IPP-QM-2: Density operators and entanglement

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MT24

The course

1. Basic quantum formalism
2. Density operators and entanglement
3. Decoherence
4. The measurement problem
5. Dynamical collapse theories
6. Bohmian mechanics
7. Everettian structure
8. Everettian probability
9. EPR and Bell's theorem
10. The Bell-CHSH inequalities and possible responses
11. Contextuality
12. The PBR theorem
13. Quantum logic
14. Pragmatism and QBism
15. Relational quantum mechanics
16. Wavefunction realism

Today

Born rule recap

Density operators

Entanglement

More on density operators

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Motivating the Born rule

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- Let $|\psi\rangle$ be the state of the system prior to measurement.

Motivating the Born rule

- Notice that

$$\langle\psi|\,\hat{1}\,|\psi\rangle = \langle\psi|\left(\sum_i |\phi_i\rangle\langle\phi_i|\right)|\psi\rangle = 1,$$

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- Writing this out, we have

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- Hence if $|\psi\rangle$ is normalised, then we can interpret the quantities $|\langle\psi|\phi_i\rangle|^2$ as probabilities, as they are positive real numbers ≤ 1 which sum to 1.

The Born rule

Born rule: For a measurement of some physical quantity represented by the self-adjoint operator $\hat{A}$, specified by a resolution of the identity in terms of the projectors $\hat{P}(a_i)$ onto subspaces of $\mathcal{H}$ corresponding to particular eigenvalues a_i of $\hat{A}$, the probability $\Pr(a_i)$ of getting outcome i, corresponding to $\hat{P}(a_i)$ is given by $\langle\psi|\,\hat{P}(a_i)\,|\psi\rangle$, for a system in the state $|\psi\rangle$.

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Note that at this point this is an *operational prescription*! Also, note that the projection postulate—closely associated with ‘wavefunction collapse’—is an optional extra here...

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  Exercise: Check that this definition is indeed independent of the basis chosen.
- Two other properties of the trace:
  1. Linearity: $\mathrm{Tr}(\alpha\hat{A} + \beta\hat{B}) = \alpha\mathrm{Tr}(\hat{A}) + \beta\mathrm{Tr}(\hat{B})$.
  2. Cyclicity: $\mathrm{Tr}(\hat{A}\hat{B}) = \mathrm{Tr}(\hat{B}\hat{A})$.

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- A special case is $\hat{\rho} = |\psi\rangle\langle\psi|$ for some vector state $|\psi\rangle$.
- In this way, any vector state can be represented by a density operator.

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- Note that whenever we write a vector state $|\psi\rangle$ in the form $|\psi\rangle \langle\psi|$, the (redundant) overall phase cancels out, so in a sense this representation is *more accurate* physically than the one given by vectors in Hilbert space.
- **Exercise:** Show that $\hat{\rho}$ is pure iff $\hat{\rho}^2 = \hat{\rho}$, iff $\det(\hat{\rho}) = 0$.

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- We'll come in due course to examples where systems do not have pure states at all, only mixed ones (i.e., a non-pure density operator is the only way in which they can be described) and where an ignorance interpretation is not possible. These systems are called *improper mixtures*.

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It's easy to see that this recovers the previous version of the Born rule. Consider some basis $\{|\phi_k\rangle\}$, let $\hat{P}_i$ be the projector $|\phi_i\rangle\langle\phi_i|$, and let $\hat{\rho}$ be associated with a system in a pure state $|\psi\rangle$, so that $\hat{\rho} = |\psi\rangle\langle\psi|$. Then:

$$\begin{aligned}\mathrm{Tr}(\hat{\rho}\hat{P}_i) &= \sum_k \langle\phi_k|\,\hat{\rho}\,|\phi_i\rangle\langle\phi_i|\phi_k\rangle = \sum_k \langle\phi_k|\,\hat{\rho}\,|\phi_i\rangle\,\delta_{ij} \\ &= \langle\phi_i|\psi\rangle\langle\psi|\phi_i\rangle = |\langle\phi_i|\psi\rangle|^2\end{aligned}$$

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- That combined system is still a quantum system, so we represent it with the 'tensor product Hilbert space', $\mathcal{H}_A \otimes \mathcal{H}_B$.
- We want to understand how $\mathcal{H}_A \otimes \mathcal{H}_B$ is built up from $\mathcal{H}_A$ and $\mathcal{H}_B$.

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- We now make the assumption that the pairs $|m_i\rangle \otimes |n_j\rangle$ of vectors from these two bases form a basis for $\mathcal{H}_A \otimes \mathcal{H}_B$: $|m_i\rangle \otimes |n_j\rangle$ gives m_i as a result of measuring M on A and n_j as a result of measuring N on B.

