Formalism, Three Dimensions, Linear Algebra

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Contents

1 Formalism

1.1 Hilbert Space

Contructs:

- state: wave function
- observables: operators
- vectors: defining conditions
- linear transformation: the operators act on vectors
- linear algebra: the natural language of Quantum Mechanics

Properties:

1. wave function live in
2. complete inner product space
3. squre-integrable

Definition 1 *Inner product of two function*

$$\langle f|g\rangle \equiv \int_a^b f(x)^* g(x)\mathrm{d}x$$

Discussion:

- Schwarz inequality:

$$\left|\int_a^b f(x)^* g(x)\mathrm{d}x\right| \le \sqrt{\int_a^b |f(x)|^2\mathrm{d}x \int_a^b |g(x)|^2\mathrm{d}x}$$

- $\langle g|f\rangle = \langle f|g\rangle^*$
- normalized $\langle f|f\rangle = 1$
- orthonormal $\langle f_m|f_n = \delta_{mn}\rangle$
- complete and orthonormal $f(x) = \sum_{n=1}^{\infty} c_n f_n(x), c_n = \langle f_n|f\rangle$

1.2 Observables

1.2.1 Hermitian Operators

Definition 2 *Hermitian Operators*

$$\langle f|\hat{Q}g\rangle = \langle \hat{Q}f|g\rangle \qquad \text{for all } f(x) \text{ and } g(x)$$

Discussion:

- Observables are represented by hermitian operators
- hermitian conjugate $\hat{Q}^\dagger = \hat{Q}$

1.2.2 Determinate State

$$\sigma^2 = \langle (Q - \langle Q \rangle)^2 \rangle = \left\langle (\Psi | (\hat{Q} - q)^2 \Psi \right\rangle = \left\langle ((\hat{Q} - q)\Psi | (\hat{Q} - q)\Psi \right\rangle = 0$$
$$\Downarrow$$
$$\hat{Q}\Psi = q\Psi$$

Discussion:

- This is eigenvalue equation for $\hat{Q}$
- Ψ if an eigenfuction of $\hat{Q}$, and q is the corresponding eigenvalue
- Determinate state of Q are eigenfuction of $\hat{Q}$
- spectrum: the collection of all the eigenvalues of an operator
- degenerate: linearly independent eigenfuctions share the same eigenvalue

1.3 Eigenfuctions of a Hermitain Operator

1.3.1 Discrete Spectra

- the eigenvalues are separated from another
- the eigenfuctions lie in Hilbert space and constitute physically realizable states

Properties of normalizable eigenfuctions of a hermitian operator:

1. Their eigenvalues are *real*
2. Eigenfuctions belonging to distinct eigenvalues are *orthognal*

1.3.2 Continuous Spectra

- the eigenvalues fill out an entire range
- the eigenfuctions are not normalizable and do not represent possible wave functions

The eigenfuctions and eigenvalues of the momentum operator (on the interval $(-\infty < x < \infty)$:

$$-i\hbar \frac{\mathrm{d}}{\mathrm{d}x} f_p(x) = p f_p(x) \quad \Rightarrow \quad f_p(x) = A e^{ipx/\hbar}$$
$$\downarrow$$
$$\int_{-\infty}^{\infty} f_{p'}^*(x) f_p(x) \mathrm{d}x = |A|^2 \int_{-\infty}^{\infty} e^{i(p-p')/\hbar} \mathrm{d}x = |A|^2 2\pi\hbar\delta(p - p')$$
$$\Downarrow$$
$$f_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$$

- Dirac orthonormality: $\langle f_{p'} | f_p \rangle = \delta(p - p')$

- Complete:

$$f(x) = \int_{-\infty}^{\infty} c(p) f_p(x) dp = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} c(p) e^{ipx/\hbar} \mathrm{d}p$$

$$\langle f_{p'} | f \rangle = \int_{-\infty}^{\infty} c(p) \langle f_{p'} | f \rangle \, \mathrm{d}p = \int_{-\infty}^{\infty} c(p) \delta(p - p') \mathrm{d}p = c(p')$$

