Quantum Foundations Lecture 6

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Properties of the Rebit Matrix Representation

• To find the eigenvectors, let's switch to polar coordinates $x = r\sin\theta$ $y = r\cos\theta$

since then $\|\boldsymbol{n}\| = r$.

In these coordinates, we have

$$\rho = \begin{pmatrix} 1 + r\cos\theta & r\sin\theta \\ r\sin\theta & 1 - r\cos\theta \end{pmatrix}$$

• It is now straightforward to check that the two orthogonal unit vectors

$$|n+\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix} = \cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2}|1\rangle \text{ and } |n-\rangle = \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \end{pmatrix} = \sin\frac{\theta}{2}|0\rangle - \cos\frac{\theta}{2}|1\rangle$$

are the eigenvectors with $\rho|n+\rangle = \lambda_{+}|n+\rangle.$

Pure Rebit States

• If the state is pure then $||n|| = \sqrt{x^2 + y^2} = 1$, so $\lambda_+ = 1$ and $\lambda_- = 0$. As a result, the density operator is

$$\rho = |n+\rangle\langle n+|$$

- This is just the projector onto the one-dimensional subspace spanned by $|n + \rangle = \cos \frac{\theta}{2} |0\rangle + \sin \frac{\theta}{2} |1\rangle$.
- In quantum mechanics, we often use the vector $|n+\rangle$ to represent a pure state rather than the projector $|n+\rangle\langle n+|$. This is just a matter of convenience.
- The space of pure states is a vector space, but you should not confuse $\rho = \frac{1}{2}\rho_1 + \frac{1}{2}\rho_2$, interpretable as a mixture, with $|\psi\rangle = \frac{1}{\sqrt{2}}|\psi_1\rangle + \frac{1}{\sqrt{2}}|\psi_1\rangle$, which is called a superposition.



3.vi) Qubits



• Consider Ω = the unit ball,

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix}$$
 s.t. $x^2 + y^2 + z^2 \le 1$.

• Lifting this to a cone gives

$$\alpha \begin{pmatrix} x \\ y \\ z \\ z \end{pmatrix} \text{s.t. } x^2 + y^2 + z^2 \le 1.$$

• This cone is self dual (similar to Hwk 1 proof for disc).

• If we also impose
$$\boldsymbol{a} \cdot \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix} \leq 1$$
 we get $\mathcal{E}(\Omega)$.

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Unfortunately, the space of 2 x 2 real symmetric matrices is only 3-dimensional, so we cannot use if here. However, if we go to the 2 x 2 complex Hermitian matrices $M^{\dagger} = M$, then this has 4 dimensions. \odot

$$\begin{pmatrix} a & c+id \\ c-id & b \end{pmatrix}$$

- This is still a real vector space. Real linear combinations of Hermitian matrices are still \odot Hermitian.
- Since we know $(N, M) = \text{Tr}(N^{\dagger}M)$ is an inner product, we can find an orthonormal basis. You can check that $\frac{\sigma_0}{\sqrt{2}}, \frac{\sigma_1}{\sqrt{2}}, \frac{\sigma_2}{\sqrt{2}}, \frac{\sigma_3}{\sqrt{2}}$ is such a basis, where \odot

$$\sigma_0 = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

This means that instead of writing our qubit vectors in \mathbb{R}^3 as $\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}$ we can write then as 2×2 matrices $\frac{1}{\sqrt{2}}(a\sigma_0 + b\sigma_1 + c\sigma_2 + d\sigma_3)$.

• Again, we usually choose a different normalization so that $\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} \rightarrow \frac{1}{2}(a\sigma_0 + b\sigma_1 + c\sigma_2 + d\sigma_3)$

• We choose to embed our state space Ω in the $\sigma_1, \sigma_2, \sigma_3$ subspace, so a normalized state is of the form

$$\rho = \frac{1}{2}(I + x\sigma_1 + y\sigma_2 + z\sigma_3) \quad \text{with} \quad x^2 + y^2 + z^2 \le 1.$$

or
$$\rho = \frac{1}{2} \begin{pmatrix} 1 + z & x - iy \\ x + iy & 1 - z \end{pmatrix}$$

 Again, let's look at the eigenvalues and eigenvectors. The characteristic equation is

$$\begin{vmatrix} 1+z-2\lambda & x-iy \\ x+iy & 1-z-2\lambda \end{vmatrix} = 0 \text{ or } 4\lambda^2 - 4\lambda + 1 - x^2 - y^2 - z^2 = 0$$

• As before, this has solutions

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$$\lambda_{\pm} = \frac{1}{2} (1 \pm \|\boldsymbol{n}\|) = \frac{1}{2} (1 \pm \sqrt{x^2 + y^2 + z^2})$$

where
$$\boldsymbol{n} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$
 with $x^2 + y^2 + z^2 \leq 1$.

