Lecture Notes

Quantum Mechanics

PHYS 501

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Fundamental Concepts

1.1. The Stern–Gerlach Experiment

1.1.1. Description of the Experiment

The Stern–Gerlach experiment (Frankfurt, 1922) provides direct evidence for the quantization of angular momentum: an initially collimated beam of neutral atoms splits into spatially separated components corresponding to discrete eigenvalues of a spin component along the direction of a nonuniform magnetic field.

Experimental Setup

A beam of neutral silver (Ag) atoms from a thermal oven is collimated and sent through a region with a strong magnetic field gradient, then collected on a distant glass plate. The beamline can be summarized schematically as

$$\text{Oven} \longrightarrow \text{Slit} \longrightarrow \text{Nonuniform magnetic field} \longrightarrow \text{Glass plate.} \tag{1.1}$$

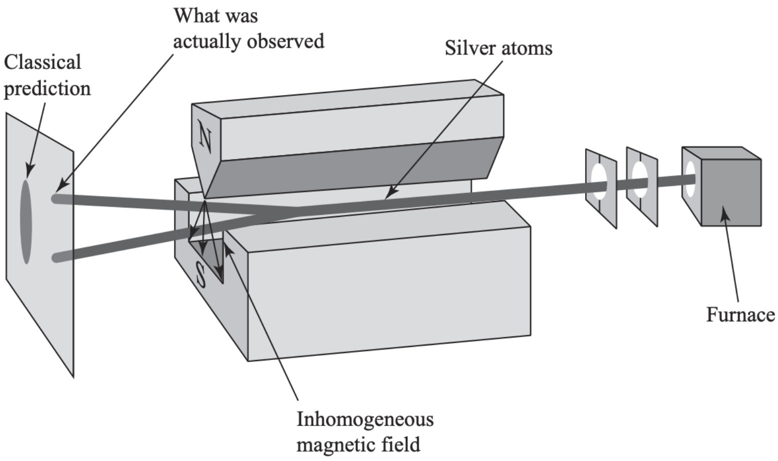

Figure 1.1: Schematic of the Stern–Gerlach experiment. Image taken from Ref. [?].

Classically, one expects a continuous smear on the plate from a continuum of magnetic moment orientations. Experimentally, two well-resolved deposits appear, symmetric about the undeflected position, evidencing two discrete values of the relevant magnetic moment component.

Properties of Silver Atoms

Silver has electron configuration [Kr] $4d^{10}5s^1$. The closed $4d^{10}$ subshell contributes no net orbital or spin moment ($L = 0,\ S = 0$). The single $5s$ electron has $l = 0$ and $s = \frac{1}{2}$, so the atom's magnetic properties are dominated by the unpaired electron's spin.

Magnetic Moment of the Unpaired Electron

Let $e > 0$ be the elementary charge, $q_e = -e$ the electron charge, and m_e the electron mass. The spin magnetic moment operator is

$$\boldsymbol{\mu}_e = -g_e\,\mu_B\,\frac{\mathbf{S}}{\hbar} = \gamma_e\,\mathbf{S}, \qquad \mu_B := \frac{e\hbar}{2m_e}, \qquad \gamma_e := g_e\left(-\frac{e}{2m_e}\right), \tag{1.2}$$

where $g_e \approx 2.0023$ is the electron g-factor and $\mathbf{S}$ is the spin operator. For spin-$\frac{1}{2}$, the eigenvalues of S_z are $m_s\hbar$ with $m_s \in \{-\frac{1}{2}, \frac{1}{2}\}$, hence

$$\mu_z = -g_e\,\mu_B\,\frac{S_z}{\hbar} \implies \mu_z^{(\pm)} = \mp\frac{g_e}{2}\,\mu_B \quad \text{for } m_s = \pm\tfrac{1}{2}. \tag{1.3}$$

Reminder – Bohr vs. nuclear magneton

$\mu_B = \dfrac{e\hbar}{2m_e}$, $\mu_N = \dfrac{e\hbar}{2m_p}$, $\dfrac{\mu_N}{\mu_B} = \dfrac{m_e}{m_p} \approx \dfrac{1}{1836}$. Thus electronic moments $\sim 10^3$ times exceed typical nuclear moments; nuclear contributions to deflection are negligible.

Magnetic Force on a Current-Carrying Wire; Potential Energy

For a wire segment carrying steady current I in a magnetic field $\mathbf{B}$, the magnetic force is

$$\mathrm{d}\mathbf{F}_B = I\,\mathrm{d}\boldsymbol{\ell} \times \mathbf{B}, \tag{1.4}$$

so that for a straight segment of vector length $\mathbf{L}$,

$$\mathbf{F}_B = I\,\mathbf{L} \times \mathbf{B}. \tag{1.5}$$

For a planar closed loop of area vector $\mathbf{A} = A\,\hat{\mathbf{n}}$, the magnetic dipole moment is

$$\boldsymbol{\mu}_{\text{loop}} = I\,\mathbf{A}. \tag{1.6}$$

Example 1.1 – Torque on a rectangular loop gives $\boldsymbol{\tau}$

Consider a rectangle of sides a, b in uniform $\mathbf{B}$. From (1.5), opposite sides experience equal and opposite forces (net force zero) but produce a net torque

$$\boldsymbol{\tau} = Iab\,\hat{\mathbf{n}} \times \mathbf{B} = (I\,\mathbf{A}) \times \mathbf{B} = \boldsymbol{\mu}_{\text{loop}} \times \mathbf{B}. \tag{1.7}$$

By partitioning a general planar loop into rectangles and passing to a limit, the result extends to any planar loop.

Let θ be the angle between $\boldsymbol{\mu}$ and $\mathbf{B}$. Using $\tau = \|\boldsymbol{\mu} \times \mathbf{B}\| = \mu B \sin\theta$ and $U'(\theta) = -\tau$, integration gives the potential energy

$$U(\theta) = -\boldsymbol{\mu} \cdot \mathbf{B}, \tag{1.8}$$

up to an additive constant chosen so that $U = 0$ at $\theta = \frac{\pi}{2}$.

Force on a Magnetic Dipole in a Nonuniform Field

In a slowly varying static field, the force on a (field-independent) dipole $\boldsymbol{\mu}$ is the negative gradient of (1.8):

$$\mathbf{F} = -\nabla U = \nabla\big(\boldsymbol{\mu} \cdot \mathbf{B}\big). \tag{1.9}$$

Reminder – Product rule for a dot product

$\nabla(\mathbf{a}\cdot\mathbf{b}) = (\mathbf{a}\cdot\nabla)\mathbf{b} + (\mathbf{b}\cdot\nabla)\mathbf{a} + \mathbf{a}\times(\nabla\times\mathbf{b}) + \mathbf{b}\times(\nabla\times\mathbf{a})$.

If $\boldsymbol{\mu}$ is spatially constant, (1.1.1) gives

$$\mathbf{F} \;=\; (\boldsymbol{\mu}\cdot\nabla)\,\mathbf{B} \;+\; \boldsymbol{\mu}\times(\nabla\times\mathbf{B}). \tag{1.10}$$

In the field region traversed by the neutral atomic beam, $\nabla\times\mathbf{B}\approx\mathbf{0}$ (no free currents), so

$$\mathbf{F} \;\approx\; (\boldsymbol{\mu}\cdot\nabla)\,\mathbf{B}. \tag{1.11}$$

If the field is predominantly along $\hat{\mathbf{z}}$ and varies mainly with z, then

$$F_z \;\approx\; \mu_z\,\frac{\partial B_z}{\partial z}. \tag{1.12}$$

Combining (1.3) with (1.12) yields the two quantum-allowed longitudinal forces

$$F_z^{(\pm)} \;=\; \mp\,\frac{g_e}{2}\,\mu_B\,\frac{\partial B_z}{\partial z}, \tag{1.13}$$

so that $\operatorname{sign}(F_z) = \operatorname{sign}(\mu_z)\,\operatorname{sign}(\partial_z B_z)$. The direction of deflection is therefore fixed by the sign of the field gradient and the eigenvalue of S_z.

Remark 1.1 – Why neutrality matters

The silver atoms are electrically neutral; no Lorentz force $q\,\mathbf{v}\times\mathbf{B}$ acts on their centers of mass. The observed splitting arises from the dipole force (1.9) due to the field gradient.

1.1.2. Sequential Stern–Gerlach Experiments

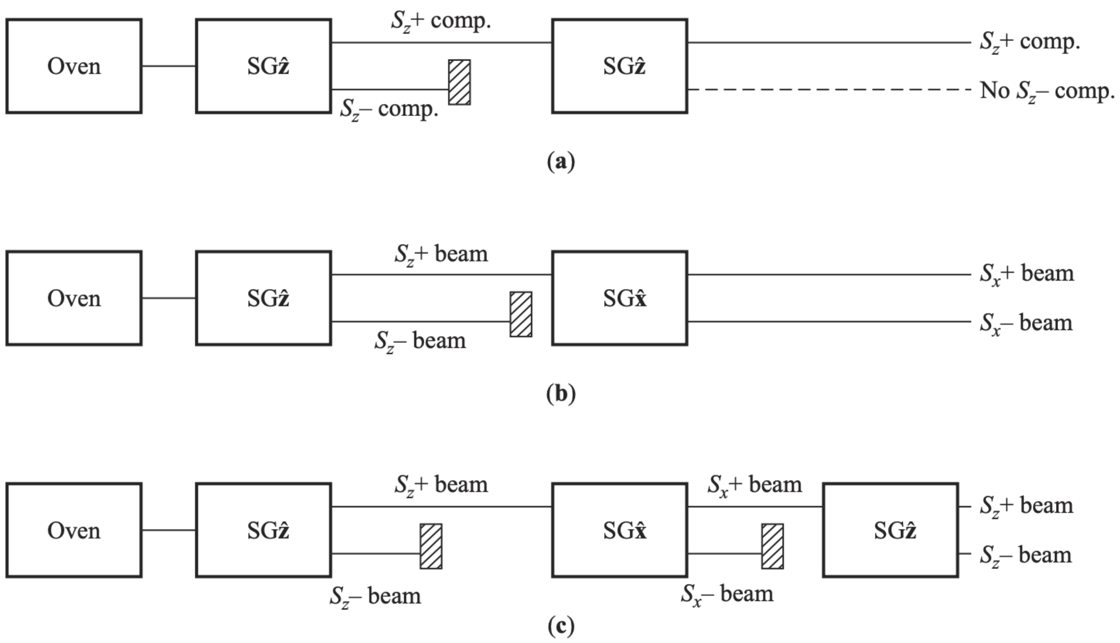

Figure 1.2: Sequential Stern–Gerlach experiments. Image taken from Ref. [?].

