CSE439 Week 12: Quantum States as Operators

This week will pivot into linear algebra and scientific computing topics that also go outside quantum mechanics: the Spectral Theorem and canonical matrices and their decompositions. We begin with the reformulation of quantum states as operators, which embraces the (IMHO philosophically fraught) extension to mixed states, and which all become matrices in the finite-dimensional case.

Mixed States

A **pure state** of n qubits is one denoted by a unit vector in $\mathbb{C}^{2^n}$. A **mixed state** is any linear combination of pure states by non-negative weights that sum to 1. That is, a mixed state is a **classical** probability distribution over pure states. Whether "mixed state" includes pure states depends on context; one can say "properly mixed" to exclude pure states.

For one qubit, every properly mixed state maps to a point interior to the Bloch Sphere. This also holds for generalizations of the Bloch Sphere to higher dimensions for more qubits. So let us have pure states $|\phi_1\rangle, \ldots, |\phi_m\rangle$ and probabilities $p_1, \ldots, p_m$ summing to 1. Then

$$p_1|\phi_1\rangle + \cdots + p_m|\phi_m\rangle$$

is the "standard" representation of the mixed state. We will see momentarily that, like writing $|\phi_k\rangle$ to begin with, it may presume more than we can directly sense. A philosophical question that comes first is whether a mixed state is a "thing", or just our lack of full knowledge about the state. Appreciating the issues needs treatment of measurements in any basis.

General Measurements and Operators

The **triple product** of a row-vector x, a matrix A, and a column vector y is just xAy. We will care about the case where x is the "bra" dual of y. Let's write $y = |\kappa\rangle$, where κ (kappa) could be any meaningful label, and further put $|\kappa\rangle = [a, b]^T$ where a and b are complex numbers such that $|a|^2 + |b|^2 = 1$. Now consider the fact that the inner product of $[1, 0]$ with $|\kappa\rangle$, i.e., of $|0\rangle$ but written it as the bra $\langle 0|$, is just a. Meanwhile the inner product $\langle\kappa| \cdot |0\rangle$ gives a^*. Furthermore,

$$a^*a = \langle\kappa| \cdot |0\rangle\langle 0| \cdot |\kappa\rangle = \langle\kappa|0\rangle \cdot \langle 0|\kappa\rangle = |\langle\kappa|0\rangle|^2 = |a|^2.$$

What this says is that we **projected** the vector denoted by κ **onto** the basis vector $|0\rangle$, and then took the magnitude of that projection. Thus $|0\rangle\langle 0|$ represents the operation of **projecting onto the** $|0\rangle$ **vector**. Moreover, look how it transforms the $|\kappa\rangle$ vector:

$$\big(|0\rangle\langle 0|\big) \cdot |\kappa\rangle = |0\rangle \cdot \langle 0|\kappa\rangle = |0\rangle(1 \cdot a + 0 \cdot b) = a|0\rangle.$$

If we let $p_0 = |a|^2$ stand for the probability of $|0\rangle$ and divide through by $\sqrt{p_0}$ then we get just $|0\rangle$. Oh wait, what we actually get is

$$\frac{1}{\sqrt{p_0}}\big(|0\rangle\langle 0|\big)\cdot|\kappa\rangle \;=\; \frac{1}{\sqrt{p_0}}a|0\rangle \;=\; \frac{a}{|a|}|0\rangle.$$

This might not be exactly $|0\rangle$, but it is **equivalent** to it since $\frac{a}{|a|}$ is always a unit complex scalar. That's good enough. Thus $\frac{1}{\sqrt{p_0}}\big(|0\rangle\langle 0|\big)$ updates the state when outcome $|0\rangle$ happens. Similarly, $\frac{1}{\sqrt{p_1}}\big(|1\rangle\langle 1|\big)$ faithfully updates the state when outcome $|1\rangle$ happens. Again, the point is how this works for any basis state, not just the standard basis. Let's trot out the general definitions first, then do the example within the $|+\rangle, |-\rangle$ basis, then use $|+\rangle, |-\rangle$ to measure κ as originally defined as $a|0\rangle + b|1\rangle$.

Definition: The **projection operator** associated to a pure state $|\phi\rangle$ is $\mathbf{P}_\phi \;=\; |\phi\rangle\langle\phi|$.

Note that $\mathbf{P}_\phi^* \;=\; \big(|\phi\rangle\cdot\langle\phi|\big)^* \;=\; \langle\phi|^*\cdot|\phi\rangle^* \;=\; |\phi\rangle\cdot\langle\phi| \;=\; \mathbf{P}_\phi$, so every projection operator is Hermitian. More generally, we define:

Definition: A matrix B is **positive semidefinite** (PSD) if there is a matrix A such that $B \;=\; AA^*$.

Definition: A matrix P computes a **projection** if it is PSD and $P^2 = P$.

By $\mathbf{P}_\phi^* = \mathbf{P}_\phi$ we also have

$$\mathbf{P}_\phi\mathbf{P}_\phi^* \;= \mathbf{P}_\phi^2 = |\phi\rangle\langle\phi|\cdot|\phi\rangle\langle\phi| \;=\; |\phi\rangle\cdot\langle\phi|\phi\rangle\cdot\langle\phi| \;=\; |\phi\rangle\cdot 1\cdot\langle\phi| \;=\; \mathbf{P}_\phi,$$

since $|\phi\rangle$ is a unit vector. So $\mathbf{P}_\phi$ is indeed a projection and is PSD.