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- An arbitrary state of $\mathcal{H}_A \otimes \mathcal{H}_B$ can now be built up from these basis vectors—a completely general expression is

$$|\psi\rangle = \sum_i \sum_j \alpha_{ij} |m_i\rangle \otimes |n_j\rangle \, .$$

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- In classical physics, we can always give the state of a combined system just by giving the states of the component systems.
- But is the same true in quantum mechanics?

Tensor product of states

- Suppose $|\chi\rangle$ and $|\phi\rangle$ are states of A and B respectively, given by

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- Then we can define their tensor product $|\chi\rangle \otimes |\phi\rangle$ by linearity:

$$\begin{aligned} |\chi\rangle \otimes |\phi\rangle &= \left(\sum_i c_i |m_i\rangle \right) \otimes \left(\sum_j d_j |n_j\rangle \right) \\ &=: \sum_i \sum_j c_i d_j |m_i\rangle \otimes |n_j\rangle \end{aligned}$$

Entanglement

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- Entangled states can be found in even the smallest systems.
- For example, if we have two spin-half particles each of which has z-spin eigenstates $|+\rangle$, $|-\rangle$, then the 'singlet' state
$$\frac{1}{\sqrt{2}} \left(|+\rangle \otimes |-\rangle - |-\rangle \otimes |+\rangle \right)$$
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- What's the spin state of system 1 or system 2 in the above joint 'singlet' states? Answer: *undefined*!

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$$\begin{aligned}\left(\hat{A} \otimes \hat{B}\right) |\Psi\rangle_{12} &= \left(\hat{A} \otimes \hat{B}\right) \left(\sum_{ij} \alpha_{ij} \, |\phi_i\rangle_1 \otimes |\chi_j\rangle_2 \right) \\ &= \sum_{ij} \alpha_{ij} \hat{A} \, |\phi_i\rangle_1 \otimes \hat{B} \, |\chi_j\rangle_2 \, .\end{aligned}$$

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Note: It is always possible to write any linear operator $\hat{O}_{12}$ acting on $\mathcal{H}_1 \otimes \mathcal{H}_2$ in the form

$$
\hat{O}_{12} = \sum_{kl} c_{kl} \hat{A}_k \otimes \hat{B}_l .
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As we'll see in Lecture 9, this is closely related to 'non-separability'.

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- Bob is lazy, and just prepared the electron in a probabilistic state (so it has x-spin or down definitely, but he makes sure there's a 50/50 chance of each).
- Alice knows Bob well, and is suspicious. She doesn't have an interferometer to hand. What could she do to check up on Bob?

The example continued

- Suppose Alice can perform linear transformations on the state that effectively rotate it: spin up states in the x direction become spin up states in the z direction (which are superpositions of x-spin states), etc.:

$$|\uparrow_x\rangle \to |\uparrow_z\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_x\rangle + |\downarrow_x\rangle\right),$$
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- What happens if Alice performs this transition on her desired superposition state? She gets a definite $|\uparrow_x\rangle$ state. (Do the calculation!)
- What happens when she performs this transformation on one of Bob's fake superpositions/really definite states? She gets a superposition state in the x basis.

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- So Alice can use the relationship between bases to uncover Bob's ploy!
- If she performs her transformation but continues to get a 50/50 mix of up and down results, she'll know they were never really superposition states!

The example continued

- So Alice can use the relationship between bases to uncover Bob's ploy!
- If she performs her transformation but continues to get a 50/50 mix of up and down results, she'll know they were never really superposition states!
- How could Bob circumvent this problem?

The example continued

- Bob could agree in advance with Alice to entangle the electrons with another electron in the singlet state:

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- Now if Alice tries to perform her rotations, she won't get a definite spin state, so she won't expect to see a difference.

Moral

Entanglement can make probabilisitic mixtures indistinguishable from superpositions (if we're not doing interference experiments)!

Today

Born rule recap

Density operators

Entanglement

More on density operators

Back to density operators

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2. A superposition of states which are not interfering (an 'improper mixture').

We've seen that if the quantum state of some (sub)system can be written only using density operators (not vectors), it is 'impure', otherwise it is 'pure'.

Entanglement and density operators

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- These are called the *reduced states* (*reduced density operators*) of a subsystem.
- When we have entanglement these reduced states will be *mixed* (by definition).
- But these are not mixtures which can be given an *ignorance interpretation*: we cannot think of these mixtures as telling us that there is some underlying pure state of which we are ignorant.