We denote by $\mathrm{SG}^{\hat{\mathbf{n}}}$ a Stern–Gerlach apparatus oriented along the unit vector $\hat{\mathbf{n}}$. Measurement of spin along $\hat{\mathbf{n}}$ is represented by the self-adjoint operator $S_{\hat{\mathbf{n}}} = \frac{\hbar}{2}\,\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}$, where $\boldsymbol{\sigma} = (\sigma_x,\sigma_y,\sigma_z)$ are the Pauli matrices.

Projective measurement of spin-$\frac{1}{2}$ For a unit vector $\hat{\mathbf{n}}$, the spectral projectors of $S_{\hat{\mathbf{n}}}$ are

$$P_{\hat{\mathbf{n}}}^{\pm} \;=\; |{+\hat{\mathbf{n}}}\rangle\langle{+\hat{\mathbf{n}}}|\,,\quad |{-\hat{\mathbf{n}}}\rangle\langle{-\hat{\mathbf{n}}}|\,,\qquad S_{\hat{\mathbf{n}}}\,|{\pm\hat{\mathbf{n}}}\rangle = \pm\tfrac{\hbar}{2}\,|{\pm\hat{\mathbf{n}}}\rangle\,. \tag{1.14}$$

Given an input state ρ (density operator), the probability of outcome $\pm$ is

$$\mathbb{P}_{\rho}\big(\pm\,;\,\hat{\mathbf{n}}\big) \;=\; \mathrm{tr}\big(P_{\hat{\mathbf{n}}}^{\pm}\rho\big)\,, \tag{1.15}$$

and the (normalized) post-measurement state conditioned on outcome $\pm$ is

$$\rho'_{\pm} \;=\; \frac{P_{\hat{\mathbf{n}}}^{\pm}\,\rho\,P_{\hat{\mathbf{n}}}^{\pm}}{\mathrm{tr}(P_{\hat{\mathbf{n}}}^{\pm}\rho)}. \tag{1.16}$$

Reminder – Pauli algebra

$$\{\sigma_i,\sigma_j\} = 2\delta_{ij}I, \qquad [\sigma_i,\sigma_j] = 2i\epsilon_{ijk}\sigma_k, \qquad S_i = \tfrac{\hbar}{2}\sigma_i.$$

First Stern–Gerlach Apparatus SG$^{\hat{\mathbf{z}}}$

An incident beam is sent through SG$^{\hat{\mathbf{z}}}$. The field gradient separates the beam into two spatially resolved components associated with the eigenstates $|{+z}\rangle$ and $|{-z}\rangle$ of S_z. Writing the projectors

$$P_z^{\pm} \;=\; |{\pm z}\rangle\langle{\pm z}|\,, \tag{1.17}$$

the two emergent beams correspond to outcomes $+\hbar/2$ and $-\hbar/2$ with probabilities given by (1.15).

Second Stern–Gerlach Apparatus SG$^{\hat{\mathbf{x}}}$

Select the $+\hat{\mathbf{z}}$ branch and feed it into SG$^{\hat{\mathbf{x}}}$. The $\hat{\mathbf{x}}$-eigenstates in the $\hat{\mathbf{z}}$-basis are

$$|{+x}\rangle \;=\; \frac{1}{\sqrt{2}}\big(|{+z}\rangle + |{-z}\rangle\big), \qquad |{-x}\rangle \;=\; \frac{1}{\sqrt{2}}\big(|{+z}\rangle - |{-z}\rangle\big). \tag{1.18}$$

Therefore, for the input $|{+z}\rangle$, the Born rule (1.15) gives

$$\mathbb{P}\big(+\,;\,\hat{\mathbf{x}}\,\big|\,+z\big) \;=\; |\langle{+x}|{+z}\rangle|^2 \;=\; \tfrac{1}{2}, \qquad \mathbb{P}\big(-\,;\,\hat{\mathbf{x}}\,\big|\,+z\big) \;=\; |\langle{-x}|{+z}\rangle|^2 \;=\; \tfrac{1}{2}. \tag{1.19}$$

Example 1.2 – Sequential run SG$^{\hat{\mathbf{z}}}$ $\to$ SG$^{\hat{\mathbf{x}}}$ $\to$ SG$^{\hat{\mathbf{z}}}$

Start with the pure state $\rho_0 = |{+z}\rangle\langle{+z}|$. After SG$^{\hat{\mathbf{x}}}$, choose the $+\hat{\mathbf{x}}$ exit (post-selection). The Lüders update (1.16) yields

$$\rho_1 \;=\; |{+x}\rangle\langle{+x}|\,. \tag{1.20}$$

Feeding ρ_1 into SG$^{\hat{\mathbf{z}}}$ gives

$$\mathbb{P}\big(+\,;\,\hat{\mathbf{z}}\,\big|\,+x\big) \;=\; |\langle{+z}|{+x}\rangle|^2 \;=\; \tfrac{1}{2}, \qquad \mathbb{P}\big(-\,;\,\hat{\mathbf{z}}\,\big|\,+x\big) \;=\; |\langle{-z}|{+x}\rangle|^2 \;=\; \tfrac{1}{2}, \tag{1.21}$$

so the final SG$^{\hat{\mathbf{z}}}$ again splits 1:1. The intermediate $\hat{\mathbf{x}}$-measurement erases prior $\hat{\mathbf{z}}$-information by projecting onto $|{\pm x}\rangle$.

Theorem 1.1 – Order dependence from noncommutativity

Let $A = \sum_a a\,P_a$ and $B = \sum_b b\,Q_b$ be two discrete observables with projectors P_a, Q_b. The joint statistics of the sequential measurements generally depend on order:

$$\mathrm{tr}\big(Q_bP_a\rho P_a\big) \;\neq\; \mathrm{tr}\big(P_aQ_b\rho Q_b\big) \quad \text{unless} \quad [P_a,Q_b]=0 \;\;\forall a,b. \tag{1.22}$$

For spin-$\frac{1}{2}$, $[S_x,S_z] = i\hbar S_y$ and $[\sigma_x,\sigma_z] = 2i\sigma_y$, therefore measurements of S_x and S_z disturb one another.

General rotations and half-angle rule

A spatial rotation about axis $\hat{\mathbf{u}}$ by angle ϕ acts on spinors via

$$U(\hat{\mathbf{u}}, \phi) \;=\; \exp\Big(-\,\tfrac{i}{2}\,\phi\,\hat{\mathbf{u}}\cdot\boldsymbol{\sigma}\Big), \tag{1.23}$$

so that if $\hat{\mathbf{n}}'$ is obtained by rotating $\hat{\mathbf{n}}$ by ϕ, then

$$|+\hat{\mathbf{n}}'\rangle \;=\; U(\hat{\mathbf{u}}, \phi)\,|+\hat{\mathbf{n}}\rangle \;=\; \cos\Big(\tfrac{\phi}{2}\Big)\,|+\hat{\mathbf{n}}\rangle - i\,\sin\Big(\tfrac{\phi}{2}\Big)\,(\hat{\mathbf{u}}\cdot\boldsymbol{\sigma})\,|+\hat{\mathbf{n}}\rangle\,. \tag{1.24}$$

Consequently,

$$\big|\,\langle+\hat{\mathbf{n}}'|+\hat{\mathbf{n}}\rangle\,\big|^2 \;=\; \cos^2\Big(\tfrac{\phi}{2}\Big), \qquad \big|\,\langle-\hat{\mathbf{n}}'|+\hat{\mathbf{n}}\rangle\,\big|^2 \;=\; \sin^2\Big(\tfrac{\phi}{2}\Big). \tag{1.25}$$

Remark 1.2 – Erasure of prior information

Equation (1.25) shows that a measurement along $\hat{\mathbf{n}}'$ with $\phi = \pi/2$ produces equal probabilities, consistent with (1.19) and (1.21). The disturbance disappears only when $[\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}, \hat{\mathbf{n}}'\cdot\boldsymbol{\sigma}] = 0$, i.e., $\hat{\mathbf{n}}' = \pm\hat{\mathbf{n}}$.

1.1.3. Analogy Between Light Polarization and Spin States

Polarization of Light

Unpolarized light has electric field directions uniformly distributed in the plane transverse to propagation. An ideal linear polarizer transmits the component along its transmission axis and blocks the orthogonal component. For an input linear polarization at angle θ to the polarizer axis, the transmitted intensity obeys Malus' law

$$I_{\text{out}} \;=\; I_{\text{in}} \cos^2\theta. \tag{1.26}$$

Sequential Polarizers

Let $\{\hat{\mathbf{x}}, \hat{\mathbf{y}}\}$ be transverse axes and define axes rotated by 45°:

$$\hat{\mathbf{x}}' \;=\; \tfrac{1}{\sqrt{2}}\big(\hat{\mathbf{x}} + \hat{\mathbf{y}}\big), \qquad \hat{\mathbf{y}}' \;=\; \tfrac{1}{\sqrt{2}}\big(-\hat{\mathbf{x}} + \hat{\mathbf{y}}\big). \tag{1.27}$$

Placing a second polarizer at 45° relative to the first transmits a fraction $\cos^2 45° = \frac{1}{2}$ of the intensity.

