Axioms of Quantum Mechanics

- quantum mechanics is a mathematical model which people have invented to fit (describe, quantify) the experimental facts for atoms, sub-atomic particles, crystals, etc.

- <u>weirdly</u>, it <u>is</u> the math of complex Hilbert spaces and their operators!

resources

I'll take postulates from here
(axiom = postulate)

1. wikipedia page for "mathematical formulation of quantum mechanics"
2. wikipedia page for "Dirac-von Neumann axioms"
3. B. Hall, Quantum Theory for Mathematicians, Springer 2013
4. any graduate-level QM book?

postulate I

Each isolated physical system is associated with a (topologically) separable complex Hilbert space H with inner product $\langle\varphi|\psi\rangle$.

Postulate I

The state of an isolated physical system is represented, at a fixed time t, by a state vector $|\psi\rangle$ belonging to a Hilbert space $\mathcal{H}$ called the *state space*.

- note Dirac decoration/style: $\psi \in \mathcal{H}$ is written "$|\psi\rangle$" and inner product $\langle\varphi,\psi\rangle$ is written "$\langle\varphi|\psi\rangle$"
- the universe is an "isolated physical system"

postulate II:

Postulate II.a

Every measurable physical quantity $\mathcal{A}$ is described by a Hermitian operator A acting in the state space $\mathcal{H}$. This operator is an observable, meaning that its eigenvectors form a basis for $\mathcal{H}$. The result of measuring a physical quantity $\mathcal{A}$ must be one of the eigenvalues of the corresponding observable A.

- this will require some unpacking ...

- name some "measurable physical quantities":

charge

mass

spin

x-coordinate of position

angular momentum

momentum

energy

mag moment

time ?

def: $A \in \mathcal{L}(\mathcal{H})$ is **Hermitian** (also known as **self-adjoint**) if

$$\langle Av, w \rangle = \langle v, Aw \rangle \text{ for all } v, w \in \mathcal{H}$$

or, equivalently, $A^* = A$

---

def: given $B \in \mathcal{L}(\mathcal{H})$, $\underline{B^*}$, the <u>adjoint of B</u>, is the operator $B^* \in \mathcal{L}(\mathcal{H})$ so that

$$\langle B^* v, w \rangle = \langle v, Bw \rangle \text{ forall } v, w \in \mathcal{H}$$

<u>def:</u> an <u>observable</u> is a Hermitian (self-adjoint) operator on $\mathcal{H}$

- II.a makes the

  <u>claim:</u> the eigenvectors of an observable form a basis for $\mathcal{H}$

- <u>Q:</u> is this true? 1

- the following lemma is the easy part...

__lemma:__ suppose $A \in \mathcal{L}(\mathcal{H})$ is hermitian (self-adjoint) and $Av_1 = \lambda_1 v_1$ and $Av_2 = \lambda_2 v_2$ for $v_1 \neq 0$, $v_2 \neq 0$, and $\lambda_1 \neq \lambda_2$. then $\langle v_1, v_2 \rangle = 0$ and $\lambda_i \in \mathbb{R}$.

__proof:__ ① $\lambda_1 \langle v_1, v_1 \rangle = \langle v_1, \lambda_1 v_1 \rangle = \langle v_1, Av_1 \rangle$

$$= \langle Av_1, v_1 \rangle = \langle \lambda_1 v_1, v_1 \rangle$$

$$= \overline{\lambda_1} \langle v_1, v_1 \rangle$$

__so:__ $(\lambda_1 - \overline{\lambda_1}) \|v_1\|^2 = 0$ so $\lambda_1 = \overline{\lambda_1}$ $\therefore \lambda_1 \in \mathbb{R}$ (also $\lambda_2 \in \mathbb{R}$)

② $\lambda_2 \langle v_1, v_2 \rangle = \langle v_1, \lambda_2 v_2 \rangle = \langle v_1, Av_2 \rangle = \langle Av_1, v_2 \rangle$

$$= \langle \lambda_1 v_1, v_2 \rangle = \lambda_1 \langle v_1, v_2 \rangle \quad \therefore \underbrace{(\lambda_1 - \lambda_2)}_{\text{notzer}} \underbrace{\langle v_1, v_2 \rangle}_{\text{zero}} = 0$$

Postulate II.a

Every measurable physical quantity $\mathcal{A}$ is described by a Hermitian operator A acting in the state space $\mathcal{H}$. This operator is an observable, meaning that its eigenvectors form a basis for $\mathcal{H}$. The result of measuring a physical quantity $\mathcal{A}$ must be one of the eigenvalues of the corresponding observable A.