The eigenfuctions and eigenvalues of the positoin operator:

$$\hat{x} g_y(x) = g_y x \quad \Rightarrow \quad g_y(x) = A\delta(x - y)$$
$$\downarrow$$
$$\int_{-\infty}^{\infty} g_{y'}^* g_y(x) \mathrm{d}x = |A|^2 \int_{-\infty}^{\infty} \delta(x - y') \delta(x - y) \mathrm{d}x = |A|^2 \delta(y - y')$$
$$\Downarrow$$
$$g_y(x) = \delta(x - y)$$

1.4 Generalized Statistical Interpretation

Observable: $Q(x, p)$
State: $\Psi(x, t)$
One of eigenvalues: $\hat{Q}(x - i\hbar d/dx)$
The probablility of getting eigenvalues(orthonormal):

1. Discrete spectrum

$$|c_n|^2, \qquad \text{where} \quad c_n = \langle f_n | \Psi \rangle \, |$$

Complete:

$$\Psi(x, t) = \sum_n c_n(t) f_n(x)$$

$$c_n(t) = \langle f_n | \Psi \rangle = \int f_n(x)^* \Psi(x, t) \mathrm{d}x$$

$$\sum_n |c_n|^2 = 1$$

The expectation value of Q:

$$\langle Q \rangle = \left\langle \Psi | \hat{Q} \Psi \right\rangle = \sum_n q_n |c_n|^2$$

2. Continuous spectrum

$$|c(z)|^2 \mathrm{d}z, \qquad \text{where} \quad c(z) = \langle f_z | \Psi \rangle \, |$$

For positoin measurements:

$$c(y) = \langle g_y | \Psi \rangle = \int_{-\infty}^{\infty} \delta(x - y) \Psi(x, t) \mathrm{d}x = \Psi(y, t)$$

For momentum measurements:

$$c(p) = \langle f_p | \Psi \rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \Psi(x, t) \mathrm{d}x$$

Fourier transformation:

$$
\Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \Psi(x,t) \mathrm{d}x
$$
$$
\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{ipx/\hbar} \Phi(p,t) \mathrm{d}p
$$

Expectation:

$$
\langle Q(x,p,t) \rangle = \begin{cases} \int \Psi^* \hat{Q} \left(x, -i\hbar\frac{\partial}{\partial x}, t\right) \Psi \, \mathrm{d}x, & \text{in position space} \\ \int \Phi^* \hat{Q} \left(i\hbar\frac{\partial}{\partial p}, p, t\right) \Phi \, \mathrm{d}p, & \text{in momentum space} \end{cases}
$$

1.5 The Uncertainty Principle

1.5.1 Proof of the Generalized Uncertainty Principle

$$
f \equiv \left(\hat{A} - \langle A \rangle\right) \Psi \quad \rightarrow \quad \sigma_A^2 \sigma_B^2 = \langle f|f \rangle \langle f|g \rangle \geq |\langle f|g \rangle|^2
$$

$$
|z|^2 \geq [\mathrm{Im}(z)]^2 = \left[\frac{1}{2i}(z - z^*)\right]^2 \quad \Rightarrow \quad \sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i}\left[\langle f|g \rangle - \langle g|f \rangle\right]\right)^2
$$

$$
\langle f|g \rangle = \langle \hat{A}|\hat{B} \rangle - \langle A \rangle \langle B \rangle
$$
$$
\Downarrow
$$
$$
\boxed{\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i}\left\langle \left[\hat{A}, \hat{B}\right] \right\rangle\right)^2}
$$

1.5.2 The Minimum-Uncertainty Wave Packet

$$
g(x) = iaf(x), \qquad \text{where } a \text{ is real}
$$
$$
\Rightarrow \left(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x} - \langle p \rangle\right) \Psi = ia(x - \langle x \rangle)\Psi
$$
$$
\Rightarrow \Psi(x) = Ae^{-a(x-\langle x \rangle)^2/2\hbar} e^{i\langle p \rangle/\hbar}
$$

1.5.3 The Energy-Time Uncertainty Principle

$$
\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\langle Q \rangle = \frac{\mathrm{d}}{\mathrm{d}t}\left\langle \Psi|\hat{Q}\Psi \right\rangle \\ i\hbar\frac{\partial \Psi}{\partial t} = \hat{H}\Psi, \quad \text{where} \qquad H = \frac{p^2}{2m} + V \end{cases} \qquad \Rightarrow
$$

$$
\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\langle Q \rangle = \frac{i}{\hbar}\left\langle \left[\hat{H}, \hat{Q}\right] \right\rangle + \left\langle \frac{\partial \hat{Q}}{\partial t} \right\rangle}
$$