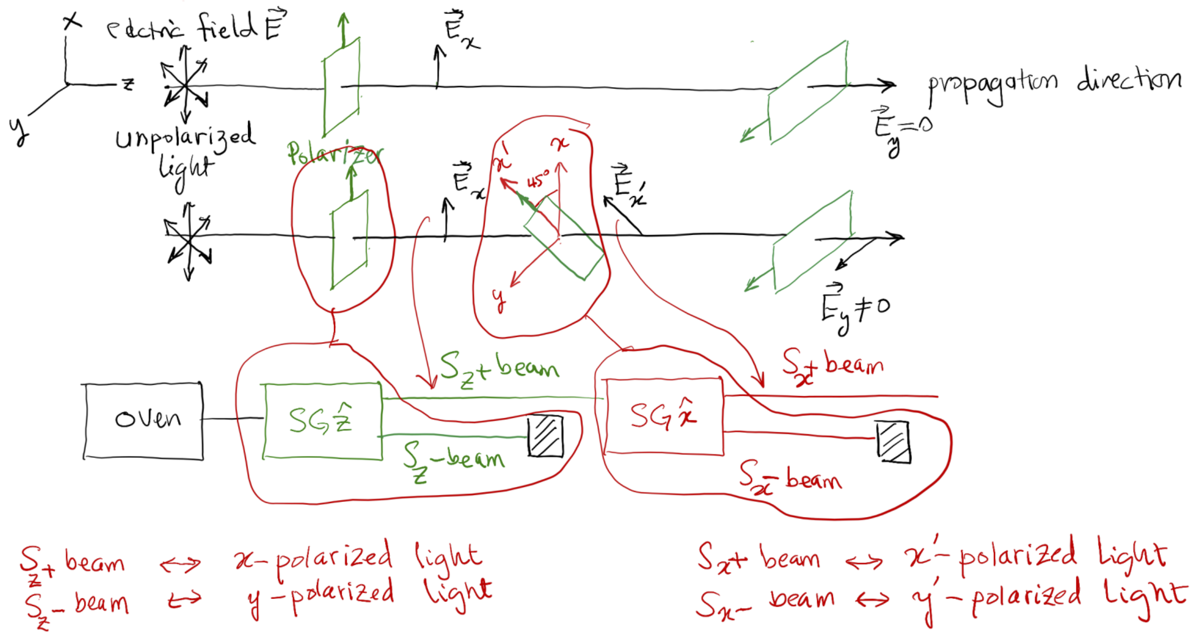

Figure 1.3: Analogy between light polarization and Stern–Gerlach splitting.

Spinor representation and the half-angle vs. Malus laws

For spin-$\frac{1}{2}$, the measurement probability between axes separated by ϕ is $\cos^2(\phi/2)$ by (1.25); for classical linear polarization the transmitted *intensity* is $\cos^2\phi$ by (1.26). The analogy is thus structural (two-dimensional state space and projection rules), but rotations act with a half-angle on spinors.
Choosing the $\hat{\mathbf{z}}$-basis,

$$|{+x}\rangle \;=\; \tfrac{1}{\sqrt{2}}\big(|{+z}\rangle + |{-z}\rangle\big), \qquad |{-x}\rangle \;=\; \tfrac{1}{\sqrt{2}}\big(|{+z}\rangle - |{-z}\rangle\big), \tag{1.28}$$

$$|{+y}\rangle \;=\; \tfrac{1}{\sqrt{2}}\big(|{+z}\rangle + i\,|{-z}\rangle\big), \qquad |{-y}\rangle \;=\; \tfrac{1}{\sqrt{2}}\big(|{+z}\rangle - i\,|{-z}\rangle\big). \tag{1.29}$$

Coordinate Transformations vs. Spin Rotations

While the geometric axes obey (1.27), the corresponding *spin* eigenstates transform under (1.23). For a rotation about $\hat{\mathbf{z}}$ by ϕ,

$$|{+x'}\rangle \;=\; e^{-i\frac{\phi}{2}\sigma_z}\,|{+x}\rangle \;=\; \cos\!\Big(\frac{\phi}{2}\Big)\,|{+x}\rangle \;-\; i\sin\!\Big(\frac{\phi}{2}\Big)\,|{-x}\rangle\,, \tag{1.30}$$

and similarly for $|{-x'}\rangle$. Setting $\phi = \frac{\pi}{4}$ (a 45° rotation) gives equal probabilities $\frac{1}{2}$ for subsequent measurement along $\hat{\mathbf{x}}$, consistent with (1.19).

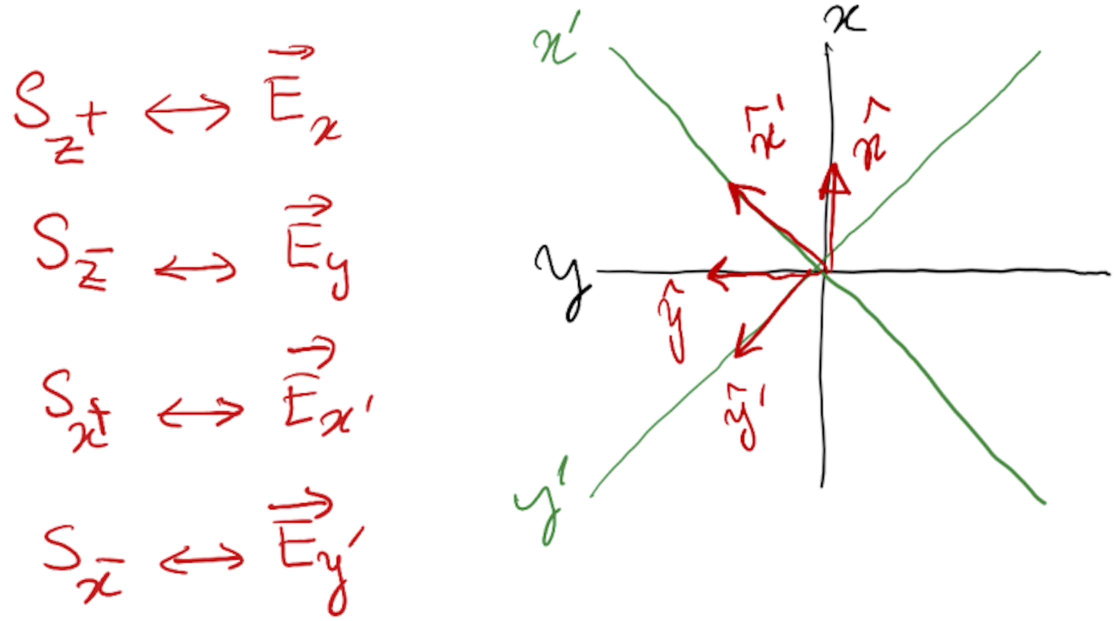

Figure 1.4: A 45° rotation of transverse axes $\hat{\mathbf{x}}, \hat{\mathbf{y}}$ to $\hat{\mathbf{x}}', \hat{\mathbf{y}}'$.

Circular Polarization and Spin States

Right- and left-circularly polarized plane waves (propagating along $+\hat{\mathbf{z}}$) can be written as

$$\mathbf{E}_R(\mathbf{r}, t) \;=\; \mathrm{Re}\left\{E_0\, e^{i(kz-\omega t)}\, \frac{\hat{\mathbf{x}} + i\hat{\mathbf{y}}}{\sqrt{2}}\right\}, \qquad \mathbf{E}_L(\mathbf{r}, t) \;=\; \mathrm{Re}\left\{E_0\, e^{i(kz-\omega t)}\, \frac{\hat{\mathbf{x}} - i\hat{\mathbf{y}}}{\sqrt{2}}\right\}. \tag{1.31}$$

The spin analog is (1.29): $|\pm y\rangle$ are obtained from $|\pm z\rangle$ by relative phase $\pm i$.

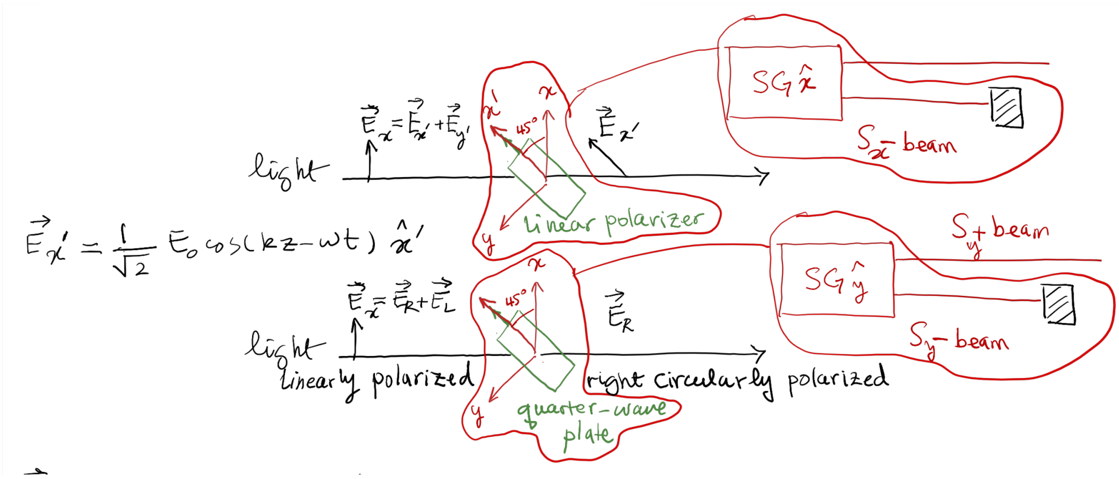

Figure 1.5: Linear vs. circular polarization and their spinor analogs.

