FY2045 Quantum Mechanics I

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Week 3

General formulation of QM

Dirac's $\langle \mathrm{bra} | \mathrm{ket} \rangle$ notation

State vector

A quantum mechanical state of a system is described by a state vector

$$|\psi\rangle$$

in a complex, linear vector space $\mathcal{H}$ — Hilbert space.

Dual vector

For each vector $|a\rangle$ we define the dual vector $\langle a|$ in the dual space $\mathcal{H}^*$,

$$|a\rangle \xleftrightarrow{\text{dual}} \langle a|,$$

so that we can define the scalar (inner) product of vectors $|a\rangle$ and $|b\rangle$

$$\langle a||b\rangle \equiv \langle a|b\rangle \in \mathbb{C},$$

with $\langle a|b\rangle = \langle b|a\rangle^*$.

Example

Probability amplitude for particle arriving at point x:

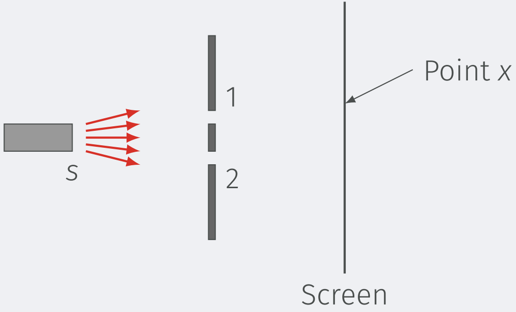
$$\langle \text{Particle arrives at } x | \text{particle leaves } s \rangle$$

or simply

$$\langle x|s \rangle.$$

Can go through either slit 1 or 2:

$$\langle x|s \rangle = \langle x|1 \rangle \langle 1|s \rangle + \langle x|2 \rangle \langle 2|s \rangle.$$



Based on Ch. 3 of Vol. III in the Feynman Lectures.

Interpretation

The wavefunction is probability amplitude of finding state $|\psi\rangle$ at point x:

$$\psi(x) = \langle x|\psi\rangle.$$

The momentum wavefunction is probability amplitude of finding state $|\psi\rangle$ with momentum p:

$$\phi(p) = \langle p|\psi\rangle.$$

The probability amplitude of finding state $|\psi\rangle$ with energy E_n:

$$\langle\psi_n|\psi\rangle.$$

Completeness

n linearly independent vectors $|1\rangle, |2\rangle, |3\rangle, \ldots$ span $\mathcal{H}$ if $\forall\ |\psi\rangle \in \mathcal{H}$ we have

$$|\psi\rangle = \sum_{k=1}^{n} c_n |k\rangle.$$

Assuming orthonormality $\langle m|k\rangle = \delta_{mk}$,

$$\Rightarrow \ |\psi\rangle = \sum_k \langle k|\psi\rangle |k\rangle = \sum_k |k\rangle\langle k||\psi\rangle,$$

meaning we have the completeness relation

$$\sum_k |k\rangle\langle k| = 1.$$

Operators

An operator $\hat{A}$ applied to a vector $|a\rangle \in \mathcal{H}$ results in a new vector $|c\rangle \in \mathcal{H}$,

$$\hat{A}|a\rangle = |c\rangle.$$

Adjoint or Hermitian conjugate of operator:

$$\langle a|\hat{A}^\dagger|b\rangle = \langle b|\hat{A}|a\rangle^* \quad \forall\ |a\rangle, |b\rangle \in \mathcal{H}.$$

meaning that we have the dual vector

$$\hat{A}|a\rangle \xleftrightarrow{\text{dual}} \langle a|\hat{A}^\dagger.$$

Properties

$$(\hat{A}^\dagger)^\dagger = \hat{A},$$
$$(\alpha\hat{A})^\dagger = \alpha^*\hat{A}^\dagger,$$
$$(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger.$$

For a Hermitian (self-adjoint) matrix

$$\hat{A}^\dagger = \hat{A}.$$

Eigenvectors and eigenvalues

The eigenvectors $|\alpha\rangle$ and eigenvalues λ_α of an operator $\hat{A}$ are defined by

$$\hat{A}|\alpha\rangle = \lambda_\alpha|\alpha\rangle.$$

The set of eigenvectors $\{|\alpha\rangle\}$ corresponding to physical quantities is assumed to be complete — they form a basis set that span $\mathcal{H}$.

