EE201/MSE207 Lecture 7

General formalism (textbook: Chapter 3 + Appendix)

In 1920s there were two quantum mechanics: "Matrix Mechanics" (developed by Heisenberg, Born, and Jordan) and Wave Mechanics (by Schrödinger); later their equivalence was proven. What we considered so far was close to "wave mechanics". Now we consider a more general point of view, which unifies both approaches.

So far we used $\Psi(x,t)$: wavefunction as a function of x, and we used operations with $\Psi(x)$: multiplication, integration, derivatives, etc.

Now a new language: wavefunction is a vector $|\Psi\rangle$ in some abstract linear space (called Hilbert space), while physical quantities ("observables": position, momentum, energy, etc.) correspond to linear operators acting on vectors (we have already started to use this language).

Why do we need this new language?

1) In some cases using $\Psi(x)$ is not possible (spin, etc.),
2) sometimes more convenient to work in a different basis (*k*-space, etc.),
3) deeper understanding of the formalism,
4) other people use it, and we need to understand them.

Most natural discussion of vectors and linear operators: linear algebra (this is why Matrix Mechanics).

Linear algebra (30-minute course)

Usually finite number of dimensions; however, almost the same with infinite number.
Functions $f(x)$ are similar to vectors – check at each step.

Vectors $|\alpha\rangle$, $|\beta\rangle$, … (this notation is widely used in QM; “ket-vector”),
scalars a, b, … (complex numbers)

We can add vectors, $|\alpha\rangle + |\beta\rangle$, and multiply them by numbers, $a\,|\alpha\rangle$
(the same with functions $f(x)$: add functions and multiply by numbers)

Components in a basis

$$|\alpha\rangle = a_1|e_1\rangle + a_2|e_2\rangle + \;\ldots$$

(similar for functions, bases can be different: δ-functions, sin/cos, etc.)

Inner product (dot-product, scalar product) $\langle\alpha|\beta\rangle$ (bracket → bra+ket)

In an orthonormal basis, if

$$|\alpha\rangle = a_1|e_1\rangle + a_2|e_2\rangle + \;\ldots$$

$$|\beta\rangle = b_1|e_1\rangle + b_2|e_2\rangle + \;\ldots$$

then

$$\langle\alpha|\beta\rangle = a_1^* b_1 + a_2^* b_2 + \;\ldots$$

Inner product properties

$|\alpha\rangle = a_1|e_1\rangle + a_2|e_2\rangle + \ ...$

$|\beta\rangle = b_1|e_1\rangle + b_2|e_2\rangle + \ ...$

$\langle\alpha|\beta\rangle = a_1^* b_1 + a_2^* b_2 + \ ...$

1) $\langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^*$

2) $\langle\alpha|\alpha\rangle \geq 0$ (real number)

} actually, definition

norm of a vector $\|\alpha\| = \sqrt{\langle\alpha|\alpha\rangle}$

3) $|\langle\alpha|\beta\rangle|^2 \leq \langle\alpha|\alpha\rangle\,\langle\beta|\beta\rangle$

(theorem, Schwartz inequality)

Proof (not important) $\quad |\gamma\rangle \equiv |\beta\rangle - \dfrac{\langle\alpha|\beta\rangle}{\langle\alpha|\alpha\rangle}\,|\alpha\rangle$

$$0 \leq \langle\gamma|\gamma\rangle = \langle\beta|\beta\rangle + \frac{|\langle\alpha|\beta\rangle|^2}{\langle\alpha|\alpha\rangle} - \frac{|\langle\alpha|\beta\rangle|^2}{\langle\alpha|\alpha\rangle} - \frac{|\langle\alpha|\beta\rangle|^2}{\langle\alpha|\alpha\rangle} = \langle\beta|\beta\rangle - \frac{|\langle\alpha|\beta\rangle|^2}{\langle\alpha|\alpha\rangle}$$

Orthogonal vectors: $\langle\beta|\alpha\rangle = 0$

Orthonormal basis $|e_i\rangle$: $\langle e_i|e_j\rangle = \delta_{ij}$

Components in orthonormal basis

$|\alpha\rangle = a_1|e_1\rangle + a_2|e_2\rangle + \ ... \quad \Rightarrow \quad a_n = \langle e_n|\alpha\rangle$

Normalization $\quad \|\alpha\| = 1 \quad \Leftrightarrow \quad \sum_i |a_i|^2 = 1$

Digression: Comparison with functions $f(x)$

Practically the same inner product

$$\langle f(x) \mid g(x) \rangle = \int_{-\infty}^{\infty} f^*(x)\, g(x)\, dx$$

But we need square-integrable functions.
Set of such functions forms a Hilbert space.

Wavefunctions $\Psi(x)$ are vectors in a Hilbert space.