Definition: A **projective measurement** is given by a set $\{\mathbf{P}_1, \ldots, \mathbf{P}_m\}$ of projections such that

$$\sum_{i=1}^{m}\mathbf{P}_i \;=\; \mathbf{I}.$$

From above, $\big\{|0\rangle\langle 0|, |1\rangle\langle 1|\big\}$ is a projective measurement. How about the $\mathbf{X}$ basis $\big\{|+\rangle\langle +|, |-\rangle\langle -|\big\}$? Using the numerics of the standard basis, we get:

$$|+\rangle\langle+| \;=\; \left[\tfrac{1}{\sqrt{2}}, \tfrac{1}{\sqrt{2}}\right]^T\left[\tfrac{1}{\sqrt{2}}, \tfrac{1}{\sqrt{2}}\right] = \tfrac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

$$|-\rangle\langle-| \;=\; \left[\tfrac{1}{\sqrt{2}}, \tfrac{-1}{\sqrt{2}}\right]^T\left[\tfrac{1}{\sqrt{2}}, \tfrac{-1}{\sqrt{2}}\right] = \tfrac{1}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

$$|+\rangle\langle+| \;+\; |-\rangle\langle-| \;=\; \tfrac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} + \tfrac{1}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \;=\; \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \;=\; \mathbf{I}.$$

So $\left\{|+\rangle\langle+|, |-\rangle\langle-|\right\}$ is a projective measurement. Note that if we used the $|+\rangle, |-\rangle$ coordinates to begin with, then the numerics would be $|+\rangle\langle+| = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ and would come out literally identical, likewise if we apply the measurement to $|\kappa'\rangle = a|+\rangle \;+\; b|-\rangle$. (Note: the third from last line on page 145 would be less confusing if it defined $|\kappa'\rangle$ this way rather than say $|\kappa\rangle$ again.) Using the standard-basis numerics:

$$|\kappa'\rangle = \left[\tfrac{a}{\sqrt{2}}, \tfrac{a}{\sqrt{2}}\right]^T + \left[\tfrac{b}{\sqrt{2}}, \tfrac{-b}{\sqrt{2}}\right]^T \;=\; \tfrac{1}{\sqrt{2}}[a+b, a-b]^T.$$

The triple product with $|+\rangle\langle+|$ is:

$$\langle\kappa'|\cdot|+\rangle\langle+|\cdot|\kappa'\rangle \;=\; \frac{1}{4}\left[a^* + b^*, a^* - b^*\right]\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}[a+b, a-b]^T = \frac{1}{4}\left[2a^*, 2a^*\right]\begin{bmatrix} a+b \\ a-b \end{bmatrix}$$

$$= \;\frac{1}{4}\left(2a^*a + 2a^*b + 2a^*a - 2a^*b\right) \;=\; \frac{1}{4}\left(4a^*a\right) \;=\; a^*a \;=\; |a|^2.$$

Similarly, we get $\langle\kappa'|\cdot|-\rangle\langle-|\cdot|\kappa'\rangle \;=\; |b|^2$. That is a lot of rigamarole to replicate the answer we got for measuring the original $|\kappa\rangle$ in the standard basis. The larger point is that the $|\kappa'\rangle$ vector with regard to the $\mathbf{X}$ basis has the same relation to it as $|\kappa\rangle$ did to the standard basis.

However, when we expressly write $|\kappa\rangle = a|0\rangle + b|1\rangle$ rather than $|\kappa\rangle = [a, b]^T$, then we are defining it in a way that is independent of a particular coordinate notation, and so it really is a different physical vector from $|\kappa'\rangle = a|+\rangle \;+\; b|-\rangle$. To underscore the point (this is an example that should be on page 146), let us measure $|\kappa\rangle$ not $|\kappa'\rangle$ in the $\mathbf{X}$ basis.

$$\langle\kappa|\cdot|+\rangle\langle+|\cdot|\kappa\rangle \;=\; \left[a^*, b^*\right]\frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}[a, b]^T = \frac{1}{2}\left[a^* + b^*, a^* + b^*\right]\begin{bmatrix} a \\ b \end{bmatrix}$$

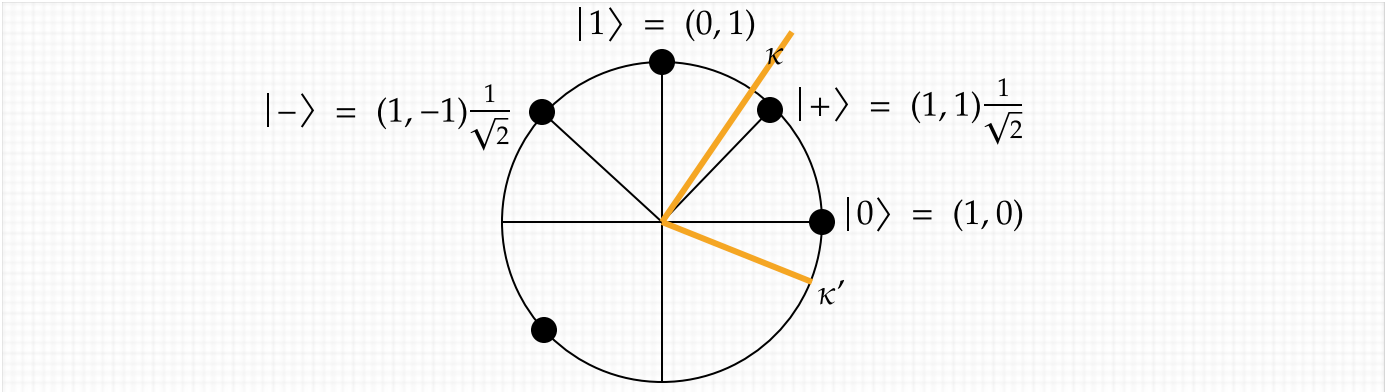
$$= \;\frac{1}{2}\left(a^*a \;+\; a^*b \;+\; b^*a + b^*b\right) \;=\; \frac{1}{2}\left(|a|^2 + |b|^2 + a^*b + b^*a\right) \;=\; \frac{1}{2} + \frac{c + c^*}{2}$$

where $c = a^*b$. What happened? The first thing to note is that the sum of a unit complex number c and its conjugate is always a real number because the imaginary parts cancel. Although in general the sum could be as big as 2 (or as low as -2), because c arises as a^*b where $|a|^2 + |b|^2 = 1$, the maximum magnitude of $c + c^*$ is 1. Hence the probability of getting the outcome $|+\rangle$ stays within the range $[0, 1]$ as required for a probability.

