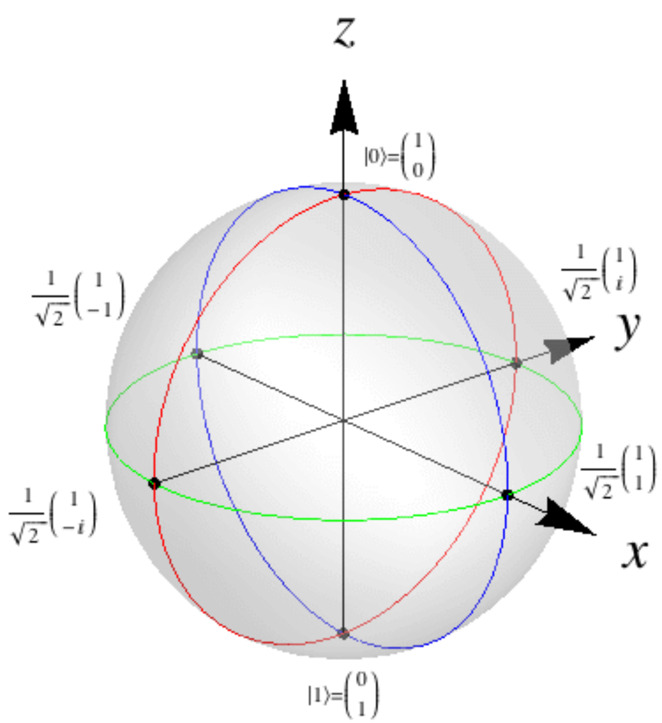
The Bloch Sphere

A single spin-1/2 state, or "qubit", is represented as a normalized state $\begin{pmatrix} a \\ b \end{pmatrix}$ where

|a|^2+|b|^2=1. The phase of this is irrelevant, so you can always multiply **both** "a" and "b" by exp(ic) without changing the state. Note that this formalism can be used for any 2D Hilbert space state; it doesn't *have* to be a spin-1/2 particle.

For any such state, you can always find a direction that you can measure the spin and **always** get a result of $\hbar/2$. This is the same direction as the expectation value of the vector of spin-operators < **S** >. This direction can be represented as a unit vector, pointing to a location on a unit sphere, or the "Bloch sphere". For example, spin-up (a=1,b=0) corresponds to the intersection of the unit sphere with the positive z-axis. Spin-down (a=0,b=1) is the -z axis.



For an arbitrary point on this sphere, measured in usual spherical coordinates (θ,ϕ), the corresponding spin-1/2 state is (see problem 4.30 in Griffiths): Eqn [4.155]:

$$\begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi} \end{pmatrix} \text{ or } \begin{pmatrix} \cos\frac{\theta}{2}e^{-i\phi/2} \\ \sin\frac{\theta}{2}e^{i\phi/2} \end{pmatrix}$$ (see why these two forms are really the same?)

Useful Exercise: Check that this works for the above cases in the diagram.

Notice the special notation for spin up: $|0\rangle$, and for spin down: $|1\rangle$. These are the "0"'s and "1"'s of a quantum computer. Of course, any single qubit state can be written in these terms: $\begin{pmatrix} a \\ b \end{pmatrix} = a|0\rangle + b|1\rangle$. (Don't forget a and b are complex.)

Single Qubit Measurements:

We already know how to do single-qubit measurements, in principle, but there is a useful shortcut when thinking about states on the Bloch sphere. For any qubit-state pointing in the **f**-direction on the Bloch sphere, suppose you measure it on the **g**-axis (for a spin-1/2 particle, you could do this by putting a magnetic field in the **g**-direction and measuring the energy.) It turns out that the probability of the outcomes only depends on the angle between **f** and **g**: call this angle θ.

It is not hard to prove (done in class) that the probability of measuring the eigenvalue corresponding to the state pointing in the the +**g** direction is $\cos^2\left(\theta/2\right)$. If this was the measurement result, we already know that the qubit would "collapse" into a state whose Bloch sphere vector pointed in the +**g** direction instead of the **f** direction.

The other possibility is that it might collapse into a state whose Bloch sphere vector pointed in the **-g** direction. Obviously, the probability of this other measurement outcome would be $\sin^2\left(\theta/2\right)$. There are no other possible outcomes for such a measurement.