Definition of a Hilbert space (not important): a complete inner product space
(i.e. a linear space with defined inner product and without "holes":
limit of a sequence of vectors belonging to this space also belongs to it).

Linear operators (matrices)

(these languages are the same)

Some definitions

1) Hermitian conjugate (adjoint) $\langle\alpha\big|(\hat{T}\beta)\rangle = \langle(\hat{T}^{\dagger}\alpha)|\beta\rangle$

for matrices $T^{\dagger} = \tilde{T}^{*}$ (transpose + complex conjugate)

2) Hermitian operator (self-adjoint) $\hat{T}^{\dagger} = \hat{T}$

(all observables in QM are Hermitian operators)

anti-Hermitian operator (skew-Hermitian) $\hat{T}^{\dagger} = -\hat{T}$

3) Inverse operator (matrix) $\hat{T}^{-1}\hat{T} = \hat{T}\ \hat{T}^{-1} = \hat{1}$

4) Unitary operator $\hat{T}^{\dagger} = \hat{T}^{-1}$ (evolution in QM)

5) Commutator $[\hat{S}, \hat{T}] = \hat{S}\hat{T} - \hat{T}\hat{S}$

Some theorems

1) $\left(\hat{S}\hat{T}\right)^{-1} = \hat{T}^{-1}\hat{S}^{-1}$

2) $\left(\hat{S}\hat{T}\right)^{\dagger} = \hat{T}^{\dagger}\hat{S}^{\dagger}$

(sometimes with hats, sometimes without)

Determinant and trace (for matrices)

$$\det(ST) = \det(S)\det(T)$$

$$\mathrm{Tr}(T) = \sum_i T_{ii}\,; \quad \mathrm{Tr}(ST) = \mathrm{Tr}(TS); \quad \mathrm{Tr}(STQ) = \mathrm{Tr}(QTS)$$

Operators in a different basis

$$\underbrace{|e_j\rangle}_{\text{old basis}} = \sum_i \underline{\underline{S_{ij}}}\, \underbrace{|f_i\rangle}_{\text{new basis}}, \quad \text{then} \quad T^{(f)} = S\,T^{(e)}S^{-1}$$

Eigenvectors and eigenvalues

$$\hat{T}\,|\alpha\rangle = \lambda\,|\alpha\rangle$$

$|\alpha\rangle$: eigenvector (in QM often called "eigenfuction" or "eigenstate"); λ: eigenvalue

(Why interesting? Because $\hat{T}$ is diagonal in the basis of eigenvectors)

Theorem

If $\hat{T}$ is Hermitian, then:

1) eigenvalues are real,
2) eigenvectors (with different eigenvalues) are orthogonal to each other,
3) eigenvectors span the whole space.

Formalism of Quantum Mechanics in a new language
(so far still consider one particle in 1D)

6 postulates (the number of postulates may be different)

1) State of the particle is described by a normalized vector $|\Psi\rangle$ in the Hilbert space.

2) Physical quantities ("observables", like position, momentum, energy, etc.) $Q(x, p, t)$ are represented by Hermitian operators $\hat{Q}(\hat{x}, \hat{p}, t)$.

3) Evolution (Schrödinger equation): $$i\hbar \frac{d|\Psi\rangle}{dt} = \hat{H}|\Psi\rangle$$

where $\hat{H}$ is the operator of energy (Hamiltonian)

4) Average ("expectation") value of observable Q for state $|\Psi\rangle$ is

$$\langle Q \rangle = \langle \Psi \big| \hat{Q}\Psi \rangle$$

usual notation $\langle \Psi \big| \hat{Q} \big| \Psi \rangle$ (Hermitian $\hat{Q}$)

Remark 1. We can calculate variance as $\langle Q^2 \rangle - \langle Q \rangle^2$ using the same rule for Q^2.

Remark 2. If $|\Psi\rangle$ is an eigenstate of $\hat{Q}$, then variance is zero $\Rightarrow$ determinate value, determinate state.

5) If we measure observable Q, the possible measurement results are only eigenvalues of $\hat{Q}$. (Remark: values in between are impossible!)

For particle in state $|\Psi\rangle$, the probability to obtain result λ is

$$P_\lambda = |\langle f_\lambda|\Psi\rangle|^2$$

where $|f_\lambda\rangle$ is normalized eigenvector ("eigenstate"), corresponding to eigenvalue λ, i.e. $\hat{Q}|f_\lambda\rangle = \lambda|f_\lambda\rangle$.

6) After measurement result λ is obtained, the state abruptly changes ("collapses") into $|f_\lambda\rangle$.