In fact, if $\kappa = |+\rangle$ then $a = b = \frac{1}{\sqrt{2}}$ so $c = \frac{1}{2}$ and $c + c^* = 1$, finally giving that the probability of getting the outcome $|+\rangle$ is 1. And the probability of getting the outcome $|-\rangle$ is:

$$\langle\kappa|\cdot|-\rangle\langle-|\cdot|\kappa\rangle = \left[a^*, b^*\right]\frac{1}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}[a, b]^T = \frac{1}{2}\left[a^* - b^*, -a^* + b^*\right]\begin{bmatrix} a \\ b \end{bmatrix}$$
$$= \frac{1}{2}\left(a^*a - b^*a - a^*b + b^*b\right) = \frac{1}{2}\left(|a|^2 + |b|^2 - a^*b - b^*a\right) = \frac{1}{2} - \frac{c + c^*}{2}$$

with $c = a^*b$ as before. This ensures that the probabilities sum to 1, regardless of what c is. It is a nice self-study exercise to repeat this with the example $|\kappa\rangle = \left[\frac{1}{2}, \frac{\sqrt{3}}{2}\right]$.



There is an essential symmetry of measurement as well. If we instead did $\langle-|\cdot|\kappa\rangle\langle\kappa|\cdot|-\rangle$ then we would get the same answer. Indeed, for a general other pure state $|\phi\rangle$, the **double action**

$$P_{|\kappa\rangle}\left(|\phi\rangle\right) = \langle\phi|\cdot|\kappa\rangle\langle\kappa|\cdot|\phi\rangle$$

is a product of the form cc^* where $c = \langle\phi|\kappa\rangle$. And $\left(cc^*\right)^* = \left(c^*\right)^*(c)^* = cc^*$ back again, so the *product* of a complex number and its conjugate is always a real number too. Some interpretations:

- The only knowledge we can *gain* about a quantum state $|\kappa\rangle$ (relative to any prior knowledge about how it was prepared) is by *measuring* it.
- All measurements of κ go through the outer product $|\kappa\rangle\langle\kappa|$.
- Hence $|\kappa\rangle\langle\kappa|$, not $|\kappa\rangle$, is the "unit of epistemology" (the origin of "episte-" is the idea of sending a message, i.e., an *epistle*). This is a Hermitian operator and a PSD matrix with real entries and a projection. All complex numbers have vamoosed.

This carries through when $|\kappa\rangle$ is a state of multiple qubits, or of multiple **qutrits**, **quarts**, **qudits** (meaning d-ary, as with card ranks where $d = 13$), and so on, even going into infinite-dimensional Hilbert spaces. The "real proof" of the principle, IMHO, comes from the extension to mixed states.

Mixed States Again

Consider a mixed state represented as $p_1|\phi_1\rangle + p_2|\phi_2\rangle + \cdots + p_m|\phi_m\rangle$ where the p_i are nonnegative and sum to 1.

Definition: The corresponding **density matrix** is

$$\rho = p_1|\phi_1\rangle\langle\phi_1| + p_2|\phi_2\rangle\langle\phi_2| + \cdots + p_m|\phi_m\rangle\langle\phi_m|.$$

Per above philosophy, ρ is all we can know about the mixed state (aside from any prior knowledge from having prepared it). The letter ρ tends to be used, without a ket or bra around it. Some more facts:

1. A density matrix is always Hermitian: $\rho^* = \rho$.
2. The matrix designates a pure state if and only if $\rho^2 = \rho$; note that this is automatic as shown above when $m = 1$.
3. The results of measuring a mixed state can be computed by applying ρ as an operator to update the state, or with the double action to compute a probability of getting a given state. By linearity, this is the same as working with each individual term and taking the linear combination.

Example: The density matrix of the mixed state $p|0\rangle + (1-p)|1\rangle$ is

$$\rho_p = p|0\rangle\langle 0| + (1-p)|1\rangle\langle 1| = p\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + (1-p)\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} p & 0 \\ 0 & 1-p \end{bmatrix}.$$

Note that $\rho_p^2 = \begin{bmatrix} p^2 & 0 \\ 0 & (1-p)^2 \end{bmatrix} \neq \rho_p$ unless $p = 1$ or $p = 0$, so this is generally not a pure state.

How about $p|+\rangle\langle +| + (1-p)|-\rangle\langle -|$? We get

$$\frac{1}{2}\left(p\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} + (1-p)\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}\right) = \frac{1}{2}\left(\begin{bmatrix} p & p \\ p & p \end{bmatrix} + \begin{bmatrix} 1-p & p-1 \\ p-1 & 1-p \end{bmatrix}\right) = \frac{1}{2}\begin{bmatrix} 1 & 1-2p \\ 1-2p & 1 \end{bmatrix}.$$

In general, this is different. But for the equal mixture $p = \frac{1}{2}$, both density matrices are the same: $\rho_{1/2} = \begin{bmatrix} 0.5 & 0 \\ 0 & 0.5 \end{bmatrix}$. In terms of the Bloch sphere, both mixtures map to the exact center of the sphere,

which is halfway down the axis between $|0\rangle$ and $|1\rangle$ at the poles, and also halfway along the equatorial axis between $|+\rangle$ and $|-\rangle$. In physical terms, that means they are *the same state*. That might come as a surprise, because:

> One is defined as a spread between the outcomes $|0\rangle$ and $|1\rangle$, the other between the outcomes $|+\rangle$ and $|-\rangle$. Isn't that like saying one is apple vs. pear, the other orange vs. grapefruit?

The ultimate point is that to probe the state, we have to choose a basis to measure against in advance. If we choose the standard basis, then to measure the probability for the outcome $|0\rangle$, even if we use the $|+\rangle$ and $|-\rangle$ mixture, we still get

$$P_{|0\rangle}(\boldsymbol{\rho}_{1/2}) = \langle 0|\big(0.5|+\rangle\langle +| + 0.5|-\rangle\langle -|\big)|0\rangle = 0.5\langle 0|+\rangle\langle +|0\rangle + 0.5\langle 0|-\rangle\langle -|0\rangle$$
$$= 0.5\frac{1}{\sqrt{2}}\cdot\frac{1}{\sqrt{2}} + 0.5\frac{1}{\sqrt{2}}\cdot\frac{1}{\sqrt{2}} = 0.5.$$

Note that this associated the terms so that the fact that the $|0\rangle$ and $|+\rangle$ vectors are 45° aligned to each other in Cartesian coordinates, likewise $|0\rangle$ and $|-\rangle$, came out as an idea. But we can get the point much more succinctly upon measuring any outcome $|\kappa\rangle$ for $\boldsymbol{\rho}_{1/2}$:

$$\langle\kappa|\boldsymbol{\rho}_{1/2}|\kappa\rangle = \left\langle\kappa\middle|\begin{bmatrix} 0.5 & 0 \\ 0 & 0.5 \end{bmatrix}\middle|\kappa\right\rangle = \langle\kappa|0.5\mathbf{I}|\kappa\rangle = 0.5\langle\kappa|\mathbf{I}|\kappa\rangle = 0.5\langle\kappa|\kappa\rangle = 0.5.$$

That's it. However we try to probe the **completely mixed state** $\boldsymbol{\rho}_{1/2}$, it just behaves like a perfect unbiased classical coin. Regardless of what we mixed to make it, there is nothing else that it is now.