The eigenvectors of a **Hermitian** operator are **real**.

Examples

Energy:

$$\hat{H}|n\rangle = E_n|n\rangle.$$

Position:

$$\hat{x}|x'\rangle = x'|x'\rangle.$$

Momentum:

$$\hat{p}|p'\rangle = p'|p'\rangle.$$

Postulates in general formulation

Postulate A

Each observable quantity F corresponds to a linear, Hermitian operator $\hat{F}$ in Hilbert space. The operators for a generalized coordinate q_n and generalized momentum p_n fulfill

$$[\hat{q}_n, \hat{p}_n] = \hat{q}_n\hat{p}_n - \hat{p}_n\hat{q}_n = i\hbar.$$

Postulate B

Each state of a physical system is represented by a state vector $|\Psi, t\rangle$ in Hilbert space with length 1, $\langle\Psi, t|\Psi t\rangle = 1$. The vector fulfills the time-dependent SE

$$i\hbar\frac{\partial}{\partial t}|\Psi, t\rangle = \hat{H}|\Psi, t\rangle.$$

Postulate C

The expectation value of an observable F, given the state $|\Psi\rangle$, is

$$\langle F\rangle = \langle\Psi|\hat{F}|\Psi\rangle.$$

Postulate D

The measurement of an observable F yields one of the eigenvalues f_n of the corresponding operator $\hat{F}$.

Position representation

Eigenvectors $|x'\rangle$ of operator $\hat{x}$:

$$\hat{x}|x'\rangle = x'|x'\rangle,$$

with eigenvalue x' taking continuous values.
$|x'\rangle$ is δ-function normalized

$$\langle x''|x'\rangle = \delta(x'' - x'),$$

with completeness relation

$$\int dx'|x'\rangle\langle x'| = \mathbb{1}.$$

Position space wavefunction

Given a state vector $|\psi\rangle$, the position space wavefunction is given by

$$\psi(x') = \langle x'|\psi\rangle,$$

the projection of $|\psi\rangle$ on the position basis vector $|x'\rangle$.

Operators

For an operator $\hat{F}$, which is a function of $\hat{x}$ and $\hat{p}$, we have

$$\langle x''|F(\hat{p},\hat{x})|x'\rangle = F\left(\frac{\hbar}{i}\frac{\partial}{\partial x''}, x''\right)\delta(x'' - x').$$

Momentum formulation

Eigenvectors $|p\rangle$ of operator $\hat{p}$:

$$\hat{p}|p\rangle = p|p\rangle,$$

with eigenvalue p taking continuous values.
$|p\rangle$ is δ-function normalized

$$\langle p'|p\rangle = \delta(p' - p),$$

with completeness relation

$$\int dp|p\rangle\langle p| = \mathbb{1}.$$

Momentum space wavefunction

Given a state vector $|\psi\rangle$, the momentum space wavefunction is given by

$$\phi(p) = \langle p|\psi\rangle,$$

the projection of $|\psi\rangle$ on the momentum basis vector $|p\rangle$.

Relation between $|p\rangle$ and $|x\rangle$

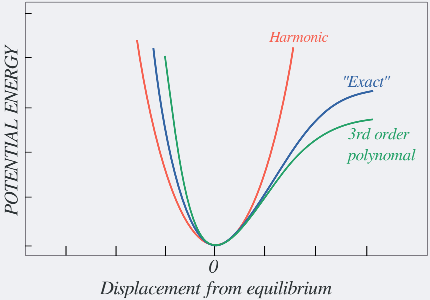
Projecting $|p\rangle$ on the position basis $|x\rangle$, we get the momentum eigenfunctions in the position formulation,

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}.$$

Harmonic oscillator

Why the harmonic oscillator again?