• Again, we have a positive matrix $0 \le \lambda_{\pm} \le 1$ with $\lambda_{+} + \lambda_{1} = 1$ or $Tr(\rho) = 1$.

• To find the eigenvectors, we switch to spherical polar coordinates $x = r\sin\theta\cos\phi$ $y = r\sin\theta\sin\phi$ $z = r\cos\theta$

so that $\|\boldsymbol{n}\| = r$.

• In these coordinates, we have $\rho = \begin{pmatrix} 1 + r\cos\theta & r\sin\theta\cos\phi - ir\sin\theta\sin\phi \\ r\sin\theta + ir\sin\theta\sin\phi & 1 - r\cos\theta \end{pmatrix} = \begin{pmatrix} 1 + r\cos\theta & r\sin\theta e^{-i\phi} \\ r\sin\theta e^{+i\phi} & 1 - r\cos\theta \end{pmatrix}$

and you can check that the two orthogonal unit vectors

$$|n+\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix} = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle \text{ and } |n-\rangle = \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \end{pmatrix} = \sin\frac{\theta}{2}|0\rangle - e^{i\phi}\cos\frac{\theta}{2}|1\rangle$$

are the eigenvectors with $\rho |n \pm \rangle = \lambda_{\pm} |n\pm \rangle$.

Pure Qubit States

• If the state is pure then $||n|| = \sqrt{x^2 + y^2 + z^2} = 1$, so $\lambda_+ = 1$ and $\lambda_- = 0$. As a result, the density operator is $\rho = |n+\rangle\langle n+|$

• This is just the projector onto the one-dimensional subspace spanned by $|n + \rangle = \cos \frac{\theta}{2} |0\rangle + e^{i\phi} \sin \frac{\theta}{2} |1\rangle$.



3.vii) Quantum Theory as a GPT

- You might have thought that, to get a general quantum state space, we have to use a hypersphere, but this is not correct.
- Instead, we generalize the complex vector space that our matrices act on to arbitrary dimensions.
- A (finite dimensional) quantum system is associated with the vector space \mathbb{C}^n .
- A state (density matrix) is a positive, Hermitian matrix ρ that satisfies

$$\mathrm{Tr}(\rho)=1.$$

- A pure state is a projector $\rho = |\psi\rangle\langle\psi|$ onto the one-dimensional subspace spanned by a unit vector $|\psi\rangle$, i.e. $\langle\psi|\psi\rangle = 1$.
 - We often just use the vector $|\psi\rangle$ to represent a pure state, but note that $e^{i\phi}|\psi\rangle$ represents the same state.

A Bit More Linear Algebra

• We now want to describe the effects and observables in quantum mechanics. But first, a few useful bits of linear algebra.

• First, the most useful result in Dirac notation:

• **Proposition:** For any orthonormal basis {|j}}, $I = \sum_{j} |j\rangle\langle j|$.

• Proof: Any vector $|\psi\rangle$ can be written as $|\psi\rangle = \sum_j a_j |j\rangle$

$$\left(\sum_{j}|j\rangle\langle j|\right)|\psi\rangle = \sum_{j}|j\rangle\langle j|\psi\rangle = \sum_{j,k}a_{k}|j\rangle\langle j|k\rangle$$
$$= \sum_{j,k}a_{k}|j\rangle\delta_{jk} = \sum_{j}a_{j}|j\rangle = |\psi\rangle$$

