Entanglement + Mixed States

– Tensor Product Hilbert Spaces

- These occur when you have more than one physical degree of freedom: multiple dimensions of motion, several qubits, multiple particles, spin and orbital angular momentum, etc

- + We can choose a factorized basis where the basis states are products of states for the separate degrees of freedom
  + Example 1: Motion in 3D by separation of variables

$$|\psi\rangle = |\psi_x\rangle|\psi_y\rangle|\psi_z\rangle \Rightarrow \psi(\vec{x}) = X(x)Y(y)Z(z)$$

or $$|\psi\rangle = |\psi_r\rangle|l,m\rangle \Rightarrow \psi(\vec{x}) = R(r)Y_l^m(\theta,\phi)$$

  + Example 2: 2 qubits w/each in the canonical basis have factorized basis $|0\rangle_1|0\rangle_2$, $|0\rangle_1|1\rangle_2$, $|1\rangle_1|0\rangle_2$, $|1\rangle_1|1\rangle_2$

  + Example 3: 2 spins have factorized basis $\{|s_1,m_1\rangle|s_2,m_2\rangle\}$

- + As matrices, the tensor product inserts each factor into the previous one. For the 2 qubits,

$$|0\rangle_1|0\rangle_2 \simeq \begin{bmatrix}1\\0\end{bmatrix}\otimes\begin{bmatrix}1\\0\end{bmatrix} \simeq \begin{bmatrix}1\begin{bmatrix}1\\0\end{bmatrix}\\0\begin{bmatrix}1\\0\end{bmatrix}\end{bmatrix} = \begin{bmatrix}1\\0\\0\\0\end{bmatrix},$$

$$|0\rangle_1|1\rangle_2 \simeq \begin{bmatrix}1\\0\end{bmatrix}\otimes\begin{bmatrix}0\\1\end{bmatrix} \simeq \begin{bmatrix}1\begin{bmatrix}0\\1\end{bmatrix}\\0\begin{bmatrix}0\\1\end{bmatrix}\end{bmatrix} = \begin{bmatrix}0\\1\\0\\0\end{bmatrix}, \text{ etc}$$

- There are non-factorizable basis sets

  + For example, if we have 2 spins (or generally 2 angular momenta), we can use the eigenbasis of total angular momentum $\{|s,m;s_1,s_2\rangle\}$ as in addition of angular momentum.
  Recall the addition of 2 $s=1/2$ spins

$$|s=1,m=1\rangle = |\uparrow\rangle_1|\uparrow\rangle_2$$

$$|s=1,m=0\rangle = \tfrac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2\right)$$

$$|1,-1\rangle = |\downarrow\rangle_1|\downarrow\rangle_2$$

$$|0,0\rangle = \tfrac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2\right)$$

+ We cannot use a factorized basis for indistinguishable particles.
Boson (integer spin) multiparticle states must be symmetric under exchange of any 2 particles
ie

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\alpha\rangle_1 |\beta\rangle_2 + |\beta\rangle_1 |\alpha\rangle_2\right) \quad \left\{ |\alpha\rangle, |\beta\rangle \text{ are } \perp \text{ 1-particle states} \right.$$

Fermion (odd 1/2 integer spin) multiparticle states are always antisymmetric when 2 particles are exchanged

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\alpha\rangle_1 |\beta\rangle_2 - |\beta\rangle_1 |\alpha\rangle_2\right)$$

- Entanglement

- Because vectors add, we know the state of a system can be a superposition of basis states (which means a state may not have a definite value

- As we've seen, a multiparticle state may be a superposition of factorizable states that does not factorize
  + Total angular momentum states or boson/fermion states are examples
  + When the full state does not factorize into separate degrees of freedom (particles), those d.o.f. are entangled

  + When two particles are entangled, neither has a definite state independent of the other. This leads to "weird" but powerful + important effects of QM

  + Two-qubit states are often written in the basis of entangled Bell states

$$|\Phi^{\pm}\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle|0\rangle \pm |1\rangle|1\rangle\right), \quad |\Psi^{\pm}\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle|1\rangle \pm |1\rangle|0\rangle\right)$$

Similar but not the same as total spin states of 2 spin 1/2 particles

+ The most famous entangled state is Schrödinger's cat. There's a cat in the box with poison released by the decay of a radioactive nucleus. At 1 ½-life

$$|\Psi(t_{1/2})\rangle = \frac{1}{\sqrt{2}}\left(|😺\rangle|N\rangle + e^{i\phi}|😿\rangle|N_1, N_2, \ldots\rangle\right)$$

We'll come back to it later

- How do we measure entanglement? How do we know if a state factorizes?