Single Qubit Gates: Rotations on the Bloch Sphere

A quantum "gate" is a transformation that you can perform on a quantum state. IMPORTANT NOTE: THIS IS NOT A MEASUREMENT. It's just a linear transformation, and can be represented by an operator: $\hat{\mathbf{Q}}|\psi\rangle = |\psi'\rangle$. In general, the gate (**Q**) takes the input state $|\psi\rangle$, and spits out the output state $|\psi'\rangle$. There is no collapse, just a transformation. (Technically, a "unitary" transformation.)

Single-qubit gates are best envisioned as <u>rotations on the Bloch sphere.</u> You can rotate around any axis, by any angle -- in fact, we already know how to do this to a spin-1/2 state with an appropriately aligned magnetic field. (The state precesses around the B-field direction.)

These gates/rotations are discussed in an important problem in Griffiths: Problem 4.56. The exponential notation in the earlier part of the problem is not needed; the upshot of this problem is the last equation [4.201] (although the book's equation drops the Identity matrix in my version). This tells us that the operator **R** corresponding to a rotation of an angle ϕ around an axis $\hat{n}$ is:

$$\mathbf{R} = \cos\left(\frac{\phi}{2}\right)\mathbf{I} + i(\hat{n}\cdot\sigma)\sin\left(\frac{\phi}{2}\right) \quad [4.201]$$

Here **I** is the 2x2 identity matrix, and σ is the vector of Pauli matrices. (So if you wanted to rotate around the z-axis, you would put in $(\hat{n}\cdot\sigma) = \sigma_z$. Obviously **R** would also be a 2x2 matrix, so that it can operate on a qubit.

(Note: These matrices are not Hermitian! They are "unitary".)

Special/useful single-qubit gates include:

The **NOT** gate (also known as the Pauli **X**-gate); a 180° rotation around the x-axis.

The Pauli-**Z** gate: a 180° rotation around the z-axis.

The Pauli-**Y** gate: a 180° rotation around the y-axis.

The $\sqrt{NOT}$ gate; a 90° rotation around the x-axis.

Phase shift gates, $R(\phi)$; a ϕ-angle rotation around the z-axis.

Useful exercise: Build these 2x2 matrices, and check that they work as advertised!

Building Two Qubit States: Tensor Products

In QM, when you have two single-particle Hilbert spaces, the total wavefunction lives in a larger Hilbert space that is the "tensor product" of those two spaces. If qubit 1 is in state $\begin{pmatrix} a \\ b \end{pmatrix}$, and qubit 2 is in state $\begin{pmatrix} c \\ d \end{pmatrix}$, then the total state of the two qubit system is: $\begin{pmatrix} a \\ b \end{pmatrix} \otimes \begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} ac \\ ad \\ bc \\ bd \end{pmatrix}$, in a 4D Hilbert space.

Now, you can also write this same equation in terms of the $|0\rangle$, $|1\rangle$ notation:

$$\left[a|0\rangle + b|1\rangle\right] \otimes \left[c|0\rangle + d|1\rangle\right] = ac|00\rangle + ad|01\rangle + bc|10\rangle + bd|11\rangle$$

Notice the new notation: The state $|00\rangle$ is just $|0\rangle \otimes |0\rangle$, etc.

You can also tensor product single-qubit operators together to make two-qubit operators. Basically, you just multiply *each* element of the first matrix by the *entire* second matrix! This clearly will make a bigger matrix:

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \otimes \begin{pmatrix} E & F \\ G & H \end{pmatrix} = \begin{pmatrix} AE & AF & BE & BF \\ AG & AH & BG & BH \\ CE & CF & DE & DF \\ CG & CH & DG & DH \end{pmatrix}$$ (see the pattern??)

If the 2x2 matrix **M** is an operator on one qubit, this clearly can't operate on a 4D Hilbert space. But the operator $\mathbf{M} \otimes \mathbf{I}$ (where **I** is the 2x2 identity) represents a measurement of **M** on qubit #1; it's a 4x4 operator. The operator $\mathbf{I} \otimes \mathbf{M}$ is what you would use to measure **M** on qubit #2.