The Spectral Theorem

Now we come to the essential connection between Hermitian and unitary matrices.

Theorem (split between theorems 14.1 and 18.1 in the text): If A is an $n \times n$ Hermitian matrix, then there are n real numbers $\lambda_1, \ldots, \lambda_n$ (not necessarily all distinct) and associated vectors $\mathbf{u}_1, \ldots, \mathbf{u}_n$ forming an orthonormal basis, such that

$$A = \lambda_1|\mathbf{u}_1\rangle\langle\mathbf{u}_1| + \lambda_2|\mathbf{u}_2\rangle\langle\mathbf{u}_2| + \cdots + \lambda_n|\mathbf{u}_n\rangle\langle\mathbf{u}_n|.$$

Furthermore, the matrix e^{iA}, which is then well-defined by

$$e^{iA} = e^{i\lambda_1}|\mathbf{u}_1\rangle\langle\mathbf{u}_1| + e^{i\lambda_2}|\mathbf{u}_2\rangle\langle\mathbf{u}_2| + \cdots + e^{i\lambda_n}|\mathbf{u}_n\rangle\langle\mathbf{u}_n|,$$

is unitary---and every unitary matrix arises in this manner.

Proof: The first part is by induction. By the fundamental theorem of algebra, the characteristic polynomial $det(A - xI)$ has n solutions over $\mathbb{C}$, counting multiplicities. If there is only one distinct solution λ, then A must equal λI. By the Hermitian property $A^* = A$, λ must be real, and we can get $A = \lambda I = \lambda|\mathbf{u}_1\rangle\langle\mathbf{u}_1| + \lambda|\mathbf{u}_2\rangle\langle\mathbf{u}_2| + \cdots + \lambda|\mathbf{u}_n\rangle\langle\mathbf{u}_n|$ from any orthonormal basis of the space. This is the base case. Note also that for $n = 1$, the basis is unique.

So suppose λ_1 is one of at least two distinct solutions. Then the subspace W of vectors $\mathbf{v}$ such that $A\mathbf{v} = \lambda_1\mathbf{v}$ is not the whole space---it has dimension m less than n. So let $\mathbf{x}$ be in W and $\mathbf{y}$ in the orthogonal complement $W^\perp$ of W. By the Hermitian property,

$$\langle x, Ay\rangle = \langle Ax, y\rangle = \langle \lambda_1^* x, y\rangle = \lambda_1^*\langle x, y\rangle = 0.$$

Since x is an arbitrary vector in W, this means that Ay always stays in the orthogonal complement $W^\perp$, as well as Ax always staying within W. Hence we can argue inductively about A acting on W and on $W^\perp$ individually. This induction also concludes, as ultimately validated on hitting the base case, that λ_1 is real, so $\lambda_1^* = \lambda_1$, and this carries through to all other (distinct) solutions. This process also builds othonormal vectors $\mathbf{u}_i$ such that

$$A = \lambda_1|\mathbf{u}_1\rangle\langle\mathbf{u}_1| + \lambda_2|\mathbf{u}_2\rangle\langle\mathbf{u}_2| + \cdots + \lambda_n|\mathbf{u}_n\rangle\langle\mathbf{u}_n|.$$

Note that these are automatically eigenvectors, because

$$\begin{aligned} A\mathbf{u}_i &= \lambda_1|\mathbf{u}_1\rangle\langle\mathbf{u}_1|\mathbf{u}_i + \lambda_2|\mathbf{u}_2\rangle\langle\mathbf{u}_2|\mathbf{u}_i + \cdots + \lambda_i|\mathbf{u}_i\rangle\langle\mathbf{u}_i|\mathbf{u}_i + \lambda_n|\mathbf{u}_n\rangle\langle\mathbf{u}_n|\mathbf{u}_i \\ &= \lambda_1\ |\mathbf{u}_1\rangle\cdot 0 + \lambda_2\ |\mathbf{u}_2\rangle\cdot 0 + \cdots + \lambda_i\ |\mathbf{u}_i\rangle\cdot 1 + \cdots + \lambda_n\ |\mathbf{u}_n\rangle\cdot 0 \\ &= \lambda_i\mathbf{u}_i \end{aligned}$$

(Well, this is because the notation $|\mathbf{u}_i\rangle$ and just $\mathbf{u}_i$ is interchangeable.) Moreover, if λ_i has multiplicity 1, i.e. is a unique eigenvalue in its eigenspace, then the associated unit eigenvector $\mathbf{u}_i$ is unique.

Now to show that e^{iA} is unitary, we note that its adjoint is

$$\overline{e^{iA}}^T = e^{-iA^T} = e^{-i\lambda_1}|\mathbf{u}_1\rangle\langle\mathbf{u}_1| + e^{-i\lambda_2}|\mathbf{u}_2\rangle\langle\mathbf{u}_2| + \cdots + e^{-i\lambda_n}|\mathbf{u}_n\rangle\langle\mathbf{u}_n|.$$

This is because, as we've seen, every self-outerproduct $|\mathbf{u}\rangle\langle\mathbf{u}|$ is Hermitian so those parts don't change under conjugate transpose. Finally, when we multiply e^{iA} by its adjoint, all of the cross-terms cancel by the orthogonality of the $\mathbf{u}_i$ vectors, leaving only the products of like terms:

$$e^{i\lambda_1}|\mathbf{u}_1\rangle\langle\mathbf{u}_1|e^{-i\lambda_1}|\mathbf{u}_1\rangle\langle\mathbf{u}_1| + \cdots + e^{i\lambda_n}|\mathbf{u}_n\rangle\langle\mathbf{u}_n|e^{-i\lambda_n}|\mathbf{u}_n\rangle\langle\mathbf{u}_n|$$

$$= e^{i\lambda_1}e^{-i\lambda_1}|\mathbf{u}_1\rangle\langle\mathbf{u}_1||\mathbf{u}_1\rangle\langle\mathbf{u}_1| + \cdots + e^{i\lambda_n}e^{-i\lambda_n}|\mathbf{u}_n\rangle\langle\mathbf{u}_n||\mathbf{u}_n\rangle\langle\mathbf{u}_n|$$

$$= |\mathbf{u}_1\rangle\langle\mathbf{u}_1| \; + \; \cdots \; + \; |\mathbf{u}_n\rangle\langle\mathbf{u}_n| \; = \; I,$$

because $e^{i\lambda_1}e^{-i\lambda_1} \; = \; e^{i(\lambda_1-\lambda_1)} = e^0 = 1$ (etc.) and the $\mathbf{u}_i$ are unit vectors. So e^{iA} is unitary.

