In Praise of the Density Matrix Formalism

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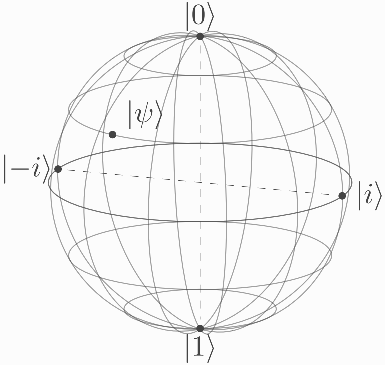
Outline

- Quantum mechanics is usually formulated using the language of state vectors
- An alternate formulation, mathematically equivalent, is based on density operators
- The density matrix formalism provides a much more convenient language for thinking about some scenarios
- And it can help in reasoning with paradoxes

Formalism

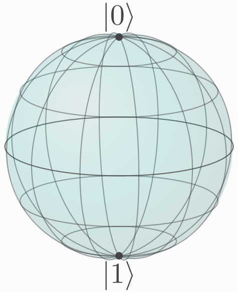
Pure states and mixed states

- The state of a qubit is a superposition $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, with $\alpha, \beta \in \mathbb{C}$ and $\langle\psi|\psi\rangle = 1$, which is not the same as a probability mixture of states.
- Even though the measurement outcome may be probabilistic, a superposition state can be known with certainty.
- Superposition states are pointwise and they can in fact be visualized as points on the Bloch sphere $|\psi\rangle = \cos\frac{\theta}{2}|1\rangle + e^{i\phi}\sin\frac{\theta}{2}|0\rangle$. They are called *pure states*.



Pure states and mixed states

- Superposition states are pointwise and they can in fact be visualized as points on the Bloch sphere. They are called *pure states*.
- In contrast, if we are not sure if a qubit is in one pure state or another pure state, then the state itself and not just its outcome is probabilistic.
- These are called *mixed states*, and they can be visualized as points in the Bloch ball



Density Matrices

- Density matrices allow probabilistic mixtures of kets
- The density matrix language provides a convenient means for describing quantum systems whose state is not completely known
- While a pure state is written using vectors, a mixed state is written using an operator called a density operator
- Since operators can be represented by matrices, often we speak of density matrices
- It should be always kept in mind that a density matrix is an operator, not a matrix, and the matrix for this operator depends on the choice of orthonormal basis

Density Matrices

- Suppose a quantum system is in one of a number of states $|\psi_i\rangle$ with respective probabilities p_i
- $\{p_i, |\psi_i\rangle\}$ is an ensemble of pure states
- The density matrix for the system is defined by the equation

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

Density Matrices

- If the evolution of a closed quantum system is described by the unitary operator U, the evolution of the density operator is

$$\sum_i p_i U|\psi_i\rangle\langle\psi_i|U^\dagger = U\rho U^\dagger$$

- Suppose we perform a measurement described by measurement operators M_m
  - If the initial state was $|\psi_i\rangle$, then the probability of getting result m is

$$p(m|i) = \langle\psi_i|M_m^\dagger M_m|\psi_i\rangle = \mathrm{Tr}\left(M_m^\dagger M_m|\psi_i\rangle\langle\psi_i|\right)$$

  - and hence

$$p(m) = \sum_i p(m|i)p_i = \mathrm{Tr}(M_m^\dagger M_m \rho)$$

  - The density operator of the system after obtaining the measurement result m is

$$\rho_m = \frac{M_m^\dagger \rho M_m}{\mathrm{Tr}\left(M_m^\dagger M_m|\psi_i\rangle\langle\psi_i|\right)}$$

Properties of Density Matrices

- $\mathrm{Tr}(\rho^2) \leq 1$
- A state is pure if and only if $\mathrm{Tr}(\rho^2) = 1$
- If a quantum system is prepared in the state ρ_i with probability p_i, the system may be described by the density matrix $\rho = \sum_i p_i \rho_i$