"Because an arbitrary smooth potential can usually be approximated as a harmonic potential at the vicinity of a stable equilibrium point, it is one of the most important model systems in quantum mechanics."[1]



[1]Wikipedia — Quantum Harmonic Oscillator.

Ladder operators

Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2.$$

Introduce **ladder operators**

$$a = \frac{1}{\sqrt{2\hbar m\omega}}(i\hat{p} + m\omega\hat{q}),$$
$$a^\dagger = \frac{1}{\sqrt{2\hbar m\omega}}(-i\hat{p} + m\omega\hat{q}),$$

with $(a)^\dagger = a^\dagger$ — they are not Hermitian.

Commutation relations for a and $a^\dagger$

Since $\hat{q}$ and $\hat{p}$ do not commute ($\hat{q}\hat{p} - \hat{p}\hat{q} = i\hbar$), neither do a and $a^\dagger$:

$$a^\dagger a = \frac{\hat{H}}{\hbar\omega} - \frac{1}{2},$$
$$aa^\dagger = \frac{\hat{H}}{\hbar\omega} + \frac{1}{2},$$

meaning we have

$$[a, a^\dagger] = aa^\dagger - a^\dagger a = 1.$$

Number operator

Define the **number operator** $\hat{N} = a^\dagger a$, and write

$$\hat{H} = \hbar\omega\left(\hat{N} + \frac{1}{2}\right).$$

Eigenvectors of $\hat{N}$ will also be eigenvectors of $\hat{H}$:

$$\hat{N}|n\rangle = n|n\rangle \quad \Rightarrow \quad \hat{H}|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle \equiv E_n|n\rangle.$$

with orthonormalized eigenvectors $|n\rangle$.

Commutation relations for $\hat{N}$

Commutators of $\hat{N}$ with a and $a^\dagger$:

$$[\hat{N}, a] = -a,$$
$$[\hat{N}, a^\dagger] = a^\dagger.$$

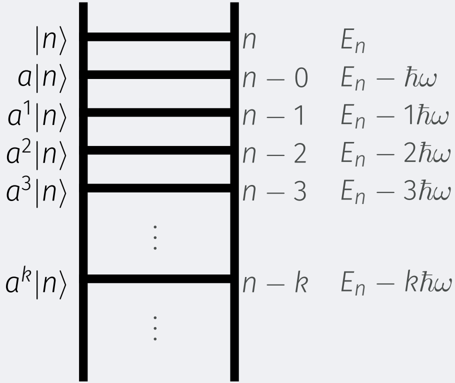
Energy spectrum

What do the ladder operators do?

$$\hat{H}a|n\rangle = (E_n - \hbar\omega)a|n\rangle.$$

If $a|n\rangle \neq 0$, $a|n\rangle$ is an eigenvector of $\hat{H}$ with eigenvalue $E_n - \hbar\omega$. a is a **lowering** or **annihilation operator**.

Can repeat this argument: If $a^k|n\rangle \neq 0$, $a^k|n\rangle$ is an eigenvector of $\hat{H}$ with eigenvalue $E_n - k\hbar\omega$.



Energy spectrum

The norm of a vector must be positive:

$$0 \leq ||a|n\rangle||^2 = \langle n|a^\dagger a|n\rangle = \langle n|\hat{N}|n\rangle = n\langle n|n\rangle = n.$$

We must require

$$a|0\rangle = 0.$$

Hence $|0\rangle$ is the ground state with energy $E_0 = \frac{1}{2}\hbar\omega$, and we get the energy eigenvalues

$$\underline{E_n = \hbar\omega\left(n + \frac{1}{2}\right), \text{ with } n = 0, 1, 2...}$$