For the converse direction, let U be any unitary matrix, and put

$$V \; = \; \frac{1}{2}\big(U + U^*\big) \text{ and } W \; = \; \frac{1}{2i}\big(U - U^*\big),$$

so that $U = V + iW$. These are intuitively trying to be the real and imaginary parts of the matrix U. Partial success is attested by the fact that they are Hermitian: $V^* = V$ and $W^* = W$. Moreover, $VW = WV$ because UU^* and U^*U both equal I.

Now a useful fact: Hermitian matrices A, B that commute can have the same orthonormal eigenbasis. For intuition, suppose λ_i has multiplicity 1 for A with unique unit eigenvector u_i. Take $v_i = Bu_i$. Then $Av_i = ABu_i = BAu_i = B\lambda_i u_i = \lambda_i Bu_i = \lambda_i v_i$. Thus v_i is also an eigenvector of A. It need not be a unit eigenvector like u_i, but it must be a multiple of u_i because the eigenspace is one-dimensional. So $Bu_i = v_i = \mu_i u_i$ for some constant μ_i. This constant can be different from λ_i, but it is an eigenvalue of B for the same eigenvector u_i. The general case of higher multiplicity is messier---and it is not the case that *every* orthonormal eigenbasis for A becomes one for B, only that *some* orthonormal eigenbasis of A carries over to B---but the basic reason it works is similar. Therefore, we can write:

$$V \; = \; \lambda_1|\mathbf{u}_1\rangle\langle\mathbf{u}_1| \; + \; \lambda_2|\mathbf{u}_2\rangle\langle\mathbf{u}_2| \; + \; \cdots \; + \; \lambda_n|\mathbf{u}_n\rangle\langle\mathbf{u}_n| \text{ and}$$
$$W \; = \; \mu_1|\mathbf{u}_1\rangle\langle\mathbf{u}_1| \; + \; \mu_2|\mathbf{u}_2\rangle\langle\mathbf{u}_2| \; + \; \cdots \; + \; \mu_n|\mathbf{u}_n\rangle\langle\mathbf{u}_n|$$

with different eigenvalues λ_i, μ_i but the same vectors u_i. So

$$U \; = \; V + iW \; = \; (\lambda_1 + i\mu_1)|\mathbf{u}_1\rangle\langle\mathbf{u}_1| + (\lambda_2 + i\mu_2)|\mathbf{u}_2\rangle\langle\mathbf{u}_2| \; + \; \cdots \; + \; (\lambda_n + i\mu_n)|\mathbf{u}_n\rangle\langle\mathbf{u}_n| \, .$$

Thus each $(\lambda_j + i\mu_j)$ is an eigenvalue of U. Since U is unitary, its eigenvalues have norm 1. Thus λ_j and μ_j are real numbers whose squares sum to 1, and they are therefore the cosine and sine of some angle θ_j. So

$$\lambda_j + i\mu_j \; = \; \cos\theta_j + i\sin\theta_j \; = \; e^{i\theta j}.$$

This finally means that taking

$$A \; = \; \theta_1|\mathbf{u}_1\rangle\langle\mathbf{u}_1| \; + \; \theta_2|\mathbf{u}_2\rangle\langle\mathbf{u}_2| \; + \; \cdots \; + \; \theta_n|\mathbf{u}_n\rangle\langle\mathbf{u}_n|$$

gives a Hermitian matrix such that $U = e^{iA}$. $\boxtimes$

Numerical Matrix Operations

One major application of the spectral representation of a matrix A (when A is Hermitian so it is available) is in representing and executing numerical functions $f(x)$ as matrix functions $f(A)$. We have seen this already with $f(x) = e^{ix}$ as defining "phased exponentiation" e^{iA}. This can be defined in general given $A = \lambda_1|\mathbf{u}_1\rangle\langle\mathbf{u}_1| + \lambda_2|\mathbf{u}_2\rangle\langle\mathbf{u}_2| + \cdots + \lambda_n|\mathbf{u}_n\rangle\langle\mathbf{u}_n|$:

$$f(A) = f(\lambda_1)|\mathbf{u}_1\rangle\langle\mathbf{u}_1| + f(\lambda_2)|\mathbf{u}_2\rangle\langle\mathbf{u}_2| + \cdots + f(\lambda_n)|\mathbf{u}_n\rangle\langle\mathbf{u}_n|.$$

When f is a function involving addition and subtraction and multiplication only (i.e., is a *polynomial function*) then this is immediately evident: only multiplication needs a second thought, and it works because terms for different orthogonal eigenvectors $\mathbf{u}_i$,$\mathbf{u}_j$ will cancel when multiplied. Provided A and B are decomposed in the same eigenbasis, this works for two-variable functions $f(x, y)$ as well: if

$$A = \lambda_1|\mathbf{u}_1\rangle\langle\mathbf{u}_1| + \lambda_2|\mathbf{u}_2\rangle\langle\mathbf{u}_2| + \cdots + \lambda_n|\mathbf{u}_n\rangle\langle\mathbf{u}_n| \text{ and}$$
$$B = \mu_1|\mathbf{u}_1\rangle\langle\mathbf{u}_1| + \mu_2|\mathbf{u}_2\rangle\langle\mathbf{u}_2| + \cdots + \mu_n|\mathbf{u}_n\rangle\langle\mathbf{u}_n|$$

then

$$f(A, B) = f(\lambda_1, \mu_1)|\mathbf{u}_1\rangle\langle\mathbf{u}_1| + f(\lambda_2, \mu_2)|\mathbf{u}_2\rangle\langle\mathbf{u}_2| + \cdots + f(\lambda_n\mu_n)|\mathbf{u}_n\rangle\langle\mathbf{u}_n|.$$