Two-Qubits: Entangled States

Not all states in 4D Hilbert spaces can be separated into two distinct single-particle states as in the above example. If they are in the form $\begin{pmatrix} a \\ b \end{pmatrix} \otimes \begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} ac \\ ad \\ bc \\ bd \end{pmatrix}$, the states are "separable"; otherwise they are "entangled". Entangled states are mathematically possible because you can add up superpositions of separable states, that no longer neatly split into two qubits. We'll try to make sense of them later.

The most general two-qubit state can be written:

$$A|00\rangle + B|01\rangle + C|10\rangle + D|11\rangle$$

One easy way to see if such a state is separable is if the quantity 2|AD-BC|=0. This quantity is called the "Concurrence", and is a measure of entanglement. (The maximum possible value is 2|AD-BC|=1; this occurs for a "maximally entangled state".)

Two-Qubit Gates

A "controlled not" or "CNOT" is an example of a gate that acts on a 2-qubit state. This operation can turn separable states into entangled states (and vice-versa) by swapping the bottom two values in this 4D Hilbert space:

$$\begin{pmatrix} e \\ f \\ g \\ h \end{pmatrix} \Rightarrow (CNOT) \Rightarrow \begin{pmatrix} e \\ f \\ h \\ g \end{pmatrix}$$

Useful Exercises: What 4x4 matrix would do this? Find a separable state that turns into a maximally-entangled state under the CNOT operation.

Obviously, two consecutive CNOTs give you back the original state.

Another two-qubit gate is the SWAP gate, which effectively swaps the two qubits.

$$\begin{pmatrix} e \\ f \\ g \\ h \end{pmatrix} \Rightarrow (SWAP) \Rightarrow \begin{pmatrix} e \\ g \\ f \\ h \end{pmatrix}$$

Useful Exercise: Check that this works as advertised for a separable state; also figure out what the 4x4 matrix might look like.

The SWAP gate cannot be used to entangle separable states; it just swaps them. But the root-SWAP, or $\sqrt{SWAP}$ gate, can do this:

$$\sqrt{\mathrm{SWAP}} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{2}(1+i) & \frac{1}{2}(1-i) & 0 \\ 0 & \frac{1}{2}(1-i) & \frac{1}{2}(1+i) & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

Useful Exercise: Check that two of these gives you a SWAP!

Two Particle Measurements:

Even if you have an entangled state, you can of course choose to measure each qubit separately. Say you choose a measurement direction for qubit 1 and a measurement direction for qubit 2. There are two possible outcomes for each direction, so there are 4 possible combined outcomes. (You would build such an operator using the Tensor Product: see above.) But finding the eigenstates of a 4x4 operator is hard; it's almost always easier to start with the two 2x2 operators separately.

The possible outcomes for qubit 1 are orthogonal eigenstates of the qubit-1 measurement operator, and so can always be represented by

$$|\psi_{1+}\rangle = \begin{pmatrix} a \\ b \end{pmatrix}, \; |\psi_{1-}\rangle = \begin{pmatrix} b^* \\ -a^* \end{pmatrix}$$ (see why these are always orthogonal?)

You can generate the first of these from the angles of the measurement setting (see first page, "The Bloch Sphere"), where the "+" outcome has Bloch sphere vector that is aligned with the setting and the "-" outcome has a vector that is anti-aligned with the setting.

In the same way, the possible outcomes for qubit 2 are determined by a **separate** setting choice; call those:

$$|\psi_{2+}\rangle = \begin{pmatrix} c \\ d \end{pmatrix}, \; |\psi_{2-}\rangle = \begin{pmatrix} d^* \\ -c^* \end{pmatrix}.$$

So the 4 measurement eigenstates of the full 4x4 operator can be generated via a tensor product. For example, the outcome "++" (both outcomes aligned with the corresponding setting) is

$$|\psi_{1+}\rangle \otimes |\psi_{2+}\rangle = \begin{pmatrix} a \\ b \end{pmatrix} \otimes \begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} ac \\ ad \\ bc \\ bd \end{pmatrix} = |++\rangle.$$

Given the actual state in the full 4D Hilbert space, the probability of the outcome of this "++" state can be found from the generalized Born rule: $|\langle ++|\psi\rangle|^2$.

If the states are normalized, the 4 probabilities will always add to one.