Light Polarization Concept	**Spin-$\frac{1}{2}$ Analog**
Horizontal / Vertical (0°/90°)	$\lvert +z\rangle$, $\lvert -z\rangle$
Linear at angle θ	$\lvert +\hat{\mathbf{n}}(\theta)\rangle$ in the xy-plane
Second polarizer at θ	Second SG along $\hat{\mathbf{n}}(\theta)$
Malus: $I \propto \cos^2\theta$	Born: $p \propto \cos^2(\theta/2)$
Right/Left circular	$\lvert +y\rangle$ / $\lvert -y\rangle$ (phase $\pm i$)

Table 1.1: Structural analogy between polarization optics and spin-$\frac{1}{2}$ measurements.

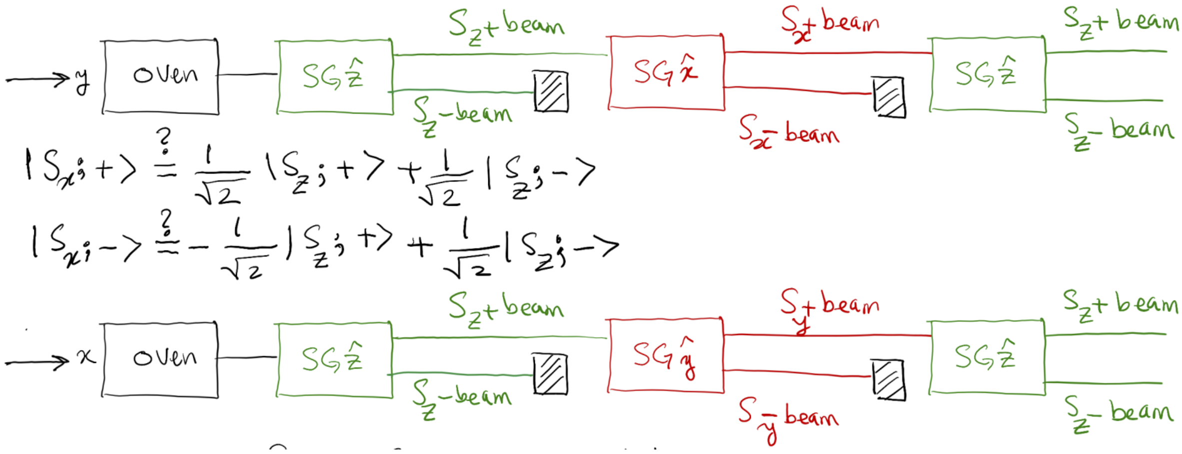

Figure 1.6: A sequential Stern–Gerlach setup emphasizing order dependence.

1.2. Kets, Bras, and Operators

1.2.1. Ket Space

Ket space and Hilbert space A *ket space* is a complex Hilbert space $\mathcal{H}$, i.e. a complex vector space over $\mathbb{C}$ equipped with an inner product $\langle\cdot\,|\,\cdot\rangle : \mathcal{H}\times\mathcal{H}\to\mathbb{C}$ that is conjugate-linear in the first slot, linear in the second, positive-definite, and complete in the induced norm

$$\|\,|\psi\rangle\,\| \;=\; \sqrt{\langle\psi\,|\,\psi\rangle}. \tag{1.32}$$

Elements of $\mathcal{H}$ are written as $|\psi\rangle$ and called *kets.*

Reminder – Selected vector space axioms

Closure: $|\psi_1\rangle + |\psi_2\rangle \in \mathcal{H}$, $\lambda|\psi\rangle \in \mathcal{H}$; Associativity/commutativity of $+$; Existence of $\mathbf{0}$ and additive inverses; Distributivity: ˆ $\alpha(|\psi_1\rangle+|\psi_2\rangle) = \alpha|\psi_1\rangle+\alpha|\psi_2\rangle$, $(\alpha+\beta)|\psi\rangle = \alpha|\psi\rangle + \beta|\psi\rangle$.

Example: a linear vector space in $\mathbb{R}^2$

Let $\mathcal{V} = \{\mathbf{v} = (v_x, v_y) \in \mathbb{R}^2\}$. With the standard basis $\{\hat{\mathbf{x}}, \hat{\mathbf{y}}\}$,

$$\mathbf{v} \;=\; v_x\,\hat{\mathbf{x}} + v_y\,\hat{\mathbf{y}}, \qquad v_x, v_y \in \mathbb{R}. \tag{1.33}$$

Closure under addition and scalar multiplication are immediate:

$$(v_x, v_y) + (w_x, w_y) = (v_x + w_x,\ v_y + w_y) \in \mathcal{V}, \quad a(v_x, v_y) = (av_x, av_y) \in \mathcal{V}. \tag{1.34}$$

Any two linearly independent vectors form a basis (e.g. $\vec{e}_1, \vec{e}_2$), hence

$$\dim(\mathcal{V}) \;=\; 2. \tag{1.35}$$

Physical states and rays

A physical (pure) state is a *ray*: the equivalence class

$$[|\psi\rangle] \;=\; \{\, c\,|\psi\rangle : c \in \mathbb{C} \setminus \{0\}\,\}. \tag{1.36}$$

Normalization chooses a representative with $\langle\psi \mid \psi\rangle = 1$.

Theorem 1.2 – State postulate (ray equivalence)

If $c \neq 0$, then $|\psi\rangle$ and $c\,|\psi\rangle$ describe the same physical state. In particular, if $|\psi_{\mathrm{N}}\rangle = |\psi\rangle /\|\,|\psi\rangle\,\|$ and $|\phi_{\mathrm{N}}\rangle = c\,|\psi\rangle /\|c\,|\psi\rangle\,\|$, then $|\phi_{\mathrm{N}}\rangle = e^{i\theta}\,|\psi_{\mathrm{N}}\rangle$ with $e^{i\theta} = c/|c|$, so all Born probabilities coincide.

Example 1.3 – Global phase and normalization leave probabilities invariant

Let $\{\,|a_k\rangle\,\}$ be eigenkets of an observable with projector $P_k = |a_k\rangle\langle a_k|$. For any $c \neq 0$,

$$\frac{\langle\psi|\,P_k\,|\psi\rangle}{\langle\psi \mid \psi\rangle} \;=\; \frac{\langle\psi|\,P_k\,|\psi\rangle}{\|\,|\psi\rangle\,\|^2} \;=\; \frac{\langle\psi|\,c^*\,P_k\,c\,|\psi\rangle}{|c|^2\,\|\,|\psi\rangle\,\|^2} \;=\; \frac{\langle c\psi|\,P_k\,|c\psi\rangle}{\langle c\psi \mid c\psi\rangle}. \tag{1.37}$$

Thus $[|\psi\rangle]$ determines all measurement probabilities.

Reminder – Inner-product conventions

Conjugate symmetry: $\langle\phi \mid \psi\rangle = \overline{\langle\psi \mid \phi\rangle}$; Linearity in second slot; conjugate-linearity in first; Cauchy–Schwarz: $|\langle\phi \mid \psi\rangle| \leq \|\,|\phi\rangle\,\|\,\|\,|\psi\rangle\,\|$.

1.2.2. Observables and Operators

An operator $\hat{A}$ acts linearly on kets:

$$\hat{A}\big(c_1\,|\psi_1\rangle + c_2\,|\psi_2\rangle\big) \;=\; c_1\,\hat{A}\,|\psi_1\rangle + c_2\,\hat{A}\,|\psi_2\rangle\,. \tag{1.38}$$

The adjoint $\hat{A}^\dagger$ is defined by

$$\langle\phi \mid \hat{A}\psi\rangle \;=\; \langle\hat{A}^\dagger\phi \mid \psi\rangle \quad \text{for all } |\phi\rangle\,, |\psi\rangle \in \mathcal{H}. \tag{1.39}$$

An *observable* is represented (in finite dimension) by a Hermitian operator, i.e. $\hat{A}^\dagger = \hat{A}$. The expectation value of $\hat{A}$ in a normalized state $|\psi\rangle$ is

$$\langle\hat{A}\rangle_\psi \;=\; \langle\psi|\,\hat{A}\,|\psi\rangle\,. \tag{1.40}$$

Theorem 1.3 – Spectral facts for Hermitian operators (finite dimension)

If $\hat{A}^\dagger = \hat{A}$ on a finite-dimensional $\mathcal{H}$, then:

1. All eigenvalues are real.
2. Eigenkets belonging to distinct eigenvalues are orthogonal.
3. There exists an orthonormal basis of $\mathcal{H}$ consisting of eigenkets of $\hat{A}$.

Proof. (i) If $\hat{A}\,|\psi\rangle = a\,|\psi\rangle$ with $|\psi\rangle \neq 0$, then $\langle\psi \mid \hat{A}\psi\rangle = a\,\langle\psi \mid \psi\rangle$. But also $\langle\psi \mid \hat{A}\psi\rangle = \langle\hat{A}\psi \mid \psi\rangle = \overline{a}\,\langle\psi \mid \psi\rangle$ by (1.39). Since $\langle\psi \mid \psi\rangle > 0$, $a = \overline{a} \in \mathbb{R}$. (ii) If $\hat{A}\,|\psi\rangle = a\,|\psi\rangle$, $\hat{A}\,|\phi\rangle = b\,|\phi\rangle$ with $a \neq b$, $(a-b)\langle\psi \mid \phi\rangle = \langle\psi \mid \hat{A}\phi\rangle - \langle\hat{A}\psi \mid \phi\rangle = \langle\psi \mid b\phi\rangle - \langle a\psi \mid \phi\rangle = 0$, so $\langle\psi \mid \phi\rangle = 0$. (iii) Follows by the spectral theorem in finite dimension. □

Eigenkets and eigenvalues

A nonzero ket $|\psi\rangle$ is an *eigenket* of $\hat{A}$ with eigenvalue $a \in \mathbb{C}$ if

$$\hat{A}\,|\psi\rangle \;=\; a\,|\psi\rangle\,. \tag{1.41}$$

For Hermitian $\hat{A}$, $a \in \mathbb{R}$ by Theorem 1.2.2, and eigenkets for different eigenvalues are orthogonal.