But the fun is that this works for just about any function f. *A fortiori*, this is because just about any function is approximable by polynomials. (I really don't know that "*a fortiori*" means, it just sounds good moving forward.) For example,

$$A^{-1} = \frac{1}{\lambda_1}|\mathbf{u}_1\rangle\langle\mathbf{u}_1| + \frac{1}{\lambda_2}|\mathbf{u}_2\rangle\langle\mathbf{u}_2| + \cdots + \frac{1}{\lambda_n}|\mathbf{u}_n\rangle\langle\mathbf{u}_n|$$

(Wait a second---we saw that many Hermitian matrices, including ones from outer-products $|\phi\rangle\langle\phi|$, are **not** invertible. So how can we do this?? Well, what happens in those cases is... As revealed in class, those matrices have 0 as an eigenvalue occurring at least once. So the above definition would try to do $\frac{1}{0}$, which blows up. So there is no contradiction here.)

This idea, plus using a polynomial approximation to the numerical function $1/x$ that works on a needed interval bounded away from $x = 0$, is the jumping point for the **HHL Algorithm** for (approximately) solving matrix equations by (*approximate*) inversion, as covered in Chapter 18. Another example is:

$$\sqrt{A} = \sqrt{\lambda_1}\cdot|\mathbf{u}_1\rangle\langle\mathbf{u}_1| + \sqrt{\lambda_2}\cdot|\mathbf{u}_2\rangle\langle\mathbf{u}_2| + \cdots + \sqrt{\lambda_n}\cdot|\mathbf{u}_n\rangle\langle\mathbf{u}_n|.$$

For unitary matrices A that happen to also be Hermitian, such as the Pauli matrices and CNOT and CZ, this gives a way to compute square roots for them. For example, on HW3 we essentially computed the following spectral representation: $\text{CNOT} =$

$$1 \cdot \left| \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \rangle\langle \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right| + 1 \cdot \left| \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \rangle\langle \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \right| + 1 \cdot \left| \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} \rangle\langle \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} \right|^{\frac{1}{2}} + (-1) \cdot \left| \begin{bmatrix} 0 \\ 0 \\ 1 \\ -1 \end{bmatrix} \rangle\langle \begin{bmatrix} 0 \\ 0 \\ 1 \\ -1 \end{bmatrix} \right|^{\frac{1}{2}}.$$

To get a 4×4 matrix B such that $B^2 = \mathbf{CNOT}$ we just take square roots of all the eigenvalues. We have a wide choice: $+1$ or -1 for the first there and i or $-i$ for the -1. Using the positive signs gives

$$B = 1 \cdot \left| \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \rangle\langle \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right| + 1 \cdot \left| \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \rangle\langle \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \right| + 1 \cdot \left| \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} \rangle\langle \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} \right|^{\frac{1}{2}} + i \cdot \left| \begin{bmatrix} 0 \\ 0 \\ 1 \\ -1 \end{bmatrix} \rangle\langle \begin{bmatrix} 0 \\ 0 \\ 1 \\ -1 \end{bmatrix} \right|^{\frac{1}{2}}$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix} + \frac{i}{2}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1+i}{2} & \frac{1-i}{2} \\ 0 & 0 & \frac{1-i}{2} & \frac{1+i}{2} \end{bmatrix}$$

This is the matrix of the controlled gate $\mathbf{CV}$ where $\mathbf{V} = \frac{1}{2}\begin{bmatrix} 1+i & 1-i \\ 1-i & 1+i \end{bmatrix}$ is also written $\mathbf{X}^{\frac{1}{2}}$ and called the **square root of NOT**. (The Wybiral circuit simulator calls it "SRNOT".) Notice also that $\mathbf{V}$ is not Hermitian like $\mathbf{X}$ is---but that's not a contradiction because i is not an eigenvalue of this basis (it isn't a real number, either).

Short Philosophical Interlude

Speaking fairly generally, a projective measurement $\mathbf{P} = \{\mathbf{P}_i\}_{i=1}^n$ can be associated to an orthonormal eigenbasis for some Hermitian matrix. When we apply $\mathbf{P}$ to measure a general (pure) state $|\phi\rangle$, we "bonk it with the basis". The measurement outcome is one of the $|\mathbf{u}_i\rangle$ vectors, with probability $|\langle \mathbf{u}_i | \phi \rangle|^2$. (Some sources further say that the associated eigenvalue λ_i "is" the outcome.) The fact that $\mathbf{P}_i^2 = \mathbf{P}_i$ lends definiteness to the measurement result---it stays the same under "repeated bonking." *Maybe* this is what enables us to *observe* the measurement result to begin with.

(By the way, note that $B = QAQ^{-1}$ is a general representation of a change of basis transformation. But if A is notationally the identity matrix, then so is B. So the specification that $\sum_i \mathbf{P}_i = \mathbf{I}$ in the definition of projective measurement does not lock us into the *notation* for the standard basis.)

Anyway, we can give a gentle partial disagreement with the Copenhagen interpretation by saying the original quantum state doesn't "collapse"---it just gets bonked. The meaningful factor going forward is: what is the role of the choice of basis to bonk it with? And is there free will in that choice? Possibly free will that leads to superluminal communication??? Let's look at a major case.

Choosing Bases to Measure In

The question that concerned Einstein is whether Bob can send a willful message to Alice through their entanglement by choices of measurement bases. My use of "willful" here is willful: *pace* quantum-based arguments against free will, it is IMHO the clearest way to frame the technical argument. All agree that Alice gains *information* of Bob's random outcomes, though that information was "pre-paid" by the interactions that set up n entangled qubits to begin with. The point of superdense coding is that Bob could distinguish among 4 willful actions by Alice *after* the initial exchange of one entnagled qubit, when it was *followed by* her sending 1 other qubit. Can something like this be done *without any further interaction*---and over time intervals shorter than the time for light to travel between Alice and Bob?