Note

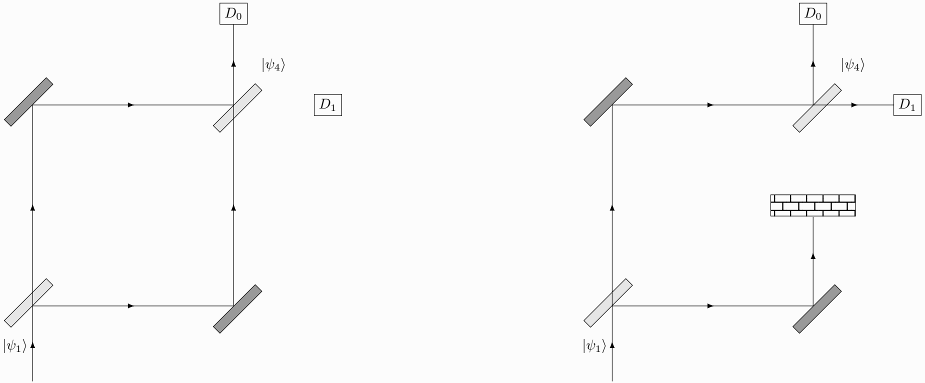
The eigenvalues and eigenvectors of a density matrix have *no* special significance with regard to the ensemble of quantum states represented by that density matrix: they just indicate one of many possible ensembles that may give rise to that specific density matrix

Properties of Density Matrices

- An operator ρ is the density operator associated to some ensemble if and only if
  - $\mathrm{Tr}(\rho) = 1$
  - ρ is a positive operator, i.e. $\langle\psi|\rho|\psi\rangle \geq 0$ for any arbitrary vector $|\psi\rangle$
- This allows to *define* a density operator as a positive operator having trace one
- The density operator representing a state of a system is defined in a unique manner, whereas the vector representing a pure state is only defined up to within a phase factor

Possible Applications

Interaction-free measurement



- In 1993, Elitzur and Vaidman proposed a gedankenexperiment based on a Mach-Zender interferometer

Interaction-free measurement

Suppose the obstacle adsorbs the photon with probability p

Input density operator $\rho_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$

Half-silvered mirror operator $S = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}$

Fully-silvered mirror operator $M = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$

Output density operator $\rho_4 = \frac{1}{2} \begin{pmatrix} 2-p & ip \\ -ip & p \end{pmatrix}$

Surprising connections

- Quantum structures (e.g., entanglement, indistinguishability, interference, and superposition) can in principle be applied to other domains, including:
  - Cognition (influencing human probability and similarity judgments, decision-making, language, and perception)
  - Socio-economic domains (behavioral economics and finance, where empirical data often deviates from classical Boolean and Kolmogorovian frameworks)
- Challenging traditional approaches can lead to a deeper understanding of underlying principles and mechanisms governing complex systems
- Quantum theory as an analogy can improve decision theory, even if the brain is not a quantum system
- Quantum interference can account for problematic situations in decision theory, such as the violation of the law of total probability when two observables are not compatible

Warm-up: Allais paradox (1953)

- The Allais paradox comes in several versions
- This is one of the simplest, slightly modified
- A participants is offered two pairs of gambles:
  - A_1 Receive \$1,000 with certainty
  - A_2 Receive \$5,000 with probability 0.8, otherwise \$0
  - B_1 Receive \$10,000 with probability 0.1, otherwise \$0
  - B_2 Receive \$50,000 with probability 0.08, otherwise \$0
- and is asked to rank A_1 vs. A_2 and B_1 vs. B_2

Ellsberg paradox (1961)

- A lottery with known probabilities is preferred to a similar but ambiguous lottery, where the decision maker does not know them
- An urn contains 30 balls, 10 of which are red. The other 20 are either black or yellow in unknown proportions. One ball will be drawn at random from this urn.
- A participants is offered two pairs of gambles:
  - A_1 Receive \$100 if the ball is red, otherwise \$0
  - A_2 Receive \$100 if the ball is black, otherwise \$0
  - B_1 Receive \$100 if the ball is either red or yellow, otherwise \$0
  - B_2 Receive \$100 if the ball is either black or yellow, otherwise \$0
- and is asked to rank A_1 vs. A_2 and B_1 vs. B_2

Ellsberg paradox

- Rank A_1 vs. A_2 and B_1 vs. B_2
  - A_1 Receive \$100 if the ball is red, otherwise \$0 ($P(\$) = 1/3$)
  - A_2 Receive \$100 if the ball is black, otherwise \$0 ($P(\$) = P(B)$)
  - B_1 Receive \$100 if the ball is either red or yellow, otherwise \$0 ($P(\$) = 1 - P(B)$)
  - B_2 Receive \$100 if the ball is either black or yellow, otherwise \$0 ($P(\$) = 2/3$)
- Ellsberg predicted (and experiments confirmed it) that most people will prefer A_1 to A_2, but B_2 to B_1
- It is as *maybe* $P(B) < 1/3$ is more relevant in the first case, but *maybe* $P(B) > 1/3$ is more relevant in the second
- La Mura (2009) applied state vector formalism to this situation


Thank You