Reduced states

- Take a composite of two systems, with Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, say in a state

$$|\Psi\rangle = \sum_i \alpha_{ij} |\psi_i\rangle \otimes |\phi_j\rangle \, .$$

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- Special cases of these observables are ones of the form $\hat{A} \otimes \hat{1}$ and $\hat{1} \otimes \hat{B}$, where $\hat{A}$ is an observable on $\mathcal{H}_1$ and $\hat{B}$ is an observable on $\mathcal{H}_2$, and $\hat{1}$ denotes the identity operator on either space.

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- The state $|\Psi\rangle$ on $\mathcal{H}_1 \otimes \mathcal{H}_2$ defines two (possibly impure) states on $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively.

The mathematics of reduced states

- We shall now discuss how to calculate the (density operators corresponding to) reduced states. This is done by means of the *partial trace*.

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- Recall that the trace of an operator is given by

$$\mathrm{Tr}(\hat{A}) = \sum_i \langle\psi_i|\,\hat{A}\,|\psi_i\rangle\,,$$

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  where $\{|\psi_i\rangle\}$ is any orthonormal basis in the Hilbert space on which $\hat{A}$ acts.
- Applied to the space $\mathcal{H}_1 \otimes \mathcal{H}_2$, the basis $\left\{|\phi_i\rangle \otimes |\psi_j\rangle\right\}$ and the pure state $|\Psi\rangle$, this yields for any observable $\hat{C}$ on $\mathcal{H}_1 \otimes \mathcal{H}_2$:

$$\mathrm{Tr}\left(|\Psi\rangle\langle\Psi| \hat{C}\right) = \sum_{i,j} \langle\phi_i| \otimes \langle\psi_j| \left[|\Psi\rangle\langle\Psi| \hat{C}\right] |\phi_i\rangle \otimes |\psi_j\rangle$$

Obtaining reduced states

If, say, $\hat{C}$ has the form $\hat{A} \otimes \hat{1}$, then this simplifies to

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$$= \sum_i \langle\phi_i|\left[\sum_j \langle\psi_j|\Psi\rangle\langle\Psi|\psi_j\rangle\right]\hat{A}\,|\phi_j\rangle$$

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&= \sum_i \langle\phi_i| \left[\sum_j \langle\psi_j|\Psi\rangle\langle\Psi|\psi_j\rangle\right] \hat{A}\,|\phi_j\rangle
\end{aligned}$$

And defining

$$\hat{\rho}_1 := \sum_j \langle\psi_j|\Psi\rangle\langle\Psi|\psi_j\rangle\,,$$

we can rewrite this as

$$\mathrm{Tr}\left(|\Psi\rangle\langle\Psi|\,\hat{A}\otimes\hat{1}\right) = \mathrm{Tr}\left(\hat{\rho}_1\hat{A}\right),$$

where the trace on the RHS is the trace in $\mathcal{H}_1$.

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- This yields the expectation values for any observable on $\mathcal{H}_1$ when the state of the total system is $|\Psi\rangle$—for recall the affinity between our previous expression and how we stated the Born rule.
- This operation is known as the *partial trace* over $\mathcal{H}_2$.

$\hat{\rho}_1$ is an operator!

Notice that, despite the notation, $\langle \psi_j | \Psi \rangle \langle \Psi | \psi_j \rangle$ is not a complex number but an operator on $\mathcal{H}_1$, since

$$|\Psi\rangle = \sum_{m,n} \alpha_{mn} |\phi_m\rangle \otimes |\psi_n\rangle \, .$$

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In fact, we can write explicitly:

$$\begin{aligned}\hat{\rho}_1 &= \sum_j \langle\psi_j| \left(\sum_{m,n} \alpha_{mn} |\phi_m\rangle \otimes |\psi_n\rangle\right) \left(\sum_{p,q} \alpha^*_{pq} \langle\phi_q| \otimes \langle\psi_q|\right) |\psi_j\rangle \\ &= \sum_{j,m,p} \alpha_{mj}\alpha^*_{pj} |\phi_m\rangle\langle\phi_p| \,,\end{aligned}$$

using the fact that $\langle\psi_i|\psi_j\rangle = \delta_{ij}$.

Matrix representation of a reduced density operator

In matrix representation, choosing $\{|\phi_j\rangle\}$ as a basis, we have

$$\hat{\rho}_1 = \begin{pmatrix} \sum_j \left|\alpha_{1j}\right|^2 & \sum_j \alpha_{1j}\alpha_{2j}^* & \cdots & \sum_j \alpha_{1j}\alpha_{nj}^* \\ \sum_j \alpha_{2j}\alpha_{1j}^* & \sum_j \left|\alpha_{2j}\right|^2 & \cdots & \sum_j \alpha_{2j}\alpha_{nj}^* \\ \vdots & \vdots & \ddots & \vdots \\ \sum_j \alpha_{nj}\alpha_{1j}^* & \sum_j \alpha_{nj}\alpha_{2j}^* & \cdots & \sum_j \left|\alpha_{nj}\right|^2 \end{pmatrix},$$

and we have something similar for $\hat{\rho}_2$ too.