Assume that Q does not depend explicity on t:

$$
\sigma_H \sigma_Q^2 \geq \left(\frac{1}{2i}\left\langle \hat{H}, \hat{Q} \right\rangle\right)^2 = \left(\frac{\hbar}{2}\right)^2 \left(\frac{d\langle Q \rangle}{dt}\right)^2
$$

$$
\begin{array}{c} \Delta E \equiv \sigma_H \\ \Delta t \equiv \dfrac{\sigma_Q}{|d\langle Q \rangle/dt|} \end{array} \qquad \Rightarrow \qquad \Delta\, t \Delta E \geq \frac{\hbar}{2}
$$

1.6 Vectors and Operators

1.6.1 Bases in Hillbert Space

$$
\begin{aligned}
\Psi(x,t) &= \langle x|\mathcal{S}(t)\rangle \\
\Phi(p,t) &= \langle p|\mathcal{S}(t)\rangle \\
c_n(t) &= \langle n|\mathcal{S}(t)\rangle
\end{aligned}
$$

$$
\begin{aligned}
|\mathcal{S}(t)\rangle \to &\int \Psi(y,t)\delta(x-y)\,\mathrm{d}y = \int \Phi(p,t)\frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}\,\mathrm{d}p \\
&\sum c_n e^{-iE_nt/\hbar}\psi_n(x)
\end{aligned}
$$

Schrodinger equation:

$$
\begin{aligned}
i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\mathcal{S}(t)\rangle = \hat{H}|\mathcal{S}(t)\rangle, &\qquad \text{Time-dependent} \\
\hat{H}|s\rangle = E|s\rangle, &\qquad \text{Time-independent}
\end{aligned}
$$

Particular example of vectors:

$$
\begin{aligned}
\hat{x}\,(\text{the position operator}) &\to \begin{cases} x & \text{(in positoin space)} \\ i\hbar\partial/\partial p & \text{(in momentum space)} \end{cases} \\
\hat{p}\,(\text{the momentum operator}) &\to \begin{cases} -i\hbar\partial/\partial x & \text{(in positoin space)} \\ p & \text{(in momentum space)} \end{cases}
\end{aligned}
$$

1.6.2 Dirac Notation

bra: $\langle\alpha|$
ket: $|\beta\rangle$
Orthonormal basis (complete):

- Discrete

$$
\langle e_m|e_n\rangle = \delta_{mn} \qquad \to \qquad \sum_n |e_n\rangle\langle e_n| = 1
$$

- Continuous

$$
\langle e_z|e_{z'}\rangle = \delta(z-z') \qquad \to \qquad \int |e_z\rangle\langle e_{z'}|\,\mathrm{d}z = 1
$$

Baker-Campbell-Hausdrff formula:

$$
e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{-\hat{C}/2}, \qquad \text{where} \qquad \hat{C} = \left[\hat{A},\hat{B}\right]
$$

1.6.3 Changing Bases in Dirac Notation

$$
\begin{aligned}
\text{the positoin eigenstats : } |x\rangle \qquad & 1 = \int dx\, |x\rangle\langle x| \\
& \to \quad |\mathcal{S}(t)\rangle = \int dx\, |x\rangle\langle x|\mathcal{S}(t)\rangle \equiv \int \Psi(x,t)\, |x\rangle\, \mathrm{d}x \\
\text{the momentum eigenstats : } |p\rangle \qquad & 1 = \int dp\, |p\rangle\langle p| \\
& \to \quad |\mathcal{S}(t)\rangle = \int dp\, |p\rangle\langle p|\mathcal{S}(t)\rangle \equiv \int \Phi(p,t)\, |p\rangle\, \mathrm{d}p \\
\text{the energy eigenstats : } |n\rangle \qquad & 1 = \sum |n\rangle\langle n| \\
& \to \quad |\mathcal{S}(t)\rangle = \sum_n |n\rangle\langle n|\mathcal{S}(t)\rangle \equiv \sum c_n(t)\, |n\rangle
\end{aligned}
$$

Operators act on kets

$$
\begin{aligned}
\langle x|\hat{x}|\mathcal{S}(t)\rangle &= \text{action of position operator in } x \text{ basis} = x\Psi(x,t) \\
\langle p|\hat{x}|\mathcal{S}(t)\rangle &= \text{action of position operator in } p \text{ basis} = i\hbar\frac{\partial \Phi}{\partial p}
\end{aligned}
$$

