

# Foundations of QM

We will discuss axioms, interpretations, + consequences

## ① Quantum States

- Definition

- Axiom: States are vectors in a complex vector space that has an inner product (with some conditions)

This type of vector space is called a Hilbert space.

- Write a vector as a "ket"  $|1\rangle$ ,  $|2\rangle$ , etc

+ You can add vectors together  $|1\rangle + |2\rangle$

+ You can multiply vectors by complex numbers (scalars)

- Basis vectors: A set of vectors in a vector space

+ In an  $N$ -dimensional space, this is a set of  $N$  vectors  $\{|e_1\rangle, |e_2\rangle, \dots, |e_N\rangle\}$  such that any vector is a linear superposition of basis vectors

$$|1\rangle = c_1 |e_1\rangle + c_2 |e_2\rangle + \dots + c_N |e_N\rangle, \quad c_i = \text{scalars.}$$

+ There are different possible basis sets for any vector space. So for different basis vectors  $\{|f_i\rangle\}$ ,

$$|1\rangle = a_1 |f_1\rangle + a_2 |f_2\rangle + \dots + a_N |f_N\rangle$$

is the same vector  $|1\rangle$  (just the representation differs)

+ Any vector space can be written in terms of column matrices by assigning basis vectors

$$|e_1\rangle \approx \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad |e_2\rangle \approx \begin{bmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{bmatrix}, \text{etc.}$$

Then

$$|1\rangle \approx \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{bmatrix} \text{ as above.}$$

If you use a different basis, you get different components in the columns. (In lin. alg., you learn about this "change of basis" in terms of matrix multiplication.)

- Inner Product: Function of 2 vectors that gives a scalar
  - + We will write the inner product of  $| \phi \rangle$  and  $| \psi \rangle$  as  $\langle \phi | \psi \rangle$ . In our complex Hilbert space, this is  $= \langle \psi | \phi \rangle^*$  (complex conjugate)
  - + The inner product is linear in right-hand argument and "anti-linear" in the left-hand argument:

$$\text{If } |\phi\rangle = a|\alpha\rangle + b|\beta\rangle \text{ and } |\psi\rangle = c|\gamma\rangle + d|\delta\rangle,$$

$$\begin{aligned}\langle \phi | \psi \rangle &= \langle \psi | (\alpha|\phi\rangle + \beta|\phi\rangle) \\ &= a^* \langle \psi | \alpha \rangle + b^* \langle \psi | \beta \rangle \\ &= a^*c \langle \psi | \alpha \rangle + b^*c \langle \psi | \beta \rangle + a^*d \langle \psi | \alpha \rangle + b^*d \langle \psi | \beta \rangle\end{aligned}$$

- + The inner product of a vector with itself is positive real. The norm of  $| \psi \rangle$  is  $\sqrt{\langle \psi | \psi \rangle}$ .

- + When we choose basis vectors, we can choose an orthonormal basis (in finite # of dimensions) meaning  $\langle e_i | e_j \rangle = \delta_{ij}$ . So  $| \psi \rangle = c_1|e_1\rangle + \dots + c_n|e_n\rangle$  and  $| \phi \rangle = b_1|e_1\rangle + \dots + b_n|e_n\rangle$  have  $\langle \phi | \psi \rangle = b_1^*c_1 + \dots + b_n^*c_n$ .
- + With an orthonormal basis  $| \psi \rangle = (c_1, \dots, c_n)$
$$| \psi \rangle = (\langle e_1 | \psi \rangle)|e_1\rangle + \dots + (\langle e_n | \psi \rangle)|e_n\rangle$$

This gives a handy way to find components/change bases

- + The left-hand argument of the inner product is written as a bra  $\langle \psi |$ . Mathematically, it is called a dual vector, which means it is an instruction to take the inner product of  $| \psi \rangle$  with any vector to the right.