Example 1.4 – Spin observable S_z and its eigenkets

In the $\{|+z\rangle\,, |-z\rangle\}$ basis,

$$S_z \;=\; \frac{\hbar}{2}\sigma_z \;=\; \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \qquad \sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{1.42}$$

The eigenvalue equations are

$$S_z\,|+z\rangle \;=\; \frac{\hbar}{2}\,|+z\rangle\,, \qquad S_z\,|-z\rangle \;=\; -\,\frac{\hbar}{2}\,|-z\rangle\,. \tag{1.43}$$

Writing a general normalized spinor $|\psi\rangle = \alpha\,|+z\rangle + \beta\,|-z\rangle$ with $|\alpha|^2 + |\beta|^2 = 1$, the expectation and variance are

$$\langle S_z\rangle_\psi \;=\; \frac{\hbar}{2}\big(|\alpha|^2 - |\beta|^2\big), \qquad \Delta S_z^2 \;=\; \big\langle (S_z - \langle S_z\rangle_\psi)^2\big\rangle_\psi \;=\; \frac{\hbar^2}{4}\big(1 - (|\alpha|^2 - |\beta|^2)^2\big). \tag{1.44}$$

Reminder – Pauli matrices

$\sigma_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$, $\sigma_y = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$, $\sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$; $\{\sigma_i, \sigma_j\} = 2\delta_{ij}I$, $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$.

1.2.3. Bra Space and Inner Products

Bra space and the Riesz map Let $\mathcal{H}$ be a complex Hilbert space with inner product $\langle\cdot\mid\cdot\rangle$ that is conjugate-linear in the first slot and linear in the second (cf. Remark 1.2.3). The *bra space* is the dual space $\mathcal{H}^* = \mathrm{Hom}_{\mathbb{C}}(\mathcal{H}, \mathbb{C})$. The Riesz representation theorem furnishes an *anti-linear* isometric isomorphism

$$J : \mathcal{H} \to \mathcal{H}^*, \qquad J(|\psi\rangle) = \langle\psi|\,, \quad \langle\psi|\phi\rangle \;=\; \langle\psi\mid\phi\rangle \;\; \forall\;|\phi\rangle \in \mathcal{H}. \tag{1.45}$$

With this convention,

$$J(c_1\,|\psi_1\rangle + c_2\,|\psi_2\rangle) \;=\; c_1^*\,\langle\psi_1| + c_2^*\,\langle\psi_2|\,, \qquad c_1, c_2 \in \mathbb{C}. \tag{1.46}$$

Reminder – Dirac conjugation rules

$\big(|\psi\rangle\big)^\dagger = \langle\psi|\,$, $\big(\langle\psi|\big)^\dagger = |\psi\rangle\,$, $\big(c\,|\psi\rangle\big)^\dagger = c^*\,\langle\psi|\,$, $\big(|\psi\rangle + |\phi\rangle\big)^\dagger = \langle\psi| + \langle\phi|\,.$

Inner products

The inner product of $\langle\beta| \in \mathcal{H}^*$ and $|\alpha\rangle \in \mathcal{H}$ is the complex scalar

$$\langle\beta|\alpha\rangle \;\in\; \mathbb{C}. \tag{1.47}$$

With our convention (conjugate-linear in the first slot, linear in the second),

$$\langle\beta|\alpha\rangle \;=\; \overline{\langle\alpha|\beta\rangle}, \qquad \langle c_1\beta_1 + c_2\beta_2|\alpha\rangle \;=\; c_1^*\,\langle\beta_1|\alpha\rangle + c_2^*\,\langle\beta_2|\alpha\rangle\,, \qquad \langle\beta|c_1\alpha_1 + c_2\alpha_2\rangle \;=\; c_1\,\langle\beta|\alpha_1\rangle + c_2\,\langle\beta|\alpha_2\rangle\,. \tag{1.48}$$

Reminder – Inner-product axioms

Conjugate symmetry: $\langle \phi \mid \psi \rangle = \overline{\langle \psi \mid \phi \rangle}$; Linearity (2nd slot) / conjugate-linearity (1st); Positive-definiteness: $\langle \psi \mid \psi \rangle \geq 0$ with equality iff $|\psi\rangle = \mathbf{0}$.

Norm, normalization, orthogonality

The norm is induced by (1.47):

$$\| \, |\alpha\rangle \, \| \;=\; \sqrt{\langle \alpha \mid \alpha \rangle}. \tag{1.49}$$

A nonzero ket $|\alpha\rangle$ can be normalized as

$$|\tilde{\alpha}\rangle \;=\; \frac{|\alpha\rangle}{\| \, |\alpha\rangle \, \|}, \qquad \langle \tilde{\alpha} \mid \tilde{\alpha} \rangle \;=\; 1. \tag{1.50}$$

Kets $|\alpha\rangle \, , |\beta\rangle$ are *orthogonal* if

$$\langle \alpha \mid \beta \rangle \;=\; 0. \tag{1.51}$$

Theorem 1.4 – Cauchy–Schwarz inequality

For all $|\phi\rangle \, , |\psi\rangle \in \mathcal{H}$,

$$\big| \langle \phi \mid \psi \rangle \big| \;\leq\; \| \, |\phi\rangle \, \| \, \| \, |\psi\rangle \, \|, \tag{1.52}$$

with equality iff $|\phi\rangle$ and $|\psi\rangle$ are linearly dependent. *Proof.* If $|\psi\rangle = \mathbf{0}$, the claim is trivial. Assume $|\psi\rangle \neq \mathbf{0}$ and consider $f(\lambda) = \| \, |\phi\rangle - \lambda \, |\psi\rangle \, \|^2 \geq 0$ for all $\lambda \in \mathbb{C}$. Expanding using (1.48),

$$f(\lambda) = \langle \phi - \lambda\psi \mid \phi - \lambda\psi \rangle = \langle \phi \mid \phi \rangle - \lambda \, \langle \phi \mid \psi \rangle - \lambda^* \, \langle \psi \mid \phi \rangle + |\lambda|^2 \, \langle \psi \mid \psi \rangle.$$

Choose $\lambda = \dfrac{\langle \psi \mid \phi \rangle}{\langle \psi \mid \psi \rangle}$. Then

$$0 \leq f(\lambda) = \langle \phi \mid \phi \rangle - \frac{|\langle \psi \mid \phi \rangle|^2}{\langle \psi \mid \psi \rangle},$$

which rearranges to (1.52). Equality holds iff $f(\lambda) = 0$, i.e. $|\phi\rangle = \lambda \, |\psi\rangle$. □

Theorem 1.5 – Triangle inequality

For all $|\phi\rangle \, , |\psi\rangle \in \mathcal{H}$,

$$\| \, |\phi\rangle + |\psi\rangle \, \| \;\leq\; \| \, |\phi\rangle \, \| + \| \, |\psi\rangle \, \|. \tag{1.53}$$

Proof. Square both sides and use $\| \, |\phi\rangle + |\psi\rangle \, \|^2 = \| \, |\phi\rangle \, \|^2 + \| \, |\psi\rangle \, \|^2 + 2 \, \mathrm{Re}\langle \phi \mid \psi \rangle$ together with $|\,\mathrm{Re}\, z| \leq |z|$ and (1.52). □

Example: spin-$\frac{1}{2}$ bras and kets

Let $\{|{+z}\rangle \, , |{-z}\rangle\}$ be an orthonormal basis, so

$$\langle +z \mid +z \rangle = 1, \quad \langle -z \mid -z \rangle = 1, \quad \langle +z \mid -z \rangle = 0. \tag{1.54}$$

A general ket has the form

$$|\psi\rangle = \alpha \, |{+z}\rangle + \beta \, |{-z}\rangle \, , \qquad \alpha, \beta \in \mathbb{C}, \tag{1.55}$$

with corresponding bra

$$\langle \psi | = \alpha^* \, \langle +z | + \beta^* \, \langle -z | \, . \tag{1.56}$$

The norm and normalization follow from (1.49):

$$\| \, |\psi\rangle \, \|^2 = \langle \psi \mid \psi \rangle = |\alpha|^2 + |\beta|^2, \qquad |\psi_{\mathrm{N}}\rangle = \frac{\alpha}{\sqrt{|\alpha|^2 + |\beta|^2}} \, |{+z}\rangle + \frac{\beta}{\sqrt{|\alpha|^2 + |\beta|^2}} \, |{-z}\rangle \, . \tag{1.57}$$

For $|\phi\rangle = a\,|{+z}\rangle + b\,|{-z}\rangle$, the inner product is

$$\langle \phi \mid \psi \rangle = a^* \alpha + b^* \beta, \tag{1.58}$$

and orthogonality $\langle \phi \mid \psi \rangle = 0$ becomes the linear constraint $a^* \alpha + b^* \beta = 0$.

1.2.4. Operators

Linear operators and equality Let $\mathcal{H}$ be a complex Hilbert space. A (linear) *operator* on $\mathcal{H}$ is a map $\hat{X} : \mathcal{H} \to \mathcal{H}$ such that for all $|\psi_1\rangle, |\psi_2\rangle \in \mathcal{H}$ and $c_1, c_2 \in \mathbb{C}$,

$$\hat{X}\big(c_1 |\psi_1\rangle + c_2 |\psi_2\rangle\big) \;=\; c_1 \hat{X} |\psi_1\rangle + c_2 \hat{X} |\psi_2\rangle . \tag{1.59}$$

Two operators $\hat{X}$ and $\hat{Y}$ are equal iff

$$\hat{X} |\psi\rangle = \hat{Y} |\psi\rangle \quad \text{for all } |\psi\rangle \in \mathcal{H}. \tag{1.60}$$

Reminder – Finite vs. infinite dimension

In finite dimension, every linear map $\mathcal{H} \to \mathcal{H}$ is everywhere defined and bounded. In infinite dimension, unbounded operators (e.g. $-i\hbar\,\partial_x$ on L^2) require a specified dense domain; here we work primarily in finite dimension unless stated otherwise.