– Pure vs Mixed States + the Density Matrix

the information content of a state?

- We are used to knowing the quantum state of the system, finding expectation values, etc. If we include the nucleus, this is even the case for Schrödinger's cat. This is called a <u>pure state</u>

- Suppose instead that I hand you a quantum system and tell you it has certain probabilities of being in states $|\psi_1\rangle$, $|\psi_2\rangle$, etc. This is called a <u>mixed state</u>

  + This is the case in statistical mechanics: if you pick 1 molecule at random from the air in a room, the probability of each single-particle state follows the Boltzmann distribution

  + A mixed state chooses a basis of states (<u>not</u> necessarily orthonormal) and assigns P_1 for $|\psi_1\rangle$, P_2 for $|\psi_2\rangle$, etc with $\sum_i P_i = 1$. Some of the P_i can $= 0$. A pure state is a mixed state when one $P_i = 1$ and the rest $= 0$

  + Note: these probabilities are <u>not</u> intrinsic like for quantum measurement. They are a measure of our ignorance instead, like how we classically don't know in advance what a coin flip will be — you just don't know all the initial conditions well enough

- The Density Matrix (or Density Operator)
  - We need a way to list probabilities that is not a vector — those represent pure states
  - If we take the (nonorthogonal) states + probabilities of the mixed state, we can define the <u>density operator</u>

$$\rho \equiv P_1 |\psi_1\rangle\langle\psi_1| + P_2 |\psi_2\rangle\langle\psi_2| + \ldots$$

  - As usual, we can write the density operator as a matrix, often also called the <u>density matrix</u> with respect to any orthonormal basis

  - If the $|\psi_i\rangle$ are orthonormal, $|\psi_i\rangle \to |e_i\rangle$, and the density matrix is diagonal

$$\rho \simeq \mathrm{diag}(P_1, P_2 \cdots P_N) \qquad (*)$$

and the $\{|e_i\rangle\}$ make an e'basis. In general, ρ is not diagonal, and you need to check the e'values for probabilities

  - <u>Example</u>: Suppose you have a single qubit. If you have a mixed state 50% $|0\rangle$ and 50% $|1\rangle$, then

$$\rho = \tfrac{1}{2}|0\rangle\langle 0| + \tfrac{1}{2}|1\rangle\langle 1| \simeq \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}$$

But if you have a pure state $|+\rangle = 1/\sqrt{2}\,(|0\rangle + |1\rangle)$

$$\rho = |+\rangle\langle +| \simeq \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix}$$

The e'values are $P=1$ for $|+\rangle$ and $P=0$ for $|-\rangle$ (the $\perp$ state)

  - You can see that $\rho^\dagger = \rho$, so it's Hermitian, so there is always an orthonormal e'basis (where ρ is diagonal)
    - Time evolution is $\rho(t) = \sum P_n |\Psi_n(t)\rangle\langle\Psi_n(t)| = U(t)\rho(0)U^\dagger(t)$

- Trace of the Density Matrix

  - Look at our examples or the diagonal ρ in $(*)$. These all have

$$\mathrm{tr}\,\rho = \sum_i \rho_{ii} = 1$$

In diagonal form, it's clear this is a sum of probabilities

+ With the relation between matrix elements + operators, the trace of an operator is

$$\operatorname{tr} A = \sum_i \langle e_i | A | e_i \rangle$$

where we sum over an entire orthonormal basis

+ We can prove generally that $\operatorname{tr} \rho = 1$:

$$\operatorname{tr} \rho = \sum_i \langle e_i | \rho | e_i \rangle = \sum_i \langle e_i | \Big(\sum_n P_n | \psi_n \rangle \langle \psi_n | \Big) | e_i \rangle$$

