Composite Systems: Two Qubits

To complete our discussion of entangling 2-qubit unitaries, let's look at the Hamiltonians that generate them to understand what entangling time evolutions correspond to physically.

The unitary CNOT can be expressed as $\Lambda(X) = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes X$

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$$Z = e^{i\theta A}$$

Take $\theta = \pi$ and $A = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} = (I - Z)$

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The CNOT Hamiltonian should do nothing if the first qubit is in the state $|0\rangle$, and if it is in the state $|1\rangle$ then it should turn on the *H* above to generate an X gate. To generate CNOT turn on

$$H_{\Lambda(X)} = |1\rangle\langle 1| \otimes (I - X)$$

For $\pi/4$ time units. Evidently the operator above is an **entangling Hamiltonian**.

Composite Systems: Two Qubits

Suppose we have two qubits and apply a spatially uniform magnetic field along the z direction. It creates an energy splitting of 2a, and assigns a higher energy to spin up $|0\rangle$ than spin down $|1\rangle$.

$$H_1 = aZ_1 \quad , \quad H_2 = aZ_2 \quad , \quad H = H_1 + H_2$$

Expanding the subscript notation, $H = a\,(Z_1 \otimes I + I \otimes Z_2)$. Is this an **entangling Hamiltonian**?

Intuitively it shouldn't be entangling, because the uniform magnetic field acts on the two qubits independently. Therefore it cannot create any correlations:

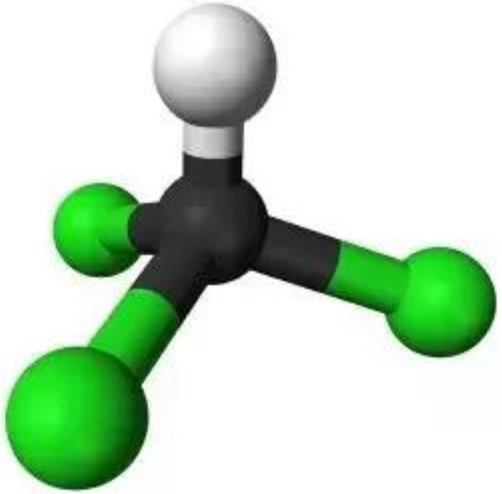
$$U = e^{i\theta a(Z_1 \otimes I + I \otimes Z_2)} = e^{i\theta a Z_1} \otimes e^{i\theta a Z_2}$$

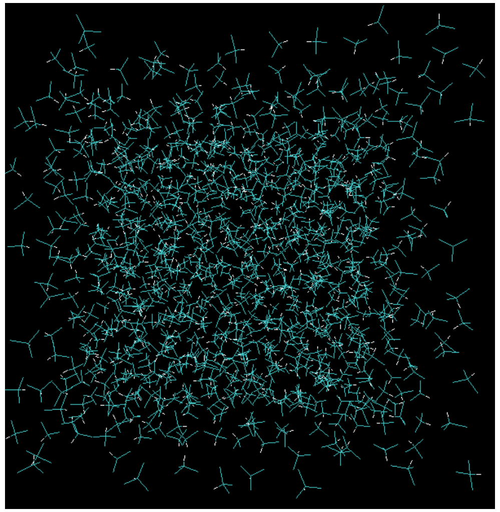
This example generalizes to any Hamiltonian that acts independently on subsystems A and B. Evidently, entangling unitaries require **physical interactions** between the subsystems.

Composite Systems: Two Qubits

Nuclear spin qubits: some of the earliest experiments to implement entangling gates used nuclear magnetic resonance (NMR).

Each Chloroform molecule (CHCL3) has two qubits, the nuclear spins of the carbon and hydrogen.





The molecules are placed in a strong magnetic field, $H = a_1 Z_1 + a_2 Z_2 + J Z_1 Z_2$.

Other single-qubit terms can be generated by oscillating RF magnetic fields.

The nuclei emit EM radiation when they are in resonance with a a weak oscillating RF magnetic field, and the resonant frequency depends on the nuclear spin state (and chemical properties). This enables measurement of the NMR qubits.