- + In terms of matrices, a bra is a row given by the Hermitian adjoint (transpose+conjugate) of the ket

$$\langle \psi | = [c_1^* \ c_2^* \ \dots \ c_n^*]^T \simeq (| \psi \rangle)^+$$

- There are other conditions on physical states:

+ A physical state has unit norm  $\langle \psi | \psi \rangle = 1$

Therefore, if  $|\psi\rangle = \sum c_i |e_i\rangle$ , then  $\sum |c_i|^2 = 1$   
(for orthonormal basis)

+ We will see that  $e^{i\theta} |\psi\rangle$  is physically equivalent to  $|\psi\rangle$  (where  $\theta$  is a real angle).

In other words, changing by an overall complex phase keeps the state the same.

### - Important examples / Generalizations

- Spin (+ Angular Momentum) States:

+ Recall that a state of definite spin has 2 quantum numbers  $S$  and  $m$ .

+  $S$  can be integer or half-integer (non-negative) and  $-S \leq m \leq S$  w/ values of  $m$  separated by integers

+ So  $S=1$  has 3 states with  $m=-1, 0, 1$

$|1, -1\rangle, |1, 0\rangle, |1, 1\rangle$ . Commonly assigned

$$|1, 1\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \quad |1, 0\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \quad |1, -1\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

+  $S=\frac{1}{2}$  has 2 states,  $m=\pm\frac{1}{2}$ ,  $|\frac{1}{2}, \frac{1}{2}\rangle = |\uparrow\rangle, |\frac{1}{2}, -\frac{1}{2}\rangle = |\downarrow\rangle$

with

$$|\uparrow\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |\downarrow\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

- Qubit (or qbit) states

+ Any 2D Hilbert space, so simplest non-trivial example.

A spin  $S=\frac{1}{2}$  system is a physical representation of a single qbit

+ The typical basis is usually written as  $|0\rangle$  and  $|1\rangle$  (orthonormal)

+ The general state of 1 qbit is

$$|1\rangle = \cos\theta |0\rangle + \sin\theta e^{i\phi} |1\rangle$$

Note: (1) normalized (2) we choose overall phase so coefficient of  $|0\rangle$  is real, positive (so  $0 \leq \theta \leq \pi/2$ )

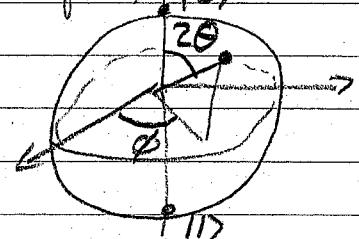
+ This qbit is a point on the (surface of the)  $|0\rangle$

+ A Black sphere, At  $\theta=0, \phi$

clearly doesn't matter. At  $\theta=\pi/2$ ,

$\phi$  becomes overall phase + also

doesn't matter — these are poles.



• Multiple particles, etc

+ Suppose you have multiple particles, one particle w/ spin + orbital angular momentum, etc.

+ States of a system with multiple parts are from a tensor product vector space. In this case, we can choose a basis where each part corresponds to a factor in the state (factorized basis)

$$\text{multiparticle state} \rightarrow |1\rangle = |\alpha\rangle_1 |\beta\rangle_2 \dots \text{single particle state}$$

+ For example, 2 qbits (with each in the usual basis) has a factorized basis

$$|0\rangle_1 |0\rangle_2, |0\rangle_1 |1\rangle_2, |1\rangle_1 |0\rangle_2, |1\rangle_1 |1\rangle_2$$

+ A non-factorized basis is often useful. For example, if there are 2 spins, a factorized state is  $|s_1, m_1\rangle |s_2, m_2\rangle$ , b/c a total angular momentum basis (think addition of angular momentum)  $|s_1, m_1; s_2, m_2\rangle$  can be helpful.

Note/

+ Remember: Identical particles can be bosons (if they have integer spin) or fermions (odd half-integer spin).