Zero and identity operators

The *null operator* $\hat{0}$ and the *identity* $\hat{I}$ are defined by

$$\hat{0} |\psi\rangle = \mathbf{0}, \qquad \hat{I} |\psi\rangle = |\psi\rangle \quad \text{for all } |\psi\rangle \in \mathcal{H}. \tag{1.61}$$

Addition and scalar multiplication

For operators $\hat{X}, \hat{Y}$ and scalar $c \in \mathbb{C}$, define

$$(\hat{X} + \hat{Y}) |\psi\rangle = \hat{X} |\psi\rangle + \hat{Y} |\psi\rangle , \qquad (c\,\hat{X}) |\psi\rangle = c\,\hat{X} |\psi\rangle . \tag{1.62}$$

Then operator addition is commutative and associative:

$$\hat{X} + \hat{Y} = \hat{Y} + \hat{X}, \qquad \hat{X} + (\hat{Y} + \hat{Z}) = (\hat{X} + \hat{Y}) + \hat{Z}. \tag{1.63}$$

Multiplication (composition)

Operator multiplication is composition:

$$(\hat{X}\hat{Y}) |\psi\rangle \;=\; \hat{X}\big(\hat{Y} |\psi\rangle\big). \tag{1.64}$$

It is associative but generally non-commutative:

$$\hat{X}(\hat{Y}\hat{Z}) = (\hat{X}\hat{Y})\hat{Z}, \qquad \hat{X}\hat{Y} \neq \hat{Y}\hat{X} \text{ in general.} \tag{1.65}$$

Theorem 1.6 – Action on bras via the adjoint

Given $\hat{X}$ and $\langle\alpha|$, define the right action on bras by

$$\langle\alpha|\, \hat{X} \;:=\; \big(\hat{X}^\dagger |\alpha\rangle\big)^\dagger, \tag{1.66}$$

so that for all $|\psi\rangle \in \mathcal{H}$,

$$\langle\alpha|\, \hat{X} |\psi\rangle \;=\; \langle\alpha|\, \big(\hat{X} |\psi\rangle\big). \tag{1.67}$$

Moreover, $\langle\beta|\,(\hat{X}\hat{Y}) = (\langle\beta|\,\hat{X})\hat{Y}$ follows from associativity and (1.66).

Reminder – Allowed vs. illegal products

Allowed: $\hat{X}\,|\psi\rangle$, $\langle\phi|\,\hat{X}$, $\langle\phi|\psi\rangle$, $|\psi\rangle\,\langle\phi|$. Illegal in a single-space setting: $|\psi\rangle\,\hat{X}$, $\hat{X}\,\langle\phi|$, $|\psi\rangle\,|\phi\rangle$, $\langle\psi|\,\langle\phi|$. (Use tensor products explicitly when different spaces are involved.)

Adjoint (Hermitian conjugate)

The *adjoint* $\hat{X}^\dagger$ is defined by

$$\langle\phi|\,\hat{X}\,|\psi\rangle \;=\; \left\langle \hat{X}^\dagger\phi \middle| \psi\right\rangle \quad \text{for all } |\phi\rangle\,,|\psi\rangle \in \mathcal{H}. \tag{1.68}$$

From (1.68) one derives, for all $\hat{X},\hat{Y}$ and $c\in\mathbb{C}$,

$$(\hat{X}+\hat{Y})^\dagger = \hat{X}^\dagger + \hat{Y}^\dagger, \qquad (c\,\hat{X})^\dagger = c^*\,\hat{X}^\dagger, \qquad (\hat{X}\hat{Y})^\dagger = \hat{Y}^\dagger\hat{X}^\dagger, \qquad (\hat{X}^\dagger)^\dagger = \hat{X}. \tag{1.69}$$

Example 1.5 – Proof of $(\hat{X}\hat{Y})^\dagger$

For arbitrary $|\phi\rangle\,,|\psi\rangle$,

$$\langle\phi|\,\hat{X}\hat{Y}\,|\psi\rangle = \left\langle \hat{X}^\dagger\phi \middle| \hat{Y}\,|\psi\rangle\right. = \left\langle \hat{Y}^\dagger\hat{X}^\dagger\phi \middle| \psi\right\rangle.$$

By the defining property (1.68), this equality for all $|\phi\rangle\,,|\psi\rangle$ implies $(\hat{X}\hat{Y})^\dagger = \hat{Y}^\dagger\hat{X}^\dagger$.

Hermitian, unitary, and positive operators

$$\text{Hermitian (self-adjoint):}\quad \hat{X}^\dagger = \hat{X}. \qquad \text{Unitary:}\quad \hat{U}^\dagger\hat{U} = \hat{U}\hat{U}^\dagger = \hat{I}. \qquad \text{Positive:}\quad \langle\psi|\,\hat{A}\,|\psi\rangle \geq 0 \quad \forall\,|\psi\rangle\,. \tag{1.70}$$

If $\hat{X}$ is Hermitian and $|\psi\rangle$ is normalized, then the expectation $\langle\psi|\,\hat{X}\,|\psi\rangle\in\mathbb{R}$ since

$$\overline{\langle\psi|\,\hat{X}\,|\psi\rangle} \;=\; \langle\psi|\,\hat{X}^\dagger\,|\psi\rangle \;=\; \langle\psi|\,\hat{X}\,|\psi\rangle\,. \tag{1.71}$$

Outer and inner products

The *outer product* $|\beta\rangle\,\langle\alpha|$ is the rank-one operator defined by

$$\big(\,|\beta\rangle\,\langle\alpha|\,\big)\,|\psi\rangle \;=\; \langle\alpha|\psi\rangle\;|\beta\rangle \quad \text{for all } |\psi\rangle\in\mathcal{H}. \tag{1.72}$$

Its adjoint is

$$\big(\,|\beta\rangle\,\langle\alpha|\,\big)^\dagger \;=\; |\alpha\rangle\,\langle\beta|\,. \tag{1.73}$$

The *inner product* $\langle\beta|\alpha\rangle$ is a scalar in $\mathbb{C}$.

Example 1.6 – Projectors and resolution of the identity

For a unit ket $|u\rangle$, the operator $\hat{P} = |u\rangle\,\langle u|$ satisfies

$$\hat{P}^2 = \hat{P}, \qquad \hat{P}^\dagger = \hat{P}, \tag{1.74}$$

so $\hat{P}$ is an orthogonal projector onto $\operatorname{span}\{|u\rangle\}$. If $\{|u_k\rangle\}_{k=1}^{n}$ is an orthonormal basis, then

$$\sum_{k=1}^{n} |u_k\rangle\,\langle u_k| \;=\; \hat{I}, \tag{1.75}$$

the *resolution of the identity*.

Remark 1.3 – Commutators and non-commutativity

The commutator $[\hat{X}, \hat{Y}] \coloneqq \hat{X}\hat{Y} - \hat{Y}\hat{X}$ vanishes iff $\hat{X}$ and $\hat{Y}$ commute. In quantum theory, non-commutativity of key observables (e.g. spin components) encodes measurement order effects and uncertainty relations.

1.2.5. The Associative Axiom

The associative property governs all *legal* compositions of kets, bras, and operators. Rebracketing does not change outcomes whenever the expressions are well-defined (cf. Remark 1.2.4).

Theorem 1.7 – Associativity for legal compositions

Let $|\alpha\rangle, |\beta\rangle, |\delta\rangle \in \mathcal{H}$ and $\hat{X}, \hat{Y}, \hat{Z}$ be operators on $\mathcal{H}$. Then:

1. **Outer/inner product associativity:**
$$\big(|\beta\rangle\langle\alpha|\big)|\delta\rangle \;=\; |\beta\rangle\big(\langle\alpha|\delta\rangle\big) \;=\; \big(\langle\alpha|\delta\rangle\big)|\beta\rangle\,. \tag{1.76}$$

2. **Associativity of operator composition on kets:**
$$(\hat{X}\hat{Y})|\alpha\rangle \;=\; \hat{X}\big(\hat{Y}|\alpha\rangle\big). \tag{1.77}$$

3. **Associativity with a bra (right action via adjoint):**
$$\langle\beta|\,(\hat{X}|\alpha\rangle) \;=\; (\langle\beta|\hat{X})\,|\alpha\rangle\,, \tag{1.78}$$

   where $\langle\beta|\hat{X}$ is defined by $\langle\beta|\hat{X} \coloneqq (\hat{X}^\dagger|\beta\rangle)^\dagger$ (see (1.66)).

Proof. (1) This is the defining action of the rank-one operator $|\beta\rangle\langle\alpha|$ in (1.72) together with the fact that $\langle\alpha|\delta\rangle \in \mathbb{C}$ acts by scalar multiplication. (2) This is the definition of operator product as composition, (1.64). (3) Combine (1.64) with the definition (1.66) to move $\hat{X}$ to the bra side. □

Reminder – Scalars and adjoints

For $c \in \mathbb{C}$: $c|\psi\rangle$ and $\langle\phi|\,c$ are legal; $(c|\psi\rangle)^\dagger = c^*\langle\psi|$, $(\langle\phi|\,c)^\dagger = c^*|\phi\rangle$. Inside $\langle\cdot\mid\cdot\rangle$: $\langle\phi\mid c\psi\rangle = c\langle\phi\mid\psi\rangle$, $\langle c\phi\mid\psi\rangle = c^*\langle\phi\mid\psi\rangle$.

