B7.3 Further Quantum Theory

Lecturer: Christopher Beem
Class Info: To Be Confirmed

Schedule: Mondays 10 – 11
Wednesdays* 11 – 12 Week 6: 12 – 1 (will be recorded due to conflict w/ Functional Analysis II)

Typed notes for previous version of course on website. Will upload my own hand written notes after each lecture.

WILL NOT FOLLOW EXACT TRAJECTORY OF TYPED NOTES. (Will try to announce upcoming topics in lectures).

Textbooks:

- An Introduction to Quantum Theory (Hannabuss) ← Main references, basis for typed notes from past years. Neither embrace Dirac bra-ket notation; will discuss in Lecture 2.
- Lectures on Quantum Mechanics (Weinberg)
- Modern Quantum Mechanics (Sakurai) ← Physics-oriented reference, does some things not found in Weinberg or in Hannabuss
- Quantum Theory for Mathematicians (Hall) Advanced text with a great deal of rigor (heavy on functional analysis).
- Principles of Quantum Mechanics (Dirac) Written by a founder of the subject, worth a look.

Problem sheets appear in weeks 1, 3, 5, 7 (start of week). First is up now, but more info on classes is TBD (hopefully by Wednesday). Maybe only subset of problems will be marked.

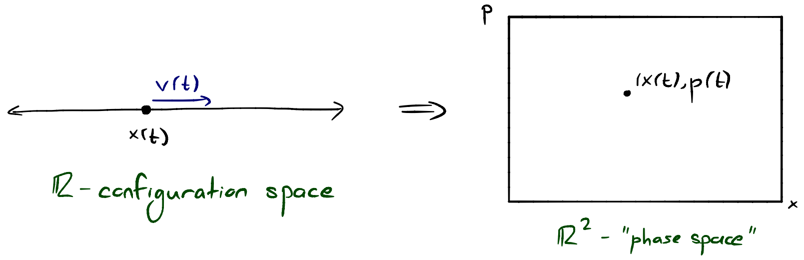
Plan for lecture 1

- Brief review of "wave mechanics" from part A.
- Postulates of quantum theory.
- Illustrating the postulates in two examples.
- Plan for next lecture.

Wave Mechanics (de Broglie, Schrödinger)

Recall basic set-up for classical dynamics (say in one dimension, $\mathbb{R}$)

States:



Observables: $f(x,p)$ (functions on phase space)

Dynamics: $\ddot{x} = \frac{1}{m}F$ (Newton)

$$\left.\begin{aligned} \dot{x} &= \frac{\partial H}{\partial p} \\ \dot{p} &= \frac{-\partial H}{\partial x} \\ H &= \frac{p^2}{2m} + V(x) \end{aligned}\right\}$$

(Hamiltonian mechanics, familiar if you took Classical Mechanics in Michaelmas term)

Hamiltonian function on phase space $\longrightarrow H$

Radically different in wave mechanics!

States: $\Psi(x,t)$ cx. wavefunction on configuration space

($|\Psi(x,t)|^2$ probability density for position $\Rightarrow \int_{-\infty}^{\infty} dx\, |\Psi(x,t)|^2 = 1$ normalization condition)

Observables: X, P act as operators on wave functions.

$$X : \psi(x) \longmapsto x\psi(x)$$
$$P : \psi(x) \longmapsto \frac{\hbar}{i}\frac{d}{dx}\psi(x)$$

$\hbar$ = "reduced Planck constant" $\approx 1.05 \times 10^{-34}$ J/s

Expectation: $\mathbb{E}_\psi\big(f(x,p)\big) = \int_{\mathbb{R}} dx\, \overline{\psi}(x)\big(f(\hat{x},\hat{p})\circ\psi\big)(x)$

Dynamics: $\frac{\partial}{\partial t}\Psi(x,t) = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t)$ [Time-dependant Schrödinger equation]

Special case of a more general framework – ideas mentioned in part A but will go into much greater depth in this course.

Postulates of Quantum Theory (see 3.1-3.3 in Weinberg, 1.1 in 2017 Notes)

P1 Quantum States

States correspond to rays in a complex Hilbert space.

A cx. Hilbert space $\mathcal{H}$ is a cx. vector space (finite or infinite dim'l) with Hermitian inner product.

$\forall \phi, \psi \in \mathcal{H} \ \forall \alpha \in \mathbb{C}$

→ $(\phi, \psi) = \overline{(\psi, \phi)}$

→ $(\phi, \alpha\psi) = \alpha(\phi, \psi)$

→ $(\alpha\phi, \psi) = \bar{\alpha}(\phi, \psi)$

convention that 2nd entry is linear while first is conjugate linear is standard in physics, but opposite of usual convention in mathematics.

Technical conditions:

→ $\mathcal{H}$ must be complete (Cauchy sequences converge)

→ $\mathcal{H}$ must admit a denumerable orthonormal basis

Both of these only relevant in ∞-dim'l case.