Marginal Probabilities

We're often interested in the probabilities of a measurement of one particular particle, independent of what happens to the other one. (The quantum no-signalling theorem says that the net probabilities of one particle can't depend on the choice of measurement setting at the other particle.) So to find the probability of a + outcome of qubit#1, we can set the qubit #2 measurement setting to anything we want, say the z-axis. Then c=1, d=0. So the two possible outcomes where particle 1 is found to be "+" are:

$$|{+}{+}\rangle = \begin{pmatrix} a \\ 0 \\ b \\ 0 \end{pmatrix}, \text{ and } |{+}{-}\rangle = \begin{pmatrix} 0 \\ a \\ 0 \\ b \end{pmatrix}.$$

To find the probability of the outcome "+" for qubit 1, we therefore need to calculate $\left|\langle{+}{+}|\psi\rangle\right|^2 + \left|\langle{+}{-}|\psi\rangle\right|^2$. In other words, we add up the probabilities of (+ on 1, + on 2) and (+ on 1, - on 2). The sum is just the total probability of measuring + on qubit 1.

We are about to learn an easier way to do this (and an easier way to make sense of the results), using something called a "partial trace" of a "density matrix".

Density Matrices: Pure States

Given the complete quantum state $|\psi\rangle$, it's possible to form a "density matrix" that encodes this state, using the equation:

$$\rho = |\psi\rangle\langle\psi|$$

This crazy-looking equation is called an "outer product"; you can figure out what it means just by plugging in the bra- and ket- in vector form. For a single qubit, this gives:

$$\rho = \begin{pmatrix} a \\ b \end{pmatrix}\begin{pmatrix} a^* & b^* \end{pmatrix} = \begin{pmatrix} aa^* & ab^* \\ a^*b & bb^* \end{pmatrix}.$$

Notice the trace of this matrix is 1. And it's automatically independent of the global phase on the original state. Also, notice that $\rho^2 = |\psi\rangle\langle\psi||\psi\rangle\langle\psi| = \rho$. For this case, when $\rho^2 = \rho$, we say this is a "pure state". (meaning, it is generated from a single, complete wavefunction). We're about to encounter other density matrices for which $\rho^2 \neq \rho$; these will be "mixed states". Every state is either pure or mixed.

Pure State of Single Qubits

$$|\psi\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi} \end{pmatrix}$$ corresponds to the state of a point on the Bloch Sphere (recall).

Building the density matrix from this state one finds:

$$\rho = \begin{pmatrix} \cos^2(\theta/2) & \cos\frac{\theta}{2}\sin\frac{\theta}{2}e^{-i\phi} \\ \cos\frac{\theta}{2}\sin\frac{\theta}{2}e^{+i\phi} & \sin^2(\theta/2) \end{pmatrix}$$

Then, using the half-angle formulas, this can be written in terms of the Pauli Matrices:

$$\rho = \frac{1}{2}\left(\mathbf{I} + \sin\theta\cos\phi\,\sigma_x + \sin\theta\cos\phi\,\sigma_y + \cos\theta\,\sigma_z\right)$$

But this is just the Cartesian coordinates of the original vector on the Bloch Sphere! (Think about the conversion from spherical to Cartesian; those are the 3 terms.) So a pure state can be written as

$$\rho = \frac{1}{2}\left(\mathbf{I} + \hat{n}\cdot\sigma\right)$$

Where "*n*" is the unit vector on the Bloch sphere. Later we'll see that we can generalize this even when "*n*" is not a unit vector! This is one of the easiest ways to get from an arbitrary single-qubit wavefunction to the vector on the Bloch sphere -- especially if you don't like using spherical coordinates.

Introduction to Mixed States

The nice thing about density matrices is that they can be combined according to ordinary probability rules. Suppose you had a machine that made the state $|\psi_1\rangle$ 30% of the time, but made the different state $|\psi_2\rangle$ 70% of the time. (This is not a superposition! Just classical ignorance.) In this case, for any given particle, you wouldn't know for sure what the state was -- and yet, your job is to make predictions all the same. This can be done by simply weighting the possible density matrices (according to their probability), and adding them up into a single density matrix: $\rho = 0.3|\psi_1\rangle\langle\psi_1| + 0.7|\psi_2\rangle\langle\psi_2|$. See how that works? You just weight the possible density matrices and add them up. It turns out that from this total density matrix you can make all the right predictions. Also, this is clearly a <u>mixed state</u>; $\rho^2 \neq \rho$. (But the trace of the mixed state density matrix is still 1.)