Properties of the Trace

• The trace of a matrix M, denoted Tr(M) is

 $\operatorname{Tr}(M) = \sum_{j} \langle j | M | j \rangle = \sum_{j} M_{jj}.$

 \odot The trace and outer products:

$$\operatorname{Tr}(|\phi\rangle\langle\psi|) = \langle\psi|\phi\rangle$$

• Proof:

$$\operatorname{Tr}(|\phi\rangle\langle\psi|) = \sum_{j} \langle j|\phi\rangle\langle\psi|j\rangle = \sum_{j} \langle\psi|j\rangle\langle j|\phi\rangle = \langle\psi|I|\phi\rangle = \langle\psi|\phi\rangle$$

• Cyclic property of the trace:

$$\operatorname{Tr}(ABC \cdots YZ) = \operatorname{Tr}(ZABC \cdots Y)$$

• Proof:

$$\operatorname{Tr}(ABC \cdots YZ) = \sum_{j} \langle j | ABC \cdots YZ | j \rangle = \sum_{j,k} \langle j | ABC \cdots Y | k \rangle \langle k | Z | j \rangle$$
$$= \sum_{j,k} \langle k | Z | j \rangle \langle j | ABC \cdots Y | k \rangle = \sum_{k} \langle k | ZABC \cdots Y | k \rangle = \operatorname{Tr}(ZABC \cdots Y)$$

Quantum Effects

- Firstly, since our normalized states ρ do not include the zero matrix, we can form the state cone by just dropping the normalization constraint $Tr(\rho) = 1$. Therefore, the state cone just consists of all positive Hermitian matrices.
- Since the inner product is $(N, M) = \text{Tr}(N^{\dagger}M)$, we know that an element of the dual cone f can be written as $f(\rho) = \text{Tr}(E\rho)$ for some $n \times n$ matrix E, such that

 $Tr(E\rho) \ge 0$ for all positive matrices ρ .

• We will show that the state cone is self dual, so *E* just has to be a positive matrix.

Quantum Effects

• **Proposition**: The cone of positive Hermitian matrices is self-dual.

- Proof: The extreme points of the state space are $\rho = |\psi\rangle\langle\psi|$, where $|\psi\rangle$ is a unit vector (pure state).
- $Tr(E\rho) \ge 0$ is guaranteed for all other matrices in the cone provided it is true on these points, i.e.

 $\operatorname{Tr}(E|\psi\rangle\langle\psi|) = \langle\psi|E|\psi\rangle \ge 0,$

but this is just the definition of a positive matrix.

Quantum Effects

• To be a valid effect, we also need $f(\rho) \le 1$ for all normalized states, or equivalently $f \le u$, where u is the unit effect.

• *u* is defined by $u(\rho) = 1$ for all normalized states. Since

 $\mathrm{Tr}(I\rho)=\mathrm{Tr}(\rho)=1,$

u is represented by the identity matrix I.

- If we introduce the partial order on matrices $E \leq F$ if F E is a positive operator, then a quantum effect is represented by a matrix E such that $0 \leq E \leq I$, where 0 is the matrix of all zeroes.
- The probability rule in quantum mechanics is therefore $Prob(E|\rho) = Tr(E\rho)$
- This is called the (generalized) Born rule.
- Note that, if $\rho = |\psi\rangle\langle\psi|$ is a pure state then

 $\operatorname{Prob}(E|\rho) = \operatorname{Tr}(E|\psi\rangle\langle\psi|) = \langle\psi|E|\psi\rangle$

Quantum Observables (POVMs)

- An observable is a set of effects $\{f_j\}$ such that $\sum_j f_j = u$.
- \odot Therefore, in quantum mechanics it is a set of positive operators $\{E_j\}$ such that

$$\sum_{j} E_{j} = I.$$

• This is called a Positive Operator Valued Measure (POVM). The operators E_i are often called POVM elements instead of effects.

• We then have

$$\operatorname{Prob}(j|\rho) = \operatorname{Tr}(E_j\rho)$$

Example: The Trine POVM



Projector Valued Measures (PVMs)

- A special class of POVMs (and the only kind of measurement usually considered in undergraduate QM) is where each POVM element P_j is a projector. This is called a *Projector Valued Measure (PVM)*.
- A PVM is also sometimes called a *sharp* observable.
- In order for $\sum_{j} P_{j} = I$ to hold, the projectors have to be orthogonal $P_{j}P_{k} = 0$, i.e. they project onto orthogonal subspaces.
- To see why, suppose P_1 and P_2 are not orthogonal and let $|\psi\rangle$ be a vector that lies in the intersection of the subspaces they project onto so that $P_1|\psi\rangle = |\psi\rangle$ and $P_2|\psi\rangle$. Then,

$$(P_1 + P_2)|\psi\rangle = 2|\psi\rangle,$$

so $\sum_{j} P_{j} \neq I$ because $I |\psi\rangle = I$.