A ray is a set of vectors in $\mathcal{H}$ that differ by (non-zero) complex multiplication, so

$$\psi \sim \lambda\psi \quad \forall \lambda \in \mathbb{C}^*$$

Taking quotient by this equivalence relation gives projective Hilbert space $\mathbb{P}(\mathcal{H}) = \mathcal{H}/\sim$. This is the true space of physically inequivalent states.

Postulates of Quantum Mechanics (cont'd)

$\boxed{\text{P2}}$ Observables

Physical observables of a quantum system with space of states $\mathbb{P}(\mathcal{H})$ are represented by Hermitian/Self-Adjoint linear operators on $\mathcal{H}$.

Given linear operator $A : \mathcal{H} \to \mathcal{H}$, define the adjoint operator $A^* : \mathcal{H} \to \mathcal{H}$ by requiring that

$$(A\phi, \psi) = (\phi, A^*\psi) \quad \forall \phi, \psi \in \mathcal{H}$$

Existence of A^* requires proof in ∞-dim'l case, which requires more fine print. Won't belabor this yet.

Useful facts about self-adjoint operators on Hilbert spaces

- Real eigenvalues*
- Orthonormal basis of eigenvectors*

  * follow from spectral theorem, but more subtleties in ∞-dim. case.
  Will see "physics" way of dealing with this in lecture 2. Justification requires more functional analysis.

- If observables A, B commute $\left([A,B] = AB - BA = 0 \right)$, can find basis of simultaneous eigenvectors.

  (Again subject to ∞-dim'l fine print.)

Postulates of Quantum Mechanics (cont'd)

$\boxed{P3}$ Measurement

When measuring an observable A, the only possible results are the eigenvalues $\{a_n\}$ of A. Let $\{\psi_n\}$ be the corresponding (complete set of) eigenvectors.

The probability that measuring A on a state ψ will yield a_n is given by the norm-square of the transition amplitude from ψ to ψ_n:

$$\text{Prob}(a_n|\psi) = |(\psi_n, \psi)|^2$$

This is known as Born's rule. Without assuming normalization,

$$\text{Prob}(a_n|\psi) = \frac{|(\psi_n,\psi)|^2}{(\psi_n,\psi_n)(\psi,\psi)}$$

if a_n is a degenerate eigenvalue, choose $\{\psi_{n,i};\ i \in I\}$ orthonormal basis for eigenspace. Then

$$\text{Prob}(a_n|\psi) = \sum_{i\in I} \frac{|(\psi_{n,i},\psi)|^2}{(\psi_{n,i},\psi_{n,i})(\psi,\psi)}$$

This defines a probability distribution for the outcome of measuring A. Can define statistical measures of this distribution...

- Expectation value $\quad \mathbb{E}_\psi(A) \equiv \langle A \rangle_\psi = \dfrac{(\psi, A\psi)}{(\psi,\psi)}$

- Dispersion
$$\Delta_\psi(A) = \left(\langle (A - \langle A\rangle_\psi)^2\rangle_\psi\right)^{1/2}$$
$$= \left(\langle A^2\rangle_\psi - \langle A\rangle_\psi^2\right)^{1/2}$$

These agree with usual notions of expected value and standard deviation; will be easy to see using notation introduced in Lecture 2.

Postulates of Quantum Mechanics (cont'd)

$\boxed{\text{P4}}$ Collapse of the Wave Function

Immediately after a measurement of the observable A yields the value a_n, the state of the system will be the corresponding eigenstate ψ_n.

This ensures that performing a second measurement immediately after the first will yield the same result.

If a_n is a degenerate eigenvalue w/ orthonormal basis $\psi_{n,i}$ $i=1,\ldots,K$ for its eigenspace, then the collapsed state is given by

$$\sum_{i=1}^{K} (\psi_{n,i}, \psi)\, \psi_{n,i} \qquad \text{(not normalized)}$$

This is the result of applying the orthogonal projection operator onto the degenerate eigenspace.

Collapse of the wave function is the subject of a huge amount of discussion by people interested in interpretational/philosophical aspects of quantum theory. I will have nothing more to say, but see e.g. Weinberg 3.7 for some comments.

Postulates of Quantum Mechanics (cont'd)

P5 Time Evolution

Time development of a state Ψ governed by the Hamiltonian observable H via the (generalized) time-dependent Schrödinger equation:

$$i\hbar \frac{d}{dt}\Psi = H\Psi$$

H can depend explicitly on time, though in many standard examples it is time independant.