II.a ← again

- II.a says that when you observe a physical quantity in an experiment you get an eigenvalue of a hermitian (self-adjoint) A
- thus experiments give real results

- **Q:** $A \in \mathcal{L}(\mathcal{H})$?

  ... do we want to require that A is bounded? ?

A. No.

postulate II.b

Postulate II.b

When the physical quantity $\mathcal{A}$ is measured on a system in a normalized state $|\psi\rangle$, the probability of obtaining an eigenvalue (denoted a_n for discrete spectra and α for continuous spectra) of the corresponding observable A is given by the *amplitude squared* of the appropriate wave function (projection onto corresponding eigenvector).

$$\mathbb{P}(a_n) = |\langle a_n|\psi\rangle|^2 \qquad \text{(Discrete, nondegenerate spectrum)}$$

$$\mathbb{P}(a_n) = \sum_i^{g_n} |\langle a_n^i|\psi\rangle|^2 \qquad \text{(Discrete, degenerate spectrum)}$$

$$d\mathbb{P}(\alpha) = |\langle \alpha|\psi\rangle|^2 d\alpha \qquad \text{(Continuous, nondegenerate spectrum)}$$

$\psi \in \mathcal{H}$, $\psi \neq 0$, $\mathcal{H} = L^2(\mathbb{R})$

$$\Rightarrow \quad \tilde{\psi} = \frac{\psi}{\|\psi\|}.$$

$$\int_{-\infty}^{\infty} |\tilde{\psi}(x)|^2 dx = \|\tilde{\psi}\|^2 = 1$$

<u>Let:</u> $p(x) = |\tilde{\psi}(x)|^2$. then

① $p \geq 0$

② $\int_{-\infty}^{\infty} p(x) dx = 1$.

- **Q.** what does it mean for $A \in \mathcal{L}(\mathcal{H})$ to have "discrete spectrum" versus "continuous spectrum"?

3

- **Q.** what does "$dP(\alpha) = |\langle\alpha|\psi\rangle|^2 d\alpha$" even mean?

4

Dirac notation:

$\mathcal{H}$ is a complex Hilbert space

A is an observable (self-adjoint op. on $\mathcal{H}$)

us:

$$v \in \mathcal{H}$$

$$Av = \underbrace{a_n}_{\in \mathbb{R}} v$$

$\ell_v(v) = 1$

$\Updownarrow$

$\|\ell_v\|_{\mathcal{H}'} = 1$

$\Updownarrow$

$$\ell_v(u) = \langle v, u \rangle \in \mathcal{H}'$$

$$\|v\|^2 = \langle v, v \rangle = 1$$

$$Pu = \langle v, u \rangle v$$

Dirac:

$$\underbrace{|a_n\rangle}_{\text{ket}} \in \mathcal{H}$$

$$A|a_n\rangle = a_n |a_n\rangle$$

$$\underbrace{\langle a_n|}_{\text{bra}} \in \mathcal{H}'$$

$$\underbrace{\langle a_n | a_n \rangle}_{\text{bracket}} = 1$$

$$P = |a_n\rangle\langle a_n|$$

- II.b says that for "discrete spectrum", if $\psi \in \mathcal{H}$ describes the current state of the system, and if $\|\psi\| = 1$, then

$$P(\text{observable quantity } \mathcal{O} \text{ yields measured value } a_n \in \mathbb{R})$$

$$= |\langle v, \psi \rangle|^2$$

where $Av = a_n v$ and $\|v\| = 1$

postulate II.c

Postulate II.c

If the measurement of the physical quantity $\mathcal{A}$ on the system in the state $|\psi\rangle$ gives the result a_n, then the state of the system immediately after the measurement is the normalized projection of $|\psi\rangle$ onto the eigensubspace associated with a_n

$$|\psi\rangle \quad \overset{a_n}{\Longrightarrow} \quad \frac{P_n|\psi\rangle}{\sqrt{\langle\psi|P_n|\psi\rangle}}$$