"Observables" In Quantum Mechanics

- In undergraduate QM, what is called an "observable" is usually a Hermitian matrix M ($M^{\dagger} = M$). Let's see how this is connected to PVMs.
- Any Hermitian operator can be written in its spectral decomposition

$$M = \sum_j \lambda_j P_j$$
,

where the λ_j 's are the eigenvalues of M and the P_j 's are the projectors onto the corresponding eigenspaces. These are orthogonal and $\sum_j P_j = 1$, so they define a PVM.

- We can think of the eigenvalues as giving values to the outcomes of the measurement, e.g. λ_j might be the position of a particle.
- Then, QM specifies the probability rule PVM with $Prob(\lambda_j | \rho) = Tr(P_j \rho)$, which is just the probability rule for the PVM $\{P_j\}$.
- If we are not interested in the values of the outcomes, just their probabilities, we can dispense with Hermitian observables and just use PVMs.

Example



Consider the matrix

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

• This has spectral decomposition

$$\sigma_1 = |+\rangle \langle +|-|-\rangle \langle -|,$$

where $|\pm\rangle = \frac{1}{\sqrt{2}} (|0\rangle \pm |1\rangle)$

- So it corresponds to the PVM $\{|+\rangle\langle+|, |-\rangle\langle-|\}$.
- The $|+\rangle\langle+|$ outcome has value +1 and The $|-\rangle\langle-|$ outcome has value -1.

Orthonormal Basis Measurements

• If the projectors in a PVM are all one-dimensional $P_j = |\phi_j\rangle\langle\phi_j|$, then $\{|\phi_j\rangle\}$ is an orthonormal basis. In this case, we can write the probabilities as

$$\Pr(\phi_j|\rho) = \operatorname{Tr}(|\phi_j\rangle\langle\phi_j|\rho) = \langle\phi_j|\rho|\phi_j\rangle.$$

• If $\rho = |\psi\rangle\langle\psi|$ is also a pure state then this can be written as

 $\Pr(\phi_j|\psi) = \langle \phi_j|\psi\rangle\langle \psi|\phi_j\rangle = |\langle \phi_j|\psi\rangle|^2,$

which is what is normally called the Born rule in undergrad QM.

 The example on the previous slide was an orthonormal basis measurement.

The Quantum Test Space

• **Theorem**: (Gleason's Theorem) Consider the test space where the outcomes are projectors $|\psi\rangle\langle\psi|$ onto unit vectors in \mathbb{C}^n and the tests are orthonormal basis measurements. If $n \ge 3$ then a state ω on this test space corresponds to a density matrix ρ , i.e. ρ is positive and $\operatorname{Tr}(\rho) = 1$, with

 $\omega(|\psi\rangle\langle\psi|) = \langle\psi|\rho|\psi\rangle.$

A. M. Gleason, "Measures on the closed subspaces of a Hilbert space", Indiana University Mathematics Journal, 6: 885–893 (1957)

 Note: There must be a test space for rebits and qubits, but it is not this "standard" quantum test space. It must include some POVMs that are not PVMs.

Conclusion

- This section was meant to persuade you that quantum theory can be understood as a generalization of probability theory, situated within a well-motivated framework for such generalizations (GPTs).
- As such, it is a Church of the Smaller Hilbert Space approach to setting up quantum theory.
- This raises the question of why this GPT and not some other? Why does nature use the orthonormal bases of \mathbb{C}^n as its test space?
 - Much work has been done on axiomatic reconstructions of quantum theory within this approach in recent years. See D'Ariano et. al. on supplemental reading list for a particularly nice example.
- In traditional undergrad. quantum theory, the analogy between quantum pure states and physical waves is used to build the theory. This is a Church of the Larger Hilbert Space approach.
- I think that which of these approaches you take more seriously biases you towards certain types of interpretation of quantum theory, and explains a lot of the talking past one another that happens in debates on interpretation.