> **Remark:** the normalization of a state is preserved under time evolution
>
> $$\frac{d}{dt}(\Psi,\Psi) = \left(\frac{d\Psi}{dt},\Psi\right) + \left(\Psi,\frac{d\Psi}{dt}\right)$$
> $$= \left(\frac{H\Psi}{i\hbar},\Psi\right) + \left(\Psi,\frac{H\Psi}{i\hbar}\right)$$
> $$= i\hbar(H\Psi,H) - i\hbar(\Psi,H\Psi) = 0$$
>
> this (plus linearity) implies that $\frac{d}{dt}(\phi,\Psi)=0 \quad \forall \phi,\Psi \in \mathcal{H}$.

Let $U(t,t_0)$ be the operator sending the state $\Psi(t_0)$ to its time development $\Psi(t)$. We have:

$$\big(\Psi(t),\Phi(t)\big) = \big(U(t,t_0)\Psi(t_0),\, U(t,t_0)\Phi(t_0)\big)$$
$$= \big(\Psi(t_0),\, U(t,t_0)^* U(t,t_0)\Phi(t_0)\big)$$
$$= \big(\Psi(t_0),\Phi(t_0)\big) \quad \text{by time-independance of overlaps}$$

So $U(t,t_0)^* = U(t,t_0)^{-1}$, i.e., $U(t,t_0)$ is a unitary operator on $\mathcal{H}$.*

*∼ ∞-dim'l subtleties

> Another perspective is to take unitary time evolution as the postulate. The Hamiltonian then arises as the infinitesimal limit of the unitary operator
>
> $$U(t+dt,t_0) = U(t,t_0) + \frac{1}{i\hbar}H\,dt \quad \text{with } H \text{ self-adjoint}$$
>
> will see more like this later.

Example of Formalism: Wave mechanics

$$\left.\begin{array}{l}\mathcal{H} = \{\text{cx. square-integrable wave functions of (say) } \mathbb{R}\} \\ (\phi(x), \psi(x)) = \int_{-\infty}^{\infty} dx\, \overline{\phi}(x)\psi(x)\,dx\end{array}\right]\ L^2(\mathbb{R})$$, ∞-dim$^{\underline{l}}$ Hilbert space

Observables: position & momentum (and functions thereof)

position $\longleftrightarrow$ $X : \psi(x) \longmapsto x\psi(x)$

momentum $\longleftrightarrow$ $P : \psi(x) \longmapsto \frac{\hbar}{i}\frac{d}{dx}\psi(x)$

Note $[X, P] = i\hbar \mathbb{1}$

identity operator

Hamiltonian normally $H = \frac{P^2}{2m} + V(X)$; find basis of "energy eigenstates" $\{\psi_n\}$ obeying $H\psi_n = E_n\psi_n$.

$$\Longrightarrow \quad U(t, t_0)\psi_n = e^{\frac{-iE_n(t-t_0)}{\hbar}}\psi_n$$

$$\Longrightarrow \quad U(t, t_0)^*\psi_n = e^{\frac{iE_n(t-t_0)}{\hbar}}\psi_n = U(t, t_0)^{-1}$$

Example of Formalism: Two state system (qubit)

$\mathcal{H} \cong \mathbb{C}^2$ (so space of states $\cong \mathbb{P}(\mathbb{C}^2) \cong \mathbb{CP}^1$)

$v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$

$w = \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}$

$(v, w) = \bar{v}_1 w_1 + \bar{v}_2 w_2 = (\bar{v})^T w$

Observables $A \in \{2\times 2 \text{ cx. matrices}\}$

$A = A^{\dagger}$ Hermitian conjugation (transpose conjugate)

Basis for these matrices: $\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{1}_{2\times 2}$

$$\left.\begin{aligned} \sigma_1 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \sigma_2 &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ \sigma_3 &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{aligned}\right\} \text{Pauli spin matrices}$$

Observe
$$\left.\begin{aligned} [\sigma_1, \sigma_2] &= i\sigma_3 \\ [\sigma_2, \sigma_3] &= i\sigma_1 \\ [\sigma_3, \sigma_1] &= i\sigma \end{aligned}\right\} [\sigma_i, \sigma_j] = \sum_k \epsilon_{ijk}\sigma_k$$

Can only measure one of these simultaneously

Suppose $H = a\sigma_0 + b\sigma_3$ (can always find a basis where this is true)

$$U(t, t_0) = e^{-\frac{i}{\hbar}(t-t_0)H} = \begin{pmatrix} e^{-\frac{i}{\hbar}(a+b)(t-t_0)} & 0 \\ 0 & e^{-\frac{i}{\hbar}(a-b)(t-t_0)} \end{pmatrix}$$

Plans for Lecture 2

- Introduce & develop Dirac's "bra-ket" notation, which renders various constructions transparent.
- Will discuss "continuum states", which are unphysical but formally useful objects to deal w/ ∞-dim'l phenomena.
- Use these to analyze propagation of free particles, build intuition.

See Sakurai 1.2–1.7 for bra-ket formalism including continuum states.

See Weinberg 3.2 for continuum states.

(Or see first ~80 pages of Dirac!)

See Sakurai 2.6 for propagators.