- this process, of "state collapse" when you do a measurement, is the biggest philosophical mystery?!

postulate III

$\mathcal{H}$ = Hilbert space
H = Hamiltonian | VS: heat eqn $\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$

$\psi(t, x)$

$$i\hbar \frac{\partial \psi}{\partial t} = \underbrace{\left(\frac{\partial^2}{\partial x^2} + x^2\right)}_{H}\psi$$

> **Postulate III**
>
> The time evolution of the state vector $|\psi(t)\rangle$ is governed by the Schrödinger equation, where $H(t)$ is the observable associated with the total energy of the system (called the Hamiltonian)
>
> $$i\hbar \frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle$$

Equivalently, the time evolution postulate can be stated as:

> **Postulate III**
>
> The time evolution of a closed system is described by a unitary transformation on the initial state.
>
> $$|\psi(t)\rangle = U(t; t_0)|\psi(t_0)\rangle$$

H is t-indep

$$U(t, t_0) = e^{-iH(t-t_0)/\hbar}$$

VS:

in $\mathbb{C}^n$: $\vec{x}\,'(t) = A\vec{x}(t)$

has soln: $\vec{x}(t) = e^{At}\vec{x}_0$

- **Q.** what kind of operator is a "Hamiltonian"?

5

partial answer:

$$\mathcal{H} = L^2(\mathbb{R})$$

$$H = -\frac{d^2}{dx^2} + V(x)$$

$f \in \mathcal{H}$

$(M_V f)(x) = V(x) f(x)$

e.g.

$$(Hf)(x) = -f''(x) + x^2 f(x)$$

special case of the "harmonic oscillator"

[but $H \notin \mathcal{L}(\mathcal{H})$! ... H is unbounded!]

- **Q.** how do we solve (or understand solutions of) the Schrödinger equation?

6

operator on $\mathcal{H} = L^2(\mathbb{R})$

e.g. harmonic oscillator

<u>Schrödinger equation</u>

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi = \underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2}}_{\text{kinetic} = \frac{p^2}{2m}} + \frac{k}{2}x^2\psi$$

$p = i\hbar\frac{\partial}{\partial x}$

8

<u>Solution?:</u>

$$\psi(t,x) = \underbrace{e^{(Ht/i\hbar)}}_{\text{exponentiate the operator } H} \overbrace{\psi(0,x)}^{\text{initial condition}}$$

"functional calculus" ⟸ bounded functional calculus

if $A \in \mathcal{L}(\mathcal{H})$ then we want to be able to form and understand new operators

$$f(A) \in \mathcal{L}(\mathcal{H})$$

actually we will do this even for unbounded operators

where e.g.

$$f(z) = e^z$$

to get

$$f(A) = e^A$$

expm(A)

Summary from "Dirac-von Neumann axioms" page:

Hilbert space formulation [edit]

The space $\mathbb{H}$ is a fixed complex Hilbert space of countably infinite dimension.

- The observables of a quantum system are defined to be the (possibly unbounded) self-adjoint operators A on $\mathbb{H}$.
- A state ψ of the quantum system is a unit vector of $\mathbb{H}$, up to scalar multiples; or equivalently, a ray of the Hilbert space $\mathbb{H}$.
- The expectation value of an observable A for a system in a state ψ is given by the inner product $\langle \psi, A\psi \rangle$.

regarding expectations:

$\left.\begin{matrix} 1, 2, 3, 4, 5, 6 \\ p = \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \dots \end{matrix}\right\} \quad \mathbb{E}(X) = \sum_{i=1}^{6} i \cdot \frac{1}{6}$

if $A \in \mathcal{L}(\mathcal{H})$ is an observable

and $A\varphi_k = \lambda_k \varphi_k$ for $k \in \mathbb{N}$ gives an ON

basis $\{\varphi_k\}_{k \in \mathbb{N}}$ of $\mathcal{H}$, then in QM the expectation

of A in state $\psi \in \mathcal{H}$ is

$$\langle A \rangle = \langle \psi, A\psi \rangle = \sum_{k=1}^{\infty} \lambda_k \left| \langle \varphi_k, \psi \rangle \right|^2$$