Composite Systems: Two Qubits

How can we use this NMR Hamiltonian to generate entanglement between the two qubits. Is the ZZ interaction capable of creating entanglement? For example we could consider:

$$U = e^{i\frac{\pi}{2} Z \otimes Z} = \begin{bmatrix} e^{i\frac{\pi}{2}} & 0 & 0 & 0 \\ 0 & e^{-i\frac{\pi}{2}} & 0 & 0 \\ 0 & 0 & e^{-i\frac{\pi}{2}} & 0 \\ 0 & 0 & 0 & e^{i\frac{\pi}{2}} \end{bmatrix}$$

A common strategy for showing that a 2-qubit gate is entangling is to apply local unitaries (tensor product unitaries) and use the freedom of global phase to relate it to a known entangling gate.

Composite Systems: Two Qubits

We are interested in entangling gates that are diagonal in the computational basis. One such gate can be produced by applying a Hadamard to the target qubit in a CNOT:

$$(I \otimes H)\,\Lambda(X)\,(I \otimes H) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

This gate, which is equivalent in entangling power to CNOT, is called CPHASE. Based on the Hamiltonian for CNOT, we can generate CPHASE using

$$A = |1\rangle\langle 1| \otimes (I - Z) = |11\rangle\langle 11| = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Composite Systems: Two Qubits

Every diagonal 4 x 4 matrix can be written using linear combinations of $\{I, Z_1, Z_2, Z_1 Z_2\}$, and so the NMR Hamiltonian must suffice for generating CPHASE.

$$A = \frac{1}{4}(I - Z_1 - Z_2 + Z_1 Z_2) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Summary: interactions are required to create entanglement and tensor product Hamiltonians are capable of generating entanglement.

Component Subsystems

So far we have discussed two-qubit states, observables, and unitary evolutions.

But suppose two qubits A and B are originally prepared in some state, which may be entangled, and A and B are sent to two keepers in different locations: Alice and Bob.

Each of the qubit keepers is allowed to probe their qubit as they see fit, but right now they are not allowed to communicate or share notes about their results.

Each keeper has a component subsystem of the same joint quantum state. If one of the keepers measures their subsystem, they will see outcomes. Our best description of the reduced state of the subsystem should account for all the observed probabilities of these outcomes.

In a probability theory, this reduced state of the subsystem would be a marginal distribution. But in quantum theory we have a distribution for each choice of basis, so it seems much more difficult to marginalize a quantum state in such a way to obtain the correct marginals on every subsystem.

Component Subystems

Take our example of an entangled state, $|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) = \frac{1}{\sqrt{2}}(|++\rangle + |--\rangle)$

Now suppose Alice holds the first qubit, and measures it in the 0/1. We can compute the probability for her to see 0 and to see 1 by finding the full measurement distribution in the 0/1 basis and computing its marginal. We find an identical result in the +/- basis:

$$\mu^A_{\Phi^+}(0) = \frac{1}{2}\ ,\ \mu^A_{\Phi^+}(1) = \frac{1}{2}\ ,\ \mu^B_{\Phi^+}(0) = \frac{1}{2}\ ,\ \mu^B_{\Phi^+}(0) = \frac{1}{2}$$

What quantum state $|\psi\rangle = \begin{bmatrix}\alpha \\ \beta\end{bmatrix}$ on Alice's subsystem is consistent with these measurements?

Component Subystems

There is no quantum state, at least of the kind we have discussed so far, which has these outcomes!

The reason this happens is that in losing or ignoring Bob’s subsystem, Alice now has incomplete information about the full system.

For all she knows, Bob could have measured or interacted with his qubit in any way whatsoever.

The state of her system is not a quantum state, it is a **probability distribution of quantum states**.

Density Matrices

Suppose A is an observable, and we have a quantum system in the state $|\psi_1\rangle$ with probability p_1 , And the state $|\psi_2\rangle$ with probability p_2 . Then the expectation of A should be

$$\langle A\rangle = p_1\langle\psi_1|A|\psi_1\rangle + p_2\langle\psi_2|A|\psi_2\rangle$$

In contrast, any superposition of $|\psi_1\rangle$ and $|\psi_2\rangle$ will give rise to unwanted cross terms like $\langle\psi_1|A|\psi_2\rangle$

As long as $|\psi_1\rangle, |\psi_2\rangle$ are orthogonal states, we can express the expectation above as

$$\langle A\rangle = \mathrm{tr}\,(A\rho) \quad , \quad \rho = p_1|\psi_1\rangle\langle\psi_1| + p_2|\psi_2\rangle\langle\psi_2|$$

This new object ρ, which represents a probability distribution over quantum states, is a Hermitian matrix with nonnegative eigenvalues that sum to 1. It is called a **density matrix** and it will suffice to describe the **reduced state of component subsystems**.