Outer products and their adjoints

Let $\hat{X} = |\beta\rangle\langle\alpha|$. Then by (1.72),
$$\hat{X}|\gamma\rangle \;=\; \big(|\beta\rangle\langle\alpha|\big)|\gamma\rangle \;=\; \langle\alpha|\gamma\rangle\,|\beta\rangle\,, \qquad \forall\,|\gamma\rangle \in \mathcal{H}, \tag{1.79}$$
and the adjoint satisfies
$$\hat{X}^\dagger \;=\; \big(|\beta\rangle\langle\alpha|\big)^\dagger \;=\; |\alpha\rangle\langle\beta|\,, \tag{1.80}$$
as in (1.73). Hence
$$\hat{X}^\dagger|\gamma\rangle \;=\; \langle\beta|\gamma\rangle\,|\alpha\rangle\,. \tag{1.81}$$

Example 1.7 – Verifying (1.76) in a basis

Let $\{|u_j\rangle\}_{j=1}^n$ be an orthonormal basis and write $|\alpha\rangle = \sum_j a_j|u_j\rangle$, $|\beta\rangle = \sum_j b_j|u_j\rangle$, $|\delta\rangle = \sum_j d_j|u_j\rangle$. Then
$$\big(|\beta\rangle\langle\alpha|\big)|\delta\rangle = \sum_k b_k|u_k\rangle\sum_j a_j^* d_j = \Big(\sum_j a_j^* d_j\Big)\sum_k b_k|u_k\rangle = \big(\langle\alpha|\delta\rangle\big)|\beta\rangle\,,$$
which is exactly (1.76).

Matrix elements and Hermitian conjugation

For any operator $\hat{X}$ and kets $|\alpha\rangle, |\beta\rangle$, the matrix element satisfies
$$\langle\beta|\hat{X}|\alpha\rangle \;=\; \big(\langle\alpha|\hat{X}^\dagger|\beta\rangle\big)^*, \tag{1.82}$$

by the defining property of the adjoint (1.68). In particular, if $\hat{X} = \hat{X}^\dagger$ (Hermitian), then

$$\langle\beta|\,\hat{X}\,|\alpha\rangle \;=\; \big(\langle\alpha|\,\hat{X}\,|\beta\rangle\big)^*. \tag{1.83}$$

Theorem 1.8 – Expanded equalities for associative rebracketing

For any $\hat{X}$, $|\alpha\rangle$, $|\beta\rangle$,

$$\langle\beta|\,\hat{X}\,|\alpha\rangle \;=\; \langle\beta|\,\big(\hat{X}\,|\alpha\rangle\big) \;=\; \big(\langle\beta|\,\hat{X}\big)\,|\alpha\rangle\,, \tag{1.84}$$

and for rank-one $\hat{X} = |\beta\rangle\,\langle\alpha|$,

$$\langle\delta|\,\hat{X}\,|\gamma\rangle \;=\; \langle\delta|\,\beta\rangle\,\langle\alpha\mid\gamma\rangle, \qquad \hat{X}\,|\gamma\rangle \;=\; \langle\alpha\mid\gamma\rangle\,|\beta\rangle\,, \qquad \langle\delta|\,\hat{X} \;=\; \langle\delta|\,\beta\rangle\,\langle\alpha|\,. \tag{1.85}$$

Proof. Identity (1.84) is Theorem 1.2.5(2)–(3). The formulas in (1.85) follow from (1.72) and (1.66). □

Reminder – Legality checklist

Legal: $\hat{X}\,|\psi\rangle$, $\langle\phi|\,\hat{X}$, $\langle\phi|\psi\rangle$, $|\psi\rangle\,\langle\phi|$. Illegal (single space): $|\psi\rangle\,\hat{X}$, $\hat{X}\,\langle\phi|$, $|\psi\rangle\,|\phi\rangle$, $\langle\psi|\,\langle\phi|$ (use tensor products for multi-space constructions).

1.3. Base Kets and Matrix Representations

1.3.1. Eigenkets of an Observable

Eigenkets and eigenvalues of an observable Let $\hat{A}$ be a (finite-dimensional) Hermitian operator on $\mathcal{H}$ representing an observable. A nonzero ket $|a\rangle$ is an *eigenket* of $\hat{A}$ with *eigenvalue* $a \in \mathbb{R}$ if

$$\hat{A}\,|a\rangle \;=\; a\;|a\rangle\,. \tag{1.86}$$

Eigenkets with distinct eigenvalues are orthogonal, and within each degenerate eigenspace one may choose an orthonormal basis.

Remark 1.4 – Hermitian vs. self-adjoint

In finite dimension, "Hermitian" ($\hat{A}^\dagger = \hat{A}$) and "self-adjoint" coincide. In infinite dimension, observables are represented by self-adjoint (densely defined) operators; symmetry alone ($\hat{A} \subseteq \hat{A}^\dagger$) is not sufficient.

Theorem 1.9 – Eigenstructure of Hermitian operators

Items (i)–(iii) of Theorem 1.2.2 apply: eigenvalues are real; eigenkets for distinct eigenvalues are orthogonal; there exists an orthonormal eigenbasis. For completeness we verify (i)–(ii).

Proof of (i) (reality). If $\hat{A}\,|a\rangle = a\,|a\rangle$ with $|a\rangle \neq 0$,

$$\langle a \mid \hat{A}a\rangle \;=\; a\,\langle a\mid a\rangle \quad\text{and}\quad \langle a\mid \hat{A}a\rangle \;=\; \langle \hat{A}a\mid a\rangle \;=\; \overline{a}\,\langle a\mid a\rangle,$$

hence $a = \overline{a} \in \mathbb{R}$.

Proof of (ii) (orthogonality). If $\hat{A}\,|a'\rangle = a'\,|a'\rangle$ and $\hat{A}\,|a''\rangle = a''\,|a''\rangle$,

$$(a' - a'')\,\langle a''\mid a'\rangle = \langle a''\mid \hat{A}a'\rangle - \langle \hat{A}a''\mid a'\rangle = \langle a''\mid \hat{A}a'\rangle - \langle a''\mid \hat{A}a'\rangle = 0,$$

so if $a' \neq a''$ then $\langle a''\mid a'\rangle = 0$. □

Reminder – Kronecker delta and ONB

For an orthonormal set $\{|a_k\rangle\}$: $\langle a_j \mid a_k\rangle = \delta_{jk}$ with $\delta_{jk} = 1$ if $j = k$ and 0 otherwise.

1.3.2. Orthonormal Bases, Components, and Completeness

Let $\{|e_j\rangle\}_{j=1}^{n}$ be an orthonormal basis (ONB) of $\mathcal{H}$. Every ket $|\psi\rangle$ admits the expansion

$$|\psi\rangle = \sum_{j=1}^{n} \psi_j \, |e_j\rangle, \qquad \psi_j = \langle e_j \mid \psi\rangle, \tag{1.87}$$

and the inner product becomes

$$\langle \phi \mid \psi\rangle = \sum_{j=1}^{n} \phi_j^* \, \psi_j. \tag{1.88}$$

Equivalently, the identity resolves as

$$\hat{I} = \sum_{j=1}^{n} |e_j\rangle \langle e_j|, \tag{1.89}$$

which is the ONB instance of (1.75).

Remark 1.5 – Degeneracy and orthonormalization

If an eigenvalue a of $\hat{A}$ has multiplicity $m > 1$, any orthonormal basis of its eigenspace $\mathcal{E}_a = \ker(\hat{A} - a\hat{I})$ is admissible; Gram–Schmidt produces $\{|a,1\rangle, \dots, |a,m\rangle\}$ with $\langle a,i \mid a,j\rangle = \delta_{ij}$.

1.3.3. Matrix Representations

Vectors (kets) and covectors (bras)

Relative to the ONB $\{|e_j\rangle\}$, identify

$$|\psi\rangle \leftrightarrow \boldsymbol{\psi} = \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_n \end{pmatrix}, \qquad \langle \phi| \leftrightarrow \boldsymbol{\phi}^\dagger = \begin{pmatrix} \phi_1^* & \cdots & \phi_n^* \end{pmatrix}. \tag{1.90}$$

Then (1.88) reads $\langle \phi \mid \psi\rangle = \boldsymbol{\phi}^\dagger \boldsymbol{\psi}$.

Operators as matrices

The matrix of $\hat{A}$ in the ONB is

$$A_{jk} = \langle e_j \mid \hat{A} \mid e_k\rangle, \qquad [\hat{A}] = (A_{jk})_{j,k=1}^{n}. \tag{1.91}$$

Using (1.89) and (1.87),

$$\hat{A}\,|\psi\rangle = \sum_{j,k} |e_j\rangle \langle e_j \mid \hat{A} \mid e_k\rangle \, \psi_k = \sum_j \Big(\sum_k A_{jk} \, \psi_k \Big) |e_j\rangle, \tag{1.92}$$

i.e. in coordinates

$$\boldsymbol{\psi}' = [\hat{A}] \, \boldsymbol{\psi}. \tag{1.93}$$

Composition and adjoint correspond to matrix product and conjugate-transpose:

$$[\hat{X}\hat{Y}] = [\hat{X}]\,[\hat{Y}], \qquad [\hat{X}^\dagger] = [\hat{X}]^\dagger. \tag{1.94}$$

Therefore $\hat{A}^\dagger = \hat{A}$ iff $[\hat{A}]^\dagger = [\hat{A}]$ (a Hermitian matrix).

Example 1.8 – Rank-one operators as outer products

Let $|\beta\rangle = \sum_j b_j |e_j\rangle$ and $|\alpha\rangle = \sum_j a_j |e_j\rangle$. The outer product $\hat{X} = |\beta\rangle \langle\alpha|$ has matrix

$$[\hat{X}] \;=\; \boldsymbol{b}\,\boldsymbol{a}^\dagger, \qquad \boldsymbol{b} = \begin{pmatrix} b_1 \\ \vdots \\ b_n \end{pmatrix}, \quad \boldsymbol{a} = \begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix}. \tag{1.95}$$

Indeed, $X_{jk} = \langle e_j \mid \beta\rangle\langle\alpha \mid e_k\rangle = b_j\, a_k^*$, and $\hat{X}\,|\psi\rangle = \langle\alpha \mid \psi\rangle\, |\beta\rangle$ matches $[\hat{X}]\,\boldsymbol{\psi} = (\boldsymbol{a}^\dagger\boldsymbol{\psi})\,\boldsymbol{b}$.