Proof:

$$
\langle p|\hat{x}|\mathcal{S}(t)\rangle = \left\langle p \middle| \hat{x} \int dx|x\rangle\langle x| \middle| \mathcal{S}(t) \right\rangle = \int \langle p|x|x\rangle\langle x|\mathcal{S}(t)\rangle dx = i\hbar\frac{\partial}{\partial p}\langle p|\mathcal{S}(t)\rangle
$$

1.7 Wave Functions in Position and Momentum Space(Addition)

NOTE: x,$f(x)$,p are operators, different form all above

1.7.1 Position-Space Wave Function

The base ket used are the position kets satisfying

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

A physical state can be expanded in terms of x'

$$
\begin{aligned}
|\alpha\rangle &= \int dx'|x'\rangle\langle x'|\alpha\rangle \\
|\langle x'|\alpha\rangle|^2 dx' & \qquad \text{probablility} \\
\langle x'|\alpha\rangle \equiv \psi_\alpha(x') & \qquad \text{wave function}
\end{aligned}
$$

Using the completness of $|x'\rangle$, we have

$$
\langle\beta|\alpha\rangle = \int dx'\, \langle\beta|x'\rangle\, \langle x'|\alpha\rangle = \int dx' \psi_\beta^*(x')\psi_\alpha^*(x')
$$

the probablility amplitude for state $|\alpha\rangle$ to be found in state $|\beta\rangle$

$f(x)$ is a function of x

$$
\begin{aligned}
\langle x'|f(x)|x''\rangle &= (\langle x'|) \cdot (f(x'')|x'') = f(x')\delta(x'-x'') \\
\langle\beta|f(x)|\alpha\rangle &= \int dx' \int dx''\, \langle\beta|x'\rangle\, \langle x'|f(x)|x''\rangle\, \langle x''|\alpha\rangle \\
&= \int dx'\, \psi_\beta^*(x')f(x')\psi_\alpha(x')
\end{aligned}
$$

1.7.2 Momentum Operator in the Position Basis

$$p|\alpha\rangle = \int dx'|x'\rangle \left(-i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\right)$$
$$\Rightarrow \langle x'|p|\alpha\rangle = -i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle$$

Properties:

$$\langle x'|p^n|x''\rangle = (-i\hbar)^n\frac{\partial^n}{\partial x'^n}\delta(x'-x'')$$
$$\langle\beta|p^n|\alpha\rangle = \int dx'\,\psi_\beta^*(x')\left((-i\hbar)^n\frac{\partial^n}{\partial x'^n}\right)\psi_\alpha(x')$$

1.7.3 Momentum-Space Wave Function

The base eigenkets in the p-basis specify

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

Same way as $|x'\rangle$

$$|\alpha\rangle = \int dp'|p'\rangle\langle p'|\alpha\rangle$$
$$|\langle p'|\alpha\rangle|^2dp' \qquad \text{probablility}$$
$$\langle p'|\alpha\rangle \equiv \phi_\alpha(p') \qquad \text{momentum-space wave function}$$

Transformation function from x to p: $\langle x'|p'\rangle$

$$\langle x'|p|p'\rangle = -i\hbar\frac{\partial}{\partial x'}\langle x'|p'\rangle = p'\langle x'|p'\rangle$$
$$\Rightarrow \langle x'|p'\rangle = N\exp\left(\frac{ip'x'}{\hbar}\right)$$

Discussion:

- the probablility amplitude for $|p'\rangle$ specified by p' to be found at positoin x'
- the wave function for $|p'\rangle$, referred to as the momentum eigenfuction (still in the x-space)
- Nomalizetion: $N = \frac{1}{\sqrt{2\pi\hbar}}$

Rewrite:

$$\begin{cases}\langle x'|\alpha\rangle = \int dp'\langle x'|p'\rangle\langle p'|\alpha\rangle \\ \langle p'|\alpha\rangle = \int dx'\langle p'|x'\rangle\langle x'|\alpha\rangle\end{cases} \quad\Leftrightarrow\quad \begin{aligned}\psi_\alpha(x') &= \left[\frac{1}{\sqrt{2\pi\hbar}}\right]\int dp'\exp\left(\frac{ip'x'}{\hbar}\right)\phi_\alpha(p') \\ \phi_\alpha(p') &= \left[\frac{1}{\sqrt{2\pi\hbar}}\right]\int dx'\exp\left(\frac{-ip'x'}{\hbar}\right)\psi_\alpha(x')\end{aligned}$$