Relative states

- The expressions we found can be made to look simpler and can often be applied more directly if we write the state of the composite,

$$|\Psi\rangle = \sum_{i,j} \alpha_{ij} |\phi_i\rangle \otimes |\psi_j\rangle$$

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  in terms of *relative states*.
- To do this, we first perform the sum over j:

$$|\Psi\rangle = \sum_i |\phi_i\rangle \otimes \left(\sum_j \alpha_{ij} |\psi_j\rangle \right) .$$

Relative states, continued

The state in round brackets is generally not normalised, so we set

$$\alpha_i := \sum_j |\alpha_{ij}|^2,$$

and write

$$\begin{aligned}
|\Psi\rangle &= \sum_i \alpha_i |\phi_i\rangle \otimes \left(\frac{1}{\alpha_i} \sum_j \alpha_{ij} |\psi_j\rangle \right) \\
&=: \sum_i \alpha_i |\phi_i\rangle \otimes |\widetilde{\psi}_i\rangle .
\end{aligned}$$

The states $|\widetilde{\psi}_i\rangle$ are the *relative states* with respect to the $|\phi_i\rangle$ in a given state $|\Psi\rangle$.

Making use of relative states

If we calculate the reduced state $\hat{\rho}_1$ by partially tracing over $\mathcal{H}_2$ we now obtain, using this notation,

$$
\begin{aligned}
\hat{\rho}_1 &= \sum_j \langle\psi_j| \left(\sum_i \alpha_i |\phi_i\rangle \otimes |\widetilde{\psi}_i\rangle \right) \left(\sum_k \langle\phi_k| \otimes \langle\widetilde{\psi}_k| \right) |\psi_j\rangle \\
&= \sum_{i,j,k} \alpha_i \alpha_k \langle\psi_j|\widetilde{\psi}_i\rangle \langle\widetilde{\psi}_k|\psi_j\rangle |\phi_i\rangle \langle\phi_k| \\
&= \sum_{i,k} \alpha_i \alpha_k \langle\widetilde{\psi}_k| \left(\sum_j |\psi_j\rangle \langle\psi_j| \right) |\widetilde{\psi}_k\rangle |\phi_i\rangle \langle\phi_k| \\
&= \sum_{i,k} \alpha_i \alpha_k \langle\widetilde{\psi}_k|\widetilde{\psi}_i\rangle |\phi_i\rangle \langle\phi_k| ,
\end{aligned}
$$

since $\sum_j |\psi_j\rangle \langle\psi_j| = \hat{1}$.

Another convenient representation of reduced density operators

Thus we can write $\hat{\rho}_1$ in matrix form as:

$$\hat{\rho}_1 = \begin{pmatrix} \alpha_1^2 & \alpha_1\alpha_2 \langle\widetilde{\psi}_2|\widetilde{\psi}_1\rangle & \cdots & \alpha_1\alpha_n \langle\widetilde{\psi}_n|\widetilde{\psi}_1\rangle \\ \alpha_2\alpha_1 \langle\widetilde{\psi}_1|\widetilde{\psi}_2\rangle & \alpha_2^2 & \cdots & \alpha_2\alpha_n \langle\widetilde{\psi}_n|\widetilde{\psi}_2\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_n\alpha_1 \langle\widetilde{\psi}_1|\widetilde{\psi}_n\rangle & \alpha_n\alpha_2 \langle\widetilde{\psi}_2|\widetilde{\psi}_n\rangle & \cdots & \alpha_n^2 \end{pmatrix}$$

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This formulation of the reduced density matrix will be very useful when we look at decoherence next time!

Reduced states as mixed

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- Consider for instance two electrons in the singlet state,

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|+\rangle\,|-\rangle - |-\rangle\,|+\rangle\right),$$

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- One can compute

  $$\hat{\rho}_1 = \hat{\rho}_2 = \frac{1}{2} \hat{1},$$

  so the subsystems cannot be in pure states!

Application to the measurement procedure

- Unitary measurement interactions *create entanglement*.

$$|\psi\rangle_S |r_0\rangle_A \mapsto \sum_i \beta_i |a_i\rangle_S |r_i\rangle_A .$$

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- Again, we'll see lots more about this next time, when we look at decoherence.

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2. Introduced density operators.
3. Introduced quantum entanglement as a qualitatively new phenomenon.
4. Showed how one can associate reduced density matrices with subsystems even in the presence of quantum entanglement.

References

Guido Bacciagaluppi, “Density Operators in Quantum Mechanics”, 1998.