Most in particular, can Alice gain any willful information---other than unstructured randomness---from how Bob orients his measurements? The answer is no. If they share $|00\rangle + |11\rangle$ (over $\sqrt{2}$) you might think Bob could guarantee a '1' by measuring in the $|+\rangle, |-\rangle$ basis, but no: that was the first decoherence example with Alice. Any basis Bob uses is the same as a unitary $\mathbf{U}$ to convert to the standard basis followed by a measurement there, and $\mathbf{U}$ has no effect on what Alice will see.

This makes it all the more amazing that there are situations where the choice of measurement basis does make a difference---one that has been quantified in actual experiments.

The CHSH Game

The initials in the CHSH Game stand for John Clauser, Michael Horne, Abner Shimony, and Richard A. Holt, who described it in a paper in 1969. The 2022 Nobel Prize in Physics was awarded to Clauser and to Alain Aspect and Anton Zeilinger. The latter two did the most notable experimental confirmations of the quantum advantage involved. Clauser and Holt are still alive; Holt is emeritus at nearby Western University in London, Ontario.

In the game, Alice and Bob share n Bell pairs $\frac{1}{\sqrt{2}}\left(|00\rangle + |11\rangle\right)$ and can have as much prior classical communication to agree on strategies as they please. Between the start and end of a *trial*---one play of

the game---they may not communicate with each other, but they may observe common sources. The common source can not only be random---such as from patterns of solar flares both Alice and Bob can see---it can be controlled by an oracle "Ozzie" who is trying to help Alice and Bob. Each trial operates via classical communication with a third party, "Ralph" (to sound like ref, referee) and goes like this:

1. Ralph sends a random bit a to Alice and a bit b to Bob. Neither can see the other's bit.
2. Alice sends a response bit u to Ralph and Bob simultaneously sends his response bit v to Ralph.
3. Ralph declares that Alice and Bob win the trial if $u \oplus v = a \wedge b$.

We may suppose that Alice and Bob receive a and b in sealed boxes, and give their respective u and v within a nanosecond of opening their boxes. Without loss of generality, we may suppose that any other influence from observations or "Ozzie" has been registered by that instant. At that point, Alice's u is a one-bit Boolean function of a alone. We use $0, 1$ for the inputs to this function but give the outputs as **Y** for "yes" or **N** for "no" in order to keep inputs and outputs visually separate. There are just four functions that she can use:

- The always-true function: yes to 0 and yes to 1, which we call **YY**.
- The always-false function, which we similarly call **NN**.
- The identity function, giving Ralph the same bit back, which is **NY**.
- Flipping the bit to Ralph, which is **YN**.

Bob has the same four options, so there are in total **16** different strategies they can use for any trial. Meanwhile, Ralph has his own four possible actions. Here is the entire matrix of possibilities. The matrix entries are numeric rather than Boolean: 1 if Alice and Bob win, 0 if they lose. The rows are the four options by Ralph, in order a, b so that for instance, if Alice and Bob adopt the strategy in the third column and find that Ralph chose $1, 0$, then Alice says **N** while Bob says **Y**---and they lose because their answers disagreed while $1 \wedge 0$ is false.

Alice	NN	NN	NN	NN	NY	NY	NY	NY	YN	YN	YN	YN	YY	YY	YY	YY
Bob	NN	NY	YN	YY	NN	NY	YN	YY	NN	NY	YN	YY	NN	NY	YN	YY
$0, 0$	1	1	0	0	1	1	0	0	0	0	1	1	0	0	1	1
$0, 1$	1	0	1	0	1	0	1	0	0	1	0	1	0	1	0	1
$1, 0$	1	1	0	0	0	0	1	1	1	1	0	0	0	0	1	1
$1, 1$	0	1	0	1	1	0	1	0	0	1	0	1	1	0	1	0

Note that when Ralph plays randomly, Alice and Bob can assure 75% winning if they choose any of the eight columns with three 1s as their joint strategy. **They cannot do better**, because every column has a case where Ralph could send them something that makes their joint strategy lose---and the randomized Ralph does so with 25% probability.

The amazing fact is that sharing one entangled Bell pair enables Alice and Bob to do much better: to win **over 85%** of the time in theory.

A side note if you are familiar with matrix game theory: could Ralph do better with non-random play if he knew Alice and Bob's strategy? Certainly if Alice and Bob always play one fixed column, such as both always saying **N**, then Ralph could always deny them by giving the one losing combination a, b. If you know the **Minimax Theorem** of zero-sum matrix game theory, then you already know that because 25% is Ralph's optimum when he has to move first, Alice and Bob *must* have a *classically randomized* strategy that assures them 75% even if Ralph is told about it in advance. We can find it easily by first removing the eight "obviously stupid" joint strategies---those with only one 1 in their column---leaving:

Alice	NN	NN	NY	NY	YN	YN	YY	YY
Bob	NN	NY	NN	YN	NY	YY	YN	YY
$0,0$	1	1	1	0	0	1	1	1
$0,1$	1	0	1	1	1	1	0	1
$1,0$	1	1	0	1	1	0	1	1
$1,1$	0	1	1	1	1	1	1	0

Now if Alice and Bob use their shared classical randomness to choose one of the leftover strategies at random with probability $1/8$, there is no way Ralph can avoid their winning 75% of the time even if Ralph knows that is their policy. If Ralph could steal their random bits by looking at solar flares *and* knowing *how* and *when* Alice and Bob will decode them, then Ralph could still always send the bad combo. But the order is: Ralph commits to the a, b combo first, then Alice and Bob have a moment to read the shared random source that determines their policies before they open their boxes.

The scientific significance does not require this detail---we just stipulate that Ralph plays randomly.