Density Matrices

To see that density matrices are the right choice for describing component subsystems, we can consider an observable A which acts only on the first qubit of an entangled state:

$$A \otimes I \quad , \quad |\psi\rangle = a|00\rangle + b|11\rangle$$

The expectation value is $\langle A \rangle = |a|^2 \langle 0|A|0\rangle + |b|^2 \langle 1|B|1\rangle$

Which can equivalently be expressed as

$$\langle A \rangle = \mathrm{tr}\,(A\rho) \quad , \quad \rho = |a|^2 |0\rangle\langle 0| + |b|^2 |1\rangle\langle 1|$$

Density Matrices

To compute the marginal of a probability distribution, we sum over all possible events on the subsystem being ignored. The density matrix ρ_A of a subsystem A , for the joint state $|\psi\rangle$ on A/B is:

$$\rho_A = \sum_{a_i, a_j} \rho_{ij}^A |a_i\rangle\langle a_j| \quad , \quad \rho_{ij}^A = \sum_{b_k} \langle a_i b_k|\psi\rangle\langle\psi|a_j b_k\rangle$$

where $\{a_i\}$ is a basis for $\mathcal{H}_A$ and $\{b_i\}$ is a basis for $\mathcal{H}_B$.

This operation which maps $|\psi_{AB}\rangle$ to ρ_A is called the **partial trace** (over the subsystem B, in this case). It is as fundamental in quantum theory as the notion of a marginal distribution in probability.

We have already seen that a joint distribution with intricate correlations can have marginal distributions that are flat and boring. A similar thing happens for entangled states! (e.g. $|\phi^+\rangle$).

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$$|\psi_{AB}\rangle \xrightarrow{\quad \mathrm{tr}_B \quad} \rho_A$$

Density Matrices

Definition: A density matrix is a probability distribution over a set of quantum states,

$$\rho = \sum_{i=1}^{m} p_i |\psi_i\rangle\langle\psi_i| \quad , \quad \sum_{i=1}^{m} p_i = 1 \quad , \quad p_i \geq 0 \; \forall i = 1, ..., m$$

Equivalently, any Hermitian operator with nonnegative eigenvalues and trace 1 can be put into the above form by diagonalization. Therefore a **density matrix** satisfies:

1. $\rho = \rho^\dagger$
2. ρ is positive semi-definite: $\langle\phi|\rho|\phi\rangle \geq 0$ for all states $|\phi\rangle \in \mathcal{H}$
3. $\mathrm{tr}\,(\rho) = 1$

Density Matrices

The quantum states we have described until now are called **pure states**. A pure state corresponds to a density matrix whose distribution is only supported on one state:

$$\Psi = |\psi\rangle\langle\psi|$$

The trace of the square of the density matrix tells us whether the state is pure, since

$$\mathrm{tr}\left(\rho^2\right) = \sum_{i=1}^{m} p_i^2 \leq \left(\sum_{i=1}^{m} p_i\right)^2 = \mathrm{tr}(\rho)^2 = 1$$

Where the inequality is saturated if and only if $p_i = 1$ for some i. Therefore

$$\mathrm{tr}(\rho^2) \leq 1$$

With equality iff ρ is a pure state.

Density Matrices

A key reason why we cannot ignore density matrices is that closed systems are an idealization. Every quantum subsystem in the real world is a subsystem (of the universe).

Whether we can describe a physical system by a pure state depends on whether it shares correlations with any other systems. If it does not (at least to a good approximation), then

$$|\psi_{\text{universe}}\rangle \approx |\psi_{\text{system}}\rangle \otimes |\psi_{\text{environment}}\rangle$$

So that the reduced state of the subsystem is relatively pure, $\Psi_{\text{system}} = |\psi_{\text{system}}\rangle\langle\psi_{\text{system}}|$. Engineering this near total lack of correlations is a major challenge, and so in general we must regard our quantum systems as open (not closed) and describe them by density operators.