Remarks to postulate 5 (and 6)

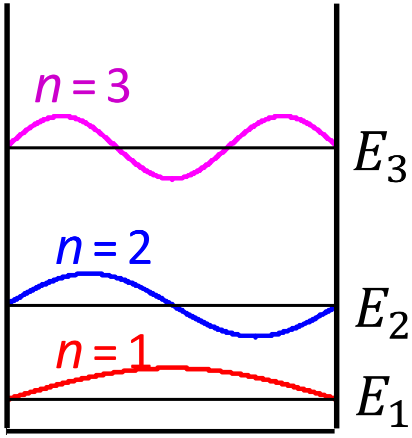
a) Actually, this is correct only if $\hat{Q}$ has discrete spectrum (discrete eigenvalues). For continuous spectrum of $\hat{Q}$, we need probability density $\mathcal{P}(\lambda)$: $\mathcal{P}(\lambda)\, d\lambda = |\langle f_\lambda|\Psi\rangle|^2\, d\lambda$, where the eigenvectors should be normalized as $\langle f_\lambda|f_\mu\rangle = \delta(\lambda-\mu)$. (A subtlety with postulate 6: accuracy of measurement.)

b) If spectrum of $\hat{Q}$ is degenerate (several orthogonal $|f\rangle$ for the same λ), then use sum of corresponding probabilities; collapse: projection onto eigenspace.

In particular, the new language allows us to consider Ψ-function not only in x-space, but also on equal footing in p-space [$\Phi(p, t)$ instead of $\Psi(x, t)$], energy space, etc.
This is called different representations (we will discuss it later).

Next: examples about measurement

Example 1



Infinite square well, $\psi = \sqrt{\frac{1}{3}}\psi_1 + \sqrt{\frac{2}{3}}\psi_2$, measure energy

We will get either E_1 or E_2, with probabilities

$P(E_1) = \frac{1}{3}$, then $\psi \to \psi_1$; $P(E_2) = \frac{2}{3}$, then $\psi \to \psi_2$.

Average result: $\frac{1}{3} E_1 + \frac{2}{3} E_2$

Compare: $$\langle E \rangle = \langle \psi | \hat{H}\psi \rangle = \left\langle \sqrt{1/3}\, \psi_1 + \sqrt{2/3}\, \psi_2 \middle| \hat{H} \left(\sqrt{1/3}\, \psi_1 + \sqrt{2/3}\, \psi_2 \right) \right\rangle =$$

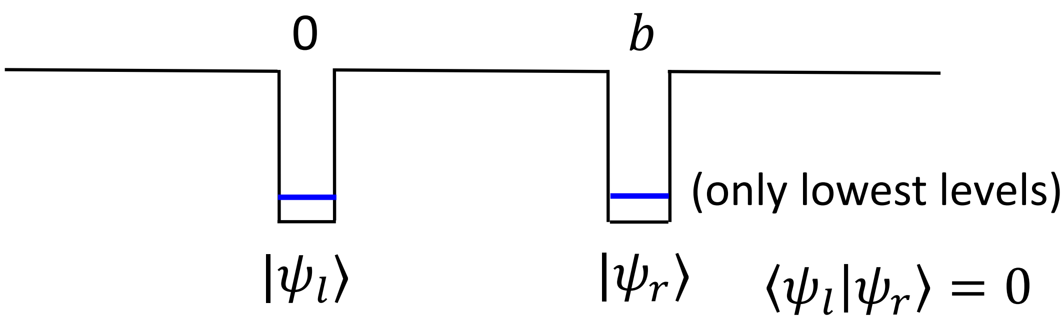
$$= \left\langle \sqrt{1/3}\, \psi_1 + \sqrt{2/3}\, \psi_2 \middle| E_1 \sqrt{1/3}\, \psi_1 + E_2 \sqrt{2/3}\, \psi_2 \right\rangle = \frac{1}{3} E_1 + \frac{2}{3} E_2$$ OK, the same

Energy is not well-defined (not determinate). "What is the energy?" – not a proper question. Proper questions: "What is the average energy?" or "What can we get if measure energy?" However, after measurement – well-determinate energy, if measure again, will get the same result (determinate state of energy). Determinate states are eigenstates of the operator.

Example 1b

Similar, but $\psi = \sqrt{\frac{1}{3}}\psi_1 + i\sqrt{\frac{2}{3}}\psi_2$. The same answers.

Example 2



$\langle \psi_l | \psi_r \rangle = 0$

Qubit: one electron in two semiconductor quantum dots

$$\psi = \sqrt{\frac{2}{5}}\psi_l + i\sqrt{\frac{3}{5}}\psi_r$$

Measure position (with accuracy, not resolving position within the dots).

Get result 0 with probability $2/5$

Get result b with probability $3/5$

After measurement the state is collapsed either to $|\psi_l\rangle$ or to $|\psi_r\rangle$

Measurement destroys the quantum state → idea of quantum cryptography.