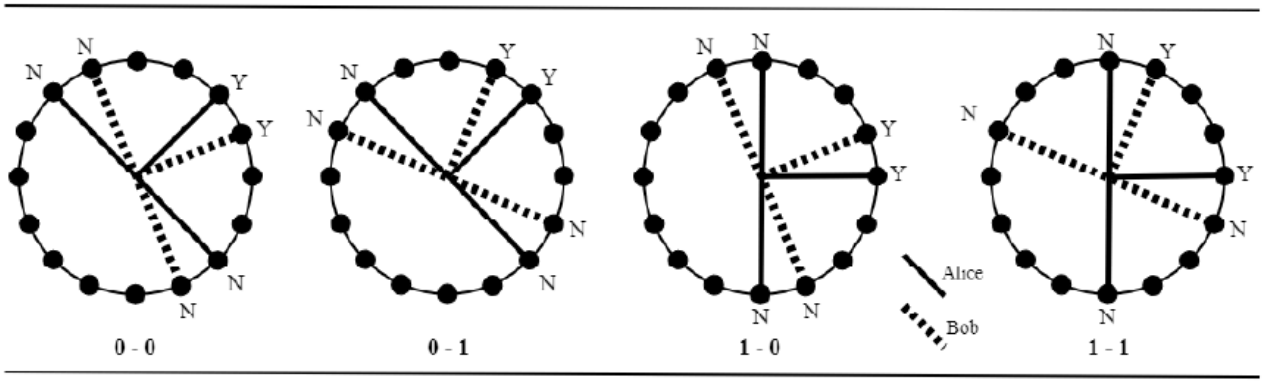
The Quantum Case

Alice and Bob get an extra option using one shared Bell pair per trial: Each can measure in a basis that depends on the bit received from Ralph. The timing of this option is synchronized as viewed by Ralph. The text describes Alice as measuring first, but we'll make Bob go first for consistency with recent lectures. By symmetry, it does not matter who goes first. What does matter, technically, is that the time lapse from opening the boxes to the second measurement---as viewed by Ralph---must be less than the time it would take light to travel from Bob to Alice. This is in order to avoid one of several possible "loopholes" that could enable a classical explanation.

Rather than the Bloch sphere, this is a case where the Cartesian diagram of state vectors is best for visualization: $|0\rangle$ at east (**E**), $|1\rangle$ at north (**N**), $|+\rangle$ between them facing northeast (**NE**), and $|-\rangle$ to the southeast (**SE**). Alice will use either the $\{|0\rangle\langle 0|, |1\rangle\langle 1|\}$ or $\{|+\rangle\langle +|, |-\rangle\langle -|\}$ measurement. We let the former outcomes stand for "yes", so we can abbreviate her options as **E** or **NE**. Bob has a funkier set of bases to choose from. He can use the basis that orients his "yes" answer at 22.5°, which we call **ENE** for east-northeast, and puts "no" at 112.5° (or equivalently, at -67.5°, i.e., 292.5°). Or Bob can use the basis that puts "yes" at $+67.5^\circ$, which is **NNE** for north-northeast. Here is the protocol:

1. Alice and Bob open their boxes simultaneously.
2. If $b = 0$, Bob measures his entangled qubit in the basis oriented **ENE**; if $b = 1$, Bob chooses **NNE**.
3. If $a = 0$, Alice instantly chooses **NE**, else she chooses **E**. No more than a nanosecond later than Bob's actions, Alice measures her qubit in her chosen basis.
4. Each sends Ralph "yes" if getting the measurement outcome designated "yes", else "no".

The upshot can be appreciated *ahead of any thinking about the underlying physical reality*, just by looking at the diagram of the choices made by Alice and Bob in the four cases Ralph can send them:



Alice's chosen orientations depend only on her bit from Ralph: northeast on 0, due east on 1. Bob likewise reacts independently of Alice. Yet the options combine to make their "yes" orientations come within 22.5° of each other in all of the 00, 01, and 10 cases from Ralph, yet 67.5° apart on 11.

If being one-fourth of a right angle apart meant a one-fourth chance of losing, then the resulting chances would be no different from the classical case: 75% frequency of winning. But in ways we can actually see for ourselves by orienting polarizing filters at these angles and telling how much light gets through, in the first three cases, the chance of her qubit instantly transformed(?) by Bob's outcome giving the same yes/no answer from her 22.5°-apart measurement is greater: $\cos^2\left(\frac{\pi}{8}\right) = 85.3553...\ \%$.

And in the fourth case, the frequency of Alice and Bob giving different answers and winning is the same.

Discussion

Well, saying "transformed" is exactly the kind of *spukhafte Fernwirkung* that Einstein objected to. But this is the straightest path to expressing the explanation for what we observe---which has been verified in actual experiments achieving over 80%. The gap between 80% and 85+% is ascribable in substantial part to the kind of slight-degrading errors we saw in the "depolarization and de-phasing" section (plus to other slight flaws in the apparatus and its nanosecond timing).

Note that no "free will" is involved on the part of Alice and Bob, nor any contextual information ("hints from Ozzie") at all. Their choices of measurement basis are determined entirely by the bit each receives from Ralph. Their only agency is the sharing of entangled Bell pairs, possession of the measuring apparatus for their respective pairs of bases, and a mechanism for reading the bit from Ralph and effecting the corresponding basis choice. Given a physical setup and timing so that their measurements are made within a picosecond of receiving the bit from Ralph and of each other, while "Alice" and "Bob" are situated more than a light-picosecond apart, Ralph is really playing solitaire. And Ralph plays randomly, so no free will is involved there either. Yet the resulting physical system "wins" with a frequency that cannot be explained by any classical theory with variables localized to "Alice" and "Bob" that obliviates the entanglements between them.

My section 14.7.3 replaces the element of Alice and Bob choosing different measurement bases with that of their choosing different *basis-change operators*, while always doing their actual measurements in the standard basis. They apply these operators **before** (and only nominally after) doing their measurements. This streamlines the physical interpretation, and yet yields the same basic math. See also the chapter end notes for further discussion. This should go hand-in-hand with the No-Communication Theorem, but the Wikipedia treatment which I've linked goes a little further afield than I had in mind for the textbook.

Finally, this example avoids objections to earlier claims of "quantum advantage"---by which the Deutsch and Deutsch-Jozsa algorithms "unfairly" restrict the classical setting; Simon's algorithm is has a discrepancy between quantum and classical that is provable but only asymptotic; Shor's algorithm is proven but factoring might be in classical (random) polynomial time after all; and Grover's algorithm gives speedups only for running times that are exponential to begin with (your HW on exercise 13.7 has some sidelight here). The ability to win more than the classical limit of 75% is concrete and experimentally proven. The only knock is that the CHSH game is for an interactive protocol, not for straight-up computation.

Section 14.8 gives a claim of quantum advantage for straight-up computation, but it has come under more of a cloud since its October 2019 unveiling (see this article by me), and is for a contrived problem anyway. We will instead seque into ideas for classical computing to take away the appearance of quantum advantage for straight-up computational problems.