The state of multiple identical bosons is always symmetric (remains the same) if any 2 <sup>single</sup> particle states switch; the state of multiple identical fermions is anti-symmetric (gives a - sign) when 2 single-particle states switch. (These generally don't factorize)

$$2 \text{ bosons} : \frac{1}{\sqrt{2}} (|1\rangle_1 |2\rangle_2 + |2\rangle_1 |1\rangle_2) \quad (K_{\alpha\beta}|\rho\rangle = 0)$$

$$2 \text{ fermions} : \frac{1}{\sqrt{2}} (|1\rangle_1 |2\rangle_2 - |2\rangle_1 |1\rangle_2)$$

### - Consequences

- Superposition:
  - + The state of a quantum system can be a linear superposition of 2 or more basis states
  - + If the assignment of basis has a physical meaning then a general state may have ambiguous physical properties of some type.
  - + This leads to the probabilistic nature of quantum mechanics (we'll return to this later)
  
- Entanglement:
  - + This is a consequence of superposition for multiparticle systems (tensor product states)
  - + Entanglement is when the full multiparticle state does not factorize
  - + That means the state of a single particle is not well-defined on its own. It depends on the state of the other particle
  - + Examples: Consider the total spin states of an electron + positron (not identical)

$$|s=0\rangle = \frac{1}{\sqrt{2}} (|1\rangle_1 |1\rangle_2 - |1\rangle_1 |2\rangle_2), \text{ entangled}$$

$$|s=1, m=1\rangle = |1\rangle_1 |1\rangle_2 \quad \text{not}$$

$$|s=1, m=0\rangle = \frac{1}{\sqrt{2}} (|1\rangle_1 |2\rangle_2 + |2\rangle_1 |1\rangle_2) \quad \text{entangled}$$

$$|s=1, m=-1\rangle = |2\rangle_1 |2\rangle_2 \quad \text{not}$$

Works for qubits,  $|1\rangle \rightarrow |0\rangle$ ,  $|2\rangle \rightarrow |1\rangle$

+ the most famous entangled state is Schrödinger's cat: cat in a box with poison controlled by a single radioactive nucleus. After 1 half-life,

$$|4\rangle \rightarrow \frac{1}{\sqrt{2}}(|\psi\rangle |N\rangle + (\text{phase}) |\bar{\psi}\rangle |N, N_{\text{--}}\rangle)$$

We'll also come back to this

- Quantum Information (very brief introduction):  
What is the information content of a state?

- Information is "what we can learn" (Claude Shannon)
  - + If we're flipping a fair coin, we don't get much information per flip — it takes a long time to get confidence odds are really 50% - 50%
  - + But if  $P(H) \gg P(T)$ , we learn a lot every time the coin comes up tails. If we flip HTHTHH..., the 2nd tail tells us a lot about  $P(T)$
  - + Information is about classical ignorance

- An alternative approach is to think about data compression
  - + Think about an alphabet w/ 4 letters a, b, c, d.
  - A simple <sup>binary</sup> encoding is a=00, b=01, c=10, d=11
  - + But this is inefficient if some letters are uncommon, say  $P(a) = 1/2$ ,  $P(b) = 1/4$ ,  $P(c) = P(d) = 1/8$
  - + A more efficient binary representation is (actually most efficient)
    - $a = 0$ ,  $b = 10$ ,  $c = 110$ ,  $d = 111$
    - i.e., max length is 3, 0 means change letters.

- + The length of a letter  $i(\text{letter}) = -\log_2(P(\text{letter}))$   
is the number of Shannon bits
- + The average length of a letter in a word / conversation  
is the Shannon entropy

$$S = -\sum P \log_2 P$$

- + The Shannon entropy formula may be familiar from statistical mechanics, and it is in fact the same idea — we are ignorant of the microstate.

- Quantum information is also about ignorance
  - + Even if we know the exact quantum state  $|1\rangle$ , there is quantum probability. This does not contribute to the information content/Shannon entropy.
  - + If the quantum state of a system is definite (even a Schrödinger cat state), it has zero entropy and is called a pure state.
  - + But suppose someone prepares a quantum state, and you don't know what it is. (This is what happens in statistical mechanics.) This is called a mixed state, and our ignorance means it contains information.
  - + We can think of a mixed state as choosing a (possibly special) basis of states and a probability for the actual state to be each one:

$P_1 |e_1\rangle, P_2 |e_2\rangle, \dots$

A pure state is a mixed state where one probability  $P_i = 1$  and the rest are zero.