$$= \sum_{k=1}^{\infty} \lambda_k \, P(\psi \text{ is in state } \varphi_k)$$

because (for any $f \in \mathcal{H}$)

$$Af = \sum_{k=1}^{\infty} \langle \varphi_k, Af \rangle \varphi_k$$

$$= \sum_{k=1}^{\infty} \langle A\varphi_k, f \rangle \varphi_k$$

$$= \sum_{k=1}^{\infty} \lambda_k \langle \varphi_k, f \rangle \varphi_k$$

$$A = \sum_{k=1}^{\infty} \lambda_k \langle \varphi_k, \cdot \rangle \varphi_k$$

$$= \sum_{k=1}^{\infty} \lambda_k |\lambda_k\rangle\langle\lambda_k|$$

so $\langle \psi, A\psi \rangle = \sum_{k=1}^{\infty} \lambda_k \langle \varphi_k, \psi \rangle \langle \psi, \varphi_k \rangle$

list of questions ← this will finish my slides

Q1 An observable is a self-adjoint operator A on $\mathcal{H}$. Is it true that its "eigenvectors form a basis" of $\mathcal{H}$?

A. Generally, no. We will define the spectrum of A as a larger subset of $\mathbb{C}$, which includes any eigenvalues. We will prove the spectral theorem (Chapter 5) to update the meaning of "basis".

Q2. An observable A in QM is a self-adjoint operator on $\mathcal{H}$. Does that mean $A \in \mathcal{L}(\mathcal{H})$?

A. No. Many observables in QM are not bounded, though they are all linear. For a single particle in 1D, where $\mathcal{H} = L^2(\mathbb{R})$, the momentum is $p = -i\hbar \frac{d}{dx}$. This is an unbounded self-adjoint operator. In Chapter 3 we define "unbounded operator", following

von Neumann (1930).

Q3 What does it mean for an observable to have "discrete" or "continuous" spectrum?

A This will come from (with) the precise statement and proof of the Spectral theorem in Chapter 5.

Q4 For continuous spectrum, postulate II.b said that the probability of getting $\alpha \in \mathbb{R}$ from observation (observable) A on state $\psi \in \mathcal{H}$ is "$dP(\alpha) = |\langle \alpha | \psi \rangle|^2 d\alpha$".

What does this mean?

A. The (rigorous) spectral theorem will also explain this.

Q5 What kind of operator is a "Hamiltonian"?

A. It is the unbounded energy operator. For each physical system one can build it based on formulas for the classical energy. For example, in the position representation $\mathcal{H} = L^2(\mathbb{R})$ we have $p = -i\hbar \frac{d}{dx}$ for momentum, and $V(x)$ is the potential energy, as a multiplication

A. cont

operator on $\mathcal{H}$. Then the Hamiltonian is

$$H = \frac{p^2}{2m} + V(x) = \frac{1}{2m}\left(-i\hbar\frac{d}{dx}\right)^2 + V(x)$$

$$= \underbrace{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}}_{\text{kinetic energy}} + \underbrace{V(x)}_{\text{potential energy}}$$

as an unbounded self-adjoint operator on $\mathcal{H}$.

Q6. How do we solve the Schrödinger equation, a PDE problem? How does the quantum state $\psi \in \mathcal{H}$ evolve in time?

A.

- H Hamiltonian, a self-adjoint unbounded operator on $\mathcal{H}$
- $i\hbar \frac{\partial \psi}{\partial t} = H\psi$ Schrödinger equation
- $U(t) = e^{-iHt/\hbar}$ Unitary, $U(t) \in \mathcal{L}(\mathcal{H})$

is created via exponentiating the Hamiltonian

- $\underbrace{\psi(t)}_{\text{state at } t} = U(t)\underbrace{\psi_0}_{\text{quantum state at time } t=0}$

- since $U(t)$ unitary:

$$\langle \psi(t), \psi(t) \rangle = \langle U(t)\psi_0, U(t)\psi_0 \rangle$$

$$= \langle U(t)^* U(t)\psi_0, \psi_0 \rangle = \langle I\psi_0, \psi_0 \rangle = \langle \psi_0, \psi_0 \rangle$$

so total probability remains 1