2 Quantum Mechanics in Three Dimensions

2.1 The Schroding Equation

2.1.1 Cartesian Coordinates

Laplacian

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Schroding's Equation

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi$$

Canonical commutation relations

$$[r_i, p_j] = i\hbar\delta_{ij} \qquad [r_i, r_j] = [p_i, p_j] = 0$$

Three-Dimensional of Ehrenfest's theorem

$$\frac{\mathrm{d}}{\mathrm{d}r}\langle \mathbf{r} \rangle = \frac{1}{m}\langle \mathbf{p} \rangle, \qquad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}t}\langle \mathbf{p} \rangle = \langle -\nabla V \rangle$$

Heisenberg's uncertainty principle

$$\sigma_{x,y,z}\sigma_{p_x,p_y,p_z} \geq \hbar/2$$

2.1.2 Spherical Coordinates

Time-independent Schrodinger equation

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial \psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial \psi}{\partial \theta}\right) + \frac{1}{r^2\sin\theta^2}\left(\frac{\partial^2\psi}{\partial \phi^2}\right)\right] + V\psi = E\psi$$

$$\Downarrow$$

$$\psi(r,\theta,\phi) = R(r)Y(\theta,\phi) \qquad \Rightarrow \qquad \begin{aligned} &\frac{1}{R}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right) - \frac{2mr^2}{\hbar^2}[V(r) - E] = \ell(\ell+1) \\ &\frac{1}{Y}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right\} = -\ell(\ell+1) \end{aligned}$$

2.1.3 The Angular Equation

$$Y(\theta,\phi) = \Theta(\theta)\Phi(\phi) \qquad \Rightarrow \qquad \begin{aligned} &\frac{1}{\Theta}\left[\sin\theta\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right)\right] + \ell(\ell+1)\sin^2\theta = m^2 \\ &\frac{1}{\Phi}\frac{\mathrm{d}^2\Theta}{\mathrm{d}\theta^2} = -m^2 \end{aligned}$$

Spherical harmonics

$$\boxed{Y_\ell^m(\theta,\phi) = \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}e^{im\phi}P_\ell^m(\cos\theta)}$$

- $\ell = 0, 1, 2\cdots$
- $m = -\ell, -\ell+1, \cdots, -1, 0, 1, \cdots, \ell-1, \ell$

2.1.4 The Radial Equation

$$u(r) \equiv rR(r)$$

$$\Rightarrow \qquad -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2 u}{\mathrm{d}r^2} + \left[V + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right]u = Eu$$

Effective potential

$$V_{\text{eff}} = V + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}$$

2.2 The Hydrogen Atom

$$V(r) = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$$

2.2.1 The Radial Wave Function

2.2.2 The Spectrum of Hydrogen

2.3 Angular Momentum

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}$$

2.3.1 Eigenvalues

Fundamental commutation relations for angular momentum

$$[L_x, L_y] = i\hbar L_z \qquad [L^2, \mathbf{L}] = 0$$

2.3.2 Eigenfunctions

2.4 Spin

2.4.1 Spin 1/2

2.4.2 Electron in a Magnetic Field

2.5 Electromagnetic Interactions

2.5.1 Minimal Coupling

2.5.2 The Aharonov-Bohm Effect

3 Linear Algebra

3.1 Vectors

(1) Addition
(2) Scalar Multiplication

$$|\alpha\rangle \leftrightarrow (a_1, a_2, \cdot, a_n)$$

3.2 Inner Product

1. $\langle\beta|\alpha\rangle = a_1^* b_a + \cdots + a_n^* b_n$

2. $\langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^*$

3. $||\alpha|| \equiv \sqrt{\langle\alpha|\alpha\rangle}$

4. orthonormal set: $\langle\alpha_i|\alpha_j\rangle = \delta_{jk}$

5. Schwarz inequality: $|\langle\beta|\alpha\rangle|^2 \leq \langle\alpha|\alpha\rangle\langle\beta|\beta\rangle$

3.3 Matrix