Density Matrices

We have already seen that $\{I, X, Y, Z\}$ is a basis for the set of 2 x 2 Hermitian matrices, so for any qubit density matrix we have

$$\rho = \frac{1}{2}(I + \alpha_x X + \alpha_y Y + \alpha_z Z) = \frac{1}{2}(I + \vec{\alpha} \cdot \vec{\sigma}) \ = \frac{1}{2}\begin{bmatrix} 1+\alpha_z & \alpha_x - i\alpha_y \\ \alpha_x + i\alpha_y & 1-\alpha_z \end{bmatrix}$$

1. Compute the determinant.
2. Find conditions on the vector $\vec{\alpha}$ which yield a valid density matrix. What about a pure state?
3. Relate the conditions on $\vec{\alpha}$ to our prior discussion of the Bloch sphere.
4. How do the components of $\vec{\alpha}$ relate to Pauli expectation values? Consider the Frobenius inner product.

Density Matrices

Suppose we have a general bipartite state $|\Psi_{AB}\rangle$, and the RDM on subsystem A is

$$\rho_A = \sum_{i=1}^{M} p_i |\psi_i^A\rangle\langle\psi_i^A|$$

Since the $\{|\psi_i^A\rangle\}$ form a basis for $\mathcal{H}_A$, we may express $|\Psi_{AB}\rangle = \sum_{i,j} \alpha_{ij} |\psi_i^A\rangle \otimes |\psi_j^B\rangle$ for some states $\{|\psi_j^B\rangle\}$ of $\mathcal{H}_B$, where $\{\alpha_{ij}\}$ are complex coefficients.

Compute $\rho_A = \mathrm{tr}_B |\Psi_{AB}\rangle\langle\Psi_{AB}|$ and show that $\langle\psi_i^B|\psi_j^B\rangle = \delta_{ij}$ and $|\alpha_{ii}|^2 = p_i$. The form

$$|\Psi_{AB}\rangle = \sum_i \sqrt{p_i} |\psi_i^A\rangle \otimes |\psi_i^B\rangle$$

is called the **Schmidt decomposition** of $|\Psi_{AB}\rangle$.

Density Matrices

The Schmidt decomposition can also be viewed as a singular value decomposition. Starting from

$$|\Psi_{AB}\rangle = \sum_{i,j} \alpha_{ij} |\psi_i^A\rangle \otimes |\psi_j^B\rangle$$

We view α_{ij} as an $N \times M$ matrix, where $N = \dim(\mathcal{H}_A), M = \dim(\mathcal{H}_B)$.

Since $\boldsymbol{\alpha}$ is not square, it does not in general have an eigendecomposition. But it does have a singular value decomposition, so there exists an $N \times N$ unitary U, an $M \times M$ unitary V, and an $N \times M$ diagonal matrix $\Sigma = \mathrm{diag}(\lambda_1, ..., \lambda_R)$ with nonnegative entries, such that

$$\boldsymbol{\alpha} = U \Sigma V^\dagger \qquad , \qquad R = \min(N, M)$$

These unitaries U,V make the decomposition of $|\Psi_{AB}\rangle$ “diagonal” ,

$$|\Psi_{AB}\rangle = \sum_i \lambda_i |\phi_i^A\rangle \otimes |\phi_i^B\rangle$$

And so the singular values $\{\lambda_i\}$ are the Schmidt coefficients in the Schmidt decomposition, and the SVD provides an alternative to the partial trace for practical computation of the RDM.

Density Matrices

The Schmidt decomposition provides us with out first quantitative definition of entanglement. The number of nonzero Schmidt values is called the **Schmidt rank** χ, and it quantifies entanglement.

$$|\Psi_{AB}\rangle = \sum_{i=1}^{\chi} \sqrt{p_i} |\phi_i^A\rangle \otimes |\phi_i^B\rangle$$

According to our definitions, $|\Psi_{AB}\rangle$ is unentangled if and only if $\chi = 1$. Larger values for χ correspond to states with "more entanglement."

What is the Schmidt rank of the Bell state $|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$? In general when the Schmidt rank across a cut is equal to the dimension of one of the subsystems, the state is **maximally entangled**.

Now we can see that $|\Psi_{AB}\rangle$ is entangled if and only if the RDMs ρ_A, ρ_B are impure. Do states with Schmidt rank 1 share any correlations across the cut?