if we simply measure them in this way. We will, later on, see that the measurement rule is more general, and we can indeed distinguish these two states with nonzero probability.