For any given mixed state density matrix, there are usually many ways to make it: different "ensembles". But even though those different ensembles may be made up of totally different quantum states, it turns out there is absolutely no way to experimentally distinguish the different ensembles, if they have the same density matrix! If you know the density matrix, you know all the probabilities that you can measure.

Extracting Probabilities

It's possible to use the rules from ordinary QM to show the expectation value of any operator Q is simply:

$\langle Q\rangle=\mathrm{Trace}(\rho Q)$

In other words, you simply multiply the density matrix times the operator matrix, and take the trace. This always works, even for mixed states! (There's also a collapse rule we may get to later.)

In principle, knowing all the expectation values gives you all the probabilities, but we'll get to exact probabilities later. (maybe!)

Time Evolution

The Schrodinger Equation also looks quite nice when written in terms of density matrices These matrices evolve with time, of course: $\rho(t)$. It solves the equation:

$$i\hbar\frac{d\rho}{dt}=[H,\rho]$$

Yes, that's a commutator! If H is constant (as usual, for us), the solution is:

$$\rho(t)=e^{-iHt/\hbar}\rho(t=0)e^{+iHt/\hbar}$$

We won't use this solution much, so don't worry about it too much. But see Griffiths problem 4.56 if you're wanting to understand what it means to have an operator in the exponent.

Gate Evolution

From the definition of the density matrix, as well as the known action of a gate operator **R** on $|\psi\rangle$, it's easy to show that if you put a density matrix into a gate **R**, the output density matrix will be simply: $\rho_{output}=\mathbf{R}\rho\mathbf{R}^{\dagger}$. Don't forget that last matrix needs to be Hermitian-conjugated.

Partial Traces: How to describe a smaller piece of a multi-qubit system.

Consider a two qubit system, $A|00\rangle + B|01\rangle + C|10\rangle + D|11\rangle$. You should be able to form the 4x4 density matrix of the whole system; it will be a pure state.

But then, as before, you may ask a question about the probabilities of a measurement on just qubit #1. If you want to describe this qubit alone, independently of the other one, it would be nice to have that qubit's 2x2 density matrix. This can be extracted from the full 4x4 matrix; the procedure is to take the "partial trace" of the full 4x4 matrix.

Basically, if you want to find the $|0\rangle\langle 0|$ entry of qubit #1's density matrix, you need to add up the $|00\rangle\langle 00|$ and the $|01\rangle\langle 01|$ components of the full 4x4 matrix. In this case, you'll get AA*+BB*. (Get it? You don't care about the second qubit, so you try both options, while keeping the first qubit fixed.) If you want to find the $|0\rangle\langle 1|$ component, you add up the $|00\rangle\langle 10|$ and the $|01\rangle\langle 11|$ components, or AC*+BD*. And so on.

It works the other way, too To find the $|0\rangle\langle 0|$ entry of qubit #2's density matrix, you add up the $|00\rangle\langle 00|$ and the $|10\rangle\langle 10|$ components of the full 4x4 matrix (keeping the second qubit fixed, summing over all possible entries for the first one.) If you want to find the $|0\rangle\langle 1|$ component for qubit #2, you add up the $|00\rangle\langle 01|$ and the $|10\rangle\langle 11|$ components.

Pieces of Entangled Systems act like Mixed States

If the original two-qubit state was separable, this partial trace procedure ends up with the proper two states for the two qubits. In this case, these would be pure states.

But if the original two-qubit state was entangled, this can't possibly work, because the state doesn't factor into two pure states. So what happens? You end up with two *mixed* states! Pieces of entangled systems act just like Mixed States!

When you find the partial trace corresponding to a single qubit, it turns out you can still always write it in the earlier form:

$$\rho = \frac{1}{2}\left(\mathbf{I} + \hat{n}\cdot\sigma\right).$$

Only now "n" is no longer a unit vector. (It's a unit vector when it's a pure state, just not when it's a mixed state.) But the Bloch sphere picture is still useful: the mixed state is a vector *inside* the sphere!! Knowing which way it's pointing is still useful, as it knowing its length. Maximally-entangled states wind up at the very center of the Bloch sphere, with n=0.

However, knowing how the two individual qubits might be measured, independently, is not the whole story. You've lost some information in the partial-trace process. What's missing is the *correlations* between the two qubits, which can only be gleaned from the full 4x4 density matrix. And this brings us to the topic of "Entanglement".