Mathematical Quantum Mechanics

Abbreviated lecture notes

1. Historical introduction

1. **Planck-Einstein relation:** photons corresponding to electromagnetic radiation of frequency ν have energy $E = h\nu$, where $h \simeq 6.63 \times 10^{-34}$ $\mathrm{J\,s}$ is **Planck's constant**.
2. **De Broglie's hypothesis:** every particle with linear momentum p has an associated wave with wavelength $\lambda = \frac{h}{p}$.
3. **Bohr's atom:** an electron orbiting a proton in a hydrogen atom can only occupy orbits with radii of the form $r = n^2 a_0$, where $n \in \mathbb{N}$ and

   $$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2} \simeq 0.53\mathring{A}$$

   is **Bohr's radius** (here ε_0 is the vacuum electric permittivity, $\hbar = \frac{h}{2\pi}$ is the reduced Planck constant, and m and $-e$ are the electron's mass and charge). Correspondingly, the electron can only have energies of the form

   $$E = -\frac{e^2}{8\pi\varepsilon_0 a_0 n^2}, \qquad n \in \mathbb{N},$$

   and whenever it jumps between allowed orbits it emits or absorbs a photon with frequency corresponding to the energy difference.
4. **Schrödinger's equation** for a particle of mass m moving under the influence of a potential energy V:

   $$i\hbar\frac{\partial\psi}{\partial t}(\mathbf{x},t) = -\frac{\hbar^2}{2m}\Delta\psi(\mathbf{x},t) + V(\mathbf{x},t)\psi(\mathbf{x},t).$$

2. Free Schrödinger PDE

1. **Free Schrödinger's equation** for a particle of mass m:

$$i\hbar\frac{\partial\psi}{\partial t}(\mathbf{x},t) = -\frac{\hbar^2}{2m}\Delta\psi(\mathbf{x},t).$$

2. Conserved quantity:

$$\|\psi(\cdot,t)\|^2_{L^2(\mathbb{R}^3)} = \int_{\mathbb{R}^3}|\psi(\mathbf{x},t)|^2d^3x.$$

3. **Born interpretation:** $|\psi(\cdot,t)|^2$ is the probability density for the position of the particle at time t. In particular, $\|\psi(\cdot,t)\|_{L^2(\mathbb{R}^3)} = 1 \Rightarrow \psi(\cdot,t)\in L^2(\mathbb{R}^3)$.
4. The solution of the 1-dimensional free Schrödinger equation,

$$i\hbar\frac{\partial\psi}{\partial t}(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}(x,t),$$

with initial data $\psi_0\in L^2(\mathbb{R})$, is

$$\psi(x,t) = \mathcal{F}^{-1}\left[e^{-\frac{i\hbar k^2 t}{2m}}\hat{\psi}_0(k)\right],$$

where $\mathcal{F}: L^2(\mathbb{R})\to L^2(\mathbb{R})$ is the Fourier transform and $\hat{\psi}_0 = \mathcal{F}[\psi_0]$.
5. The average of the probability distribution $|\psi(\cdot,t)|^2$ is

$$\langle X\rangle = \int_{\mathbb{R}} x\,|\psi(x,t)|^2dx = \langle X\rangle_0 + \frac{\langle P\rangle}{m}t,$$

where

$$\langle X\rangle_0 = \int_{\mathbb{R}} x\,|\psi_0(x)|^2dx$$

and

$$\langle P\rangle = \int_{\mathbb{R}}\hbar k\,|\hat{\psi}_0(k)|^2dk.$$

6. Defining, on appropriate subspaces of $L^2(\mathbb{R})$, the operators X and P given by

$$(Xf)(x) = xf(x) \qquad \text{and} \qquad (Pf)(x) = \frac{\hbar}{i}\frac{df}{dx}(x),$$

we have

$$\langle X\rangle = \langle\psi, X\psi\rangle_{L^2(\mathbb{R})} \qquad \text{and} \qquad \langle P\rangle = \langle\psi, P\psi\rangle_{L^2(\mathbb{R})}.$$

7. The variance of the probability distribution $|\psi(\cdot,t)|^2$ is

$$\langle X^2\rangle - \langle X\rangle^2 = \int_{\mathbb{R}} x^2|\psi(x,t)|^2dx - \langle X\rangle^2 = \frac{\langle P^2\rangle - \langle P\rangle^2}{m^2}t^2 + b_1t + b_0,$$

where b_1 and b_0 are constants and

$$\langle P^2\rangle = \int_{\mathbb{R}}\hbar^2k^2\,|\hat{\psi}_0(k)|^2dk = \langle\psi, P^2\psi\rangle_{L^2(\mathbb{R})}.$$

8. The 1-dimensional free Schrödinger equation can be written as

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi,$$

where

$$H = \frac{P^2}{2m}.$$

9. We have, for f, g on appropriate subspaces of $L^2(\mathbb{R})$,

$$\langle f, Xg\rangle_{L^2(\mathbb{R})} = \langle Xf, g\rangle_{L^2(\mathbb{R})},$$

$$\langle f, Pg\rangle_{L^2(\mathbb{R})} = \langle Pf, g\rangle_{L^2(\mathbb{R})},$$

$$\langle f, Hg\rangle_{L^2(\mathbb{R})} = \langle Hf, g\rangle_{L^2(\mathbb{R})}.$$

10. **Heisenberg's commutation relation**: $[X, P] \equiv XP - PX = i\hbar I$ on an appropriate subspace of $L^2(\mathbb{R})$.

3. The axioms of quantum mechanics

1. A **Hilbert space** is a complex vector space H with an inner product which is **complete**. We will assume H to be **separable**, that is, to have a countable dense subset.
2. A linear operator $A : H \to H$ is said to be **bounded** if there exists a constant $C > 0$ such that $\|Av\| \leq C\|v\|$ for all $v \in H$.
3. A linear operator is bounded if and only if it is continuous.
4. The set of eigenvalues of a bounded operator is bounded.
5. Riesz Representation Theorem: If $\alpha : H \to \mathbb{C}$ is a bounded linear functional then there exists a unique vector $u \in H$ such that $\alpha(v) = \langle u, v\rangle$ for all $v \in H$.
6. If $A : H \to H$ is a bounded linear operator then its **adjoint** is the bounded linear operator $A^* : H \to H$ is defined as follows: A^*u is the unique vector representing the bounded linear functional $v \mapsto \langle u, Av\rangle$ (so that $\langle u, Av\rangle = \langle A^*u, v\rangle$).
7. If $A : H \to H$ is a linear operator such that $\langle u, Av\rangle = \langle Au, v\rangle$ for all $u, v \in H$ then L is bounded.
8. An **unbounded operator** is a linear map $A : D(A) \to H$, where $D(A) \subset H$ is a dense subspace. The **adjoint** of an unbounded operator $A : D(A) \to H$ is the unbounded operator $A^* : D(A^*) \to H$ defined by choosing $D(A^*) = \{u \in H : v \mapsto \langle u, Av\rangle \text{ is bounded}\}$ and taking A^*u to be the unique vector representing the bounded linear functional $v \mapsto \langle u, Av\rangle$ (so that $\langle u, Av\rangle = \langle A^*u, v\rangle$).
9. An unbounded operator $A : D(A) \to H$ is called:
   (i) **symmetric** if $\langle u, Av\rangle = \langle Au, v\rangle$ for all $u, v \in D(A)$;