- Density Matrix (or Density Operator):
  - + A pure state is mathematically described by a normalized ket. What is a mixed state?
  - + We need a way to list probabilities  $P_i$ . Ket is not a vector (bc those represent kets).
  - + But we can use a matrix. Define the density matrix in the  $\{|e_i\rangle\}$  basis as

$$\rho = \text{diag}(P_1, P_2, \dots, P_N)$$

Can change basis  
 by similarity  
 transformation

+ This is Hermitian  $\rho^\dagger = \rho$  and has  $\text{Tr}(\rho) = \sum P_i = 1$

+ We can define  $\rho_{ij}$  as an operator

$$\rho = P_1 |e_1\rangle\langle e_1| + P_2 |e_2\rangle\langle e_2| + \dots$$

+ Each term is called a dyad and acts on a ket  $|4\rangle$  by  $\rho|4\rangle = \sum_i P_i (\langle e_i | 4 \rangle) |e_i\rangle$

This is equivalent to matrix multiplication of  $\rho$  on the column describing  $|4\rangle$  in the  $|e_i\rangle$  basis

+ Each dyad is a column  $\times$  row = square matrix  
+ A pure state  $|e_i\rangle \equiv |4\rangle$  has density matrix

$$\rho = |4\rangle\langle 4|$$

+ Suppose we want to write  $\rho$  as a matrix in another basis  $\{|f_i\rangle\}$ . Take the dyad form. Then the matrix elements are

$$\rho_{ij} = \langle f_i | \rho | f_j \rangle = \sum_k P_k \langle f_i | e_k \rangle \langle e_k | f_j \rangle$$

+ Examples: Suppose we know an electron has 50% chance of being spin up  $|1\rangle$  or down  $|1\rangle$ . In the usual basis  $(|e_1\rangle = |1\rangle, |e_2\rangle = |1\rangle)$

$$\rho = \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}$$

BUT if it is "spin right"  $|4\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)$ ,

$$\rho = |4\rangle\langle 4| \cong \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix}$$

So here we don't have  $\{|1\rangle, |2\rangle\} = \{|e_1\rangle, |e_2\rangle\}$   
b/c  $\rho$  is not diagonal. If we diagonalize it,  
the probabilities are  $P_1 = 1$  and  $P_2 = 0$ .

### Entropy + the density matrix

+ For a diagonal matrix  $M$ , with diagonal entries  $M_1, M_2, \dots$ ,  
a function  $f(M) = \text{diag}(f(M_1), f(M_2), \dots)$

+ So

$$S = -\text{Tr } \rho \log_2(\rho) = -\sum_i P_i \log_2 P_i$$

generalizes Shannon entropy to quantum form.  
So we see a pure state has zero entropy. The entropy of a mixed state is our ignorance.

+ But the universe is in a pure state, presumably.  
How do we get a mixed state? It's b/c we only know about part of the full system

- + Simplest example: suppose we have an electron + positron. In spin state  $|14\rangle = \frac{1}{\sqrt{2}}(|1\rangle, |2\rangle_2 - |1\rangle, |2\rangle_2)$ . But if we only have the electron, it doesn't have a well-defined pure state by itself. We can make a mixed state for the electron by "tracing" over the positron states

$$\rho_1 \equiv \frac{1}{2}|\!\langle 14\rangle\langle 4|1\rangle_2 + \langle 1|\!\langle 4|\langle 41\rangle_2 \\ = \frac{1}{2}|1\rangle\langle 1| + \frac{1}{2}|1\rangle\langle 1|$$

This is a mixed state and has entropy!

- + This is a key property of entanglement: if you start with multiple particles in a pure state and "trace out" some of them, the remaining particles are in a mixed state iff the multiparticle pure state is entangled. The entropy of the remaining particles is the entanglement entropy and measures the entanglement.
- There are many other aspects of quantum information theory and it is rapidly becoming a critical subject to learn for many fields of physics