(for convergent sums) completeness

$$= \sum_n P_n \langle \psi_n | \Big(\sum_i | e_i \rangle \langle e_i | \Big) | \psi_n \rangle = \sum_n P_n \langle \psi_n | \psi_n \rangle$$

$$= \sum_n P_n = 1 \quad \text{by normalization}$$

+ The trace is the same no matter what orthonormal basis you use to calculate it. Proof: also reorders sums + uses completeness

+ The trace is cyclic: $\operatorname{tr}(AB) = \operatorname{tr}(BA)$ etc. Similar proof. (Have to be careful for infinite-dimensional Hilbert spaces)

→ Partial Traces + Entanglement: entanglement leads to mixed states

• Suppose we have a Hilbert space with multiple degrees of freedom. Due to tensor structure, we can take a partial trace of just one factor of Hilbert space.

+ Take a Hilbert space w/ 2 factors (you can just group a bunch of factors together) and write a factorized basis $\{ | e_i \rangle_1 | f_j \rangle_2 \}$

+ The partial trace over factor 2 is defined as

$$\operatorname{tr}_2 \rho = \sum_j {}_2\langle f_j | \rho | f_j \rangle_2 \equiv \rho_1$$

This leaves an operator ρ_1 on factor 1 called the reduced density matrix

+ Simplest example : 2 qubits, In a pure state

$$|0\rangle_1 |0\rangle_2 \simeq \begin{bmatrix}1\\0\end{bmatrix} \otimes \begin{bmatrix}1\\0\end{bmatrix} \Rightarrow \rho = \left(|0\rangle\langle 0|\right)_1 \left(|0\rangle\langle 0|\right)_2$$

$$\simeq \left([1\ 0]\begin{bmatrix}1\\0\end{bmatrix}\right)_1 \otimes \left([1\ 0]\begin{bmatrix}1\\0\end{bmatrix}\right)_2 = \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix}_1 \otimes \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix}_2$$

The partial trace is just the trace over the 2nd factor

$$\rho_1 = \mathrm{tr}_2(\rho) = \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix}_1$$

+ Example : Suppose our 2 qubits are in the entangled Bell state $|\Phi\pm\rangle$. Then

$$\rho = |\Phi^\pm\rangle\langle\Phi^\pm|$$
$$= \tfrac{1}{2}\{ |0\rangle_1|0\rangle_2 \langle 0|_1\langle 0|_2 \pm |1\rangle_1|1\rangle_2 \langle 0|_1\langle 0|_2$$
$$\pm |0\rangle_1|0\rangle_2 \langle 1|_1\langle 1|_2 + |1\rangle_1|1\rangle_2 \langle 1|_1\langle 1|_2 \}$$

The reduced density matrix is

$$\rho_1 = {}_2\langle 0|\rho|0\rangle_2 + {}_2\langle 1|\rho|1\rangle_2 = \tfrac{1}{2}|0\rangle_1\langle 0|_1 + \tfrac{1}{2}|1\rangle_1\langle 1|_1$$

This is the mixed state $\rho_1 \simeq \begin{bmatrix}1/2 & 0\\0 & 1/2\end{bmatrix}$!

+ The state of a 2-part system is entangled iff the reduced density matrix is a mixed state ;
We say the 2-part state is maximally entangled when the probabilities for factor 1 of the Hilbert space are all = $1/N$, where N is the Hilbert space dimension (maximally mixed)

∘ Purification : any mixed state can be written as a partial trace of an entangled pure state

+ Suppose $\rho_1 = \sum_n P_n |\psi_n\rangle\langle\psi_n|$ for some system 1.
Then

$$|\Psi\rangle = \sum_n \sqrt{P_n}\, |\psi_n\rangle_1 |f_n\rangle_2 \text{ and } \rho = |\Psi\rangle\langle\Psi|$$

gives ρ_1 on partial trace over system 2 if $\{|f_n\rangle_2\}$ are part of an orthonormal basis for system 2.

+ We can think of any mixed states we deal with as reflections of our ignorance about the pure state of the larger system/universe.