Reminder – Matrix adjoint

For $M = (M_{jk})$, $M^\dagger = (\overline{M_{kj}})$. Thus M Hermitian $\Leftrightarrow M_{jk} = \overline{M_{kj}}$.

1.3.4. Spectral Decomposition and Projectors

With an orthonormal eigenbasis $\{|a_k\rangle\}$ of $\hat{A}$ and spectral projectors $P_k = |a_k\rangle \langle a_k|$, one has

$$\hat{A} \;=\; \sum_k a_k\, P_k, \qquad P_k P_\ell \;=\; \delta_{k\ell}\, P_k, \qquad \sum_k P_k \;=\; \hat{I}. \tag{1.96}$$

In a degenerate eigenspace $\mathcal{E}_a$, $P_a = \sum_{i=1}^{m_a} |a,i\rangle \langle a,i|$ is independent of the orthonormal basis chosen in $\mathcal{E}_a$.

Example 1.9 – Spin-1/2:

With $|e_1\rangle = |{+z}\rangle$, $|e_2\rangle = |{-z}\rangle$,

$$[S_z] \;=\; \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \big[\,|{+z}\rangle\,\langle{+z}|\,\big] \;=\; \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad \big[\,|{-z}\rangle\,\langle{-z}|\,\big] \;=\; \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \tag{1.97}$$

The resolution $\hat{I} = |{+z}\rangle\,\langle{+z}| + |{-z}\rangle\,\langle{-z}|$ is the 2×2 identity, and $[\cdot]^\dagger = [\cdot]$ for these projectors, consistent with (1.94).

1.3.5. Change of Basis and Unitary Transformations

Let $\{|e_j\rangle\}$ and $\{|f_k\rangle\}$ be ONBs, and define the unitary

$$U_{kj} \;=\; \langle f_k \mid e_j\rangle, \qquad U^\dagger U = UU^\dagger = I. \tag{1.98}$$

The coordinate column of $|\psi\rangle$ transforms as

$$\boldsymbol{\psi}^{(f)} \;=\; U\,\boldsymbol{\psi}^{(e)}, \qquad \psi_k^{(f)} \;=\; \sum_j U_{kj}\,\psi_j^{(e)}, \tag{1.99}$$

and operator matrices transform by unitary congruence,

$$[\hat{A}]^{(f)} \;=\; U\,[\hat{A}]^{(e)}\,U^\dagger. \tag{1.100}$$

Therefore spectra are basis-independent, and Hermiticity is preserved under change of ONB.

1.3.6. Eigenkets as Base Kets

Theorem 1.10 – Completeness and expansion in an eigenbasis

Let $\hat{A}$ be a Hermitian operator on a finite-dimensional Hilbert space $\mathcal{H}$. Then there exists an orthonormal eigenbasis $\{|a^{(i)}\rangle\}_{i=1}^{N}$ with real eigenvalues $\{a^{(i)}\}$ such that

$$\hat{I} = \sum_{i=1}^{N} \left|a^{(i)}\right\rangle\left\langle a^{(i)}\right|, \tag{1.101}$$

and every ket $|\psi\rangle \in \mathcal{H}$ admits the unique expansion

$$|\psi\rangle = \sum_{i=1}^{N} c_{a^{(i)}} \left|a^{(i)}\right\rangle, \qquad c_{a^{(i)}} = \left\langle a^{(i)}\middle|\,\psi\right\rangle. \tag{1.102}$$

Proof. By Theorem 1.3.1, $\hat{A}$ has an orthonormal eigenbasis. Then the ONB resolution (1.89) gives (1.101). For (1.102),

$$|\psi\rangle = \hat{I}\,|\psi\rangle = \sum_{i=1}^{N} \left|a^{(i)}\right\rangle\left\langle a^{(i)}\middle|\,\psi\right\rangle = \sum_{i=1}^{N} \left(\left\langle a^{(i)}\middle|\,\psi\right\rangle\right)\left|a^{(i)}\right\rangle,$$

and uniqueness follows by taking $\left\langle a^{(j)}\right|$ and using orthonormality. □

Reminder – Orthonormality and coefficients

$\langle a^{(i)} \mid a^{(j)}\rangle = \delta_{ij}$. In (1.102), coefficients are projections: $c_{a^{(i)}} = \langle a^{(i)} \mid \psi\rangle$.

Remark 1.6 – Degeneracies and spectral projectors

If a has multiplicity m_a, choose an ONB $\{|a,j\rangle\}_{j=1}^{m_a}$ of the eigenspace $\mathcal{E}_a$. The orthogonal projector onto $\mathcal{E}_a$ is

$$P_a = \sum_{j=1}^{m_a} |a,j\rangle\langle a,j|, \tag{1.103}$$

and the completeness relation reads

$$\hat{I} = \sum_{a\in\sigma(\hat{A})} P_a = \sum_{a\in\sigma(\hat{A})} \sum_{j=1}^{m_a} |a,j\rangle\langle a,j|. \tag{1.104}$$

In particular, $\dim\mathcal{H} = \sum_a m_a = N$.

Reminder – Continuous spectra (for later)

For continuous spectra one replaces sums by integrals, e.g. $\hat{I} = \int |a\rangle\langle a|\,\mathrm{d}\mu(a)$ with $\langle a \mid a'\rangle = \delta(a-a')$.

Applications of completeness

Example 1.10 – Insertion of the identity and Parseval

Using (1.101), the norm of $|\alpha\rangle$ satisfies

$$\langle\alpha \mid \alpha\rangle \;=\; \langle\alpha \mid \hat{I} \mid \alpha\rangle \;=\; \sum_{i=1}^{N}\langle\alpha \mid a^{(i)}\rangle\langle a^{(i)} \mid \alpha\rangle \;=\; \sum_{i=1}^{N}\left|\langle a^{(i)} \mid \alpha\rangle\right|^{2}. \tag{1.105}$$

Hence, if $|\alpha\rangle$ is normalized, then

$$\sum_{i=1}^{N}\left|c_{a^{(i)}}\right|^{2} \;=\; 1, \qquad c_{a^{(i)}} = \langle a^{(i)} \mid \alpha\rangle. \tag{1.106}$$

Example 1.11 – Matrix elements via double completeness

For any operator $\hat{B}$,

$$\langle\phi \mid \hat{B} \mid \psi\rangle \;=\; \sum_{i,j=1}^{N}\langle\phi \mid a^{(i)}\rangle\,\langle a^{(i)} \mid \hat{B} \mid a^{(j)}\rangle\,\langle a^{(j)} \mid \psi\rangle, \tag{1.107}$$

obtained by inserting $\hat{I} = \sum_i \left|a^{(i)}\right\rangle\!\left\langle a^{(i)}\right|$ to the left and right of $\hat{B}$.

Example 1.12 – Three-dimensional case

Let $\mathcal{H}$ be three-dimensional with eigenkets $\{\left|a^{(1)}\right\rangle, \left|a^{(2)}\right\rangle, \left|a^{(3)}\right\rangle\}$. Any $|\psi\rangle$ expands as

$$|\psi\rangle \;=\; c_{a^{(1)}}\left|a^{(1)}\right\rangle + c_{a^{(2)}}\left|a^{(2)}\right\rangle + c_{a^{(3)}}\left|a^{(3)}\right\rangle, \qquad c_{a^{(i)}} = \langle a^{(i)} \mid \psi\rangle, \tag{1.108}$$

and $\langle\psi \mid \psi\rangle = |c_{a^{(1)}}|^2 + |c_{a^{(2)}}|^2 + |c_{a^{(3)}}|^2$ by (1.105).

1.3.7. Matrix Representations

Theorem 1.11 – Matrix representation via completeness

Let $\{|a^{(i)}\rangle\}_{i=1}^{N}$ be an orthonormal eigenbasis (cf. Theorem 1.3.6) so that

$$\hat{I} \;=\; \sum_{i=1}^{N} \left|a^{(i)}\right\rangle\left\langle a^{(i)}\right|. \tag{1.109}$$

For any operator $\hat{X} : \mathcal{H} \to \mathcal{H}$,

$$\hat{X} \;=\; \hat{I}\,\hat{X}\,\hat{I} \;=\; \sum_{i=1}^{N}\sum_{j=1}^{N} \left|a^{(i)}\right\rangle\left\langle a^{(i)}\right|\,\hat{X}\,\left|a^{(j)}\right\rangle\left\langle a^{(j)}\right| \;=\; \sum_{i=1}^{N}\sum_{j=1}^{N} \langle a^{(i)} \mid \hat{X} \mid a^{(j)}\rangle\;\left|a^{(i)}\right\rangle\left\langle a^{(j)}\right|. \tag{1.110}$$

Define the **matrix elements** of $\hat{X}$ in this basis by

$$X_{ij} \;:=\; \langle a^{(i)} \mid \hat{X} \mid a^{(j)}\rangle, \tag{1.111}$$

so that $\hat{X} = \sum_{i,j} X_{ij}\;|a^{(i)}\rangle\langle a^{(j)}|$.

Reminder – Index convention

X_{ij} means *row* i and *column* j: left bra $\left\langle a^{(i)}\right|$, right ket $\left|a^{(j)}\right\rangle$.

The matrix and its action on coordinates

Let $\boldsymbol{X} = [X_{ij}]_{i,j=1}^{N}$ be the $N \times N$ matrix of $\hat{X}$ in the basis $\{\left|a^{(i)}\right\rangle\}$. For a ket

$$|\psi\rangle = \sum_{j=1}^{N} c_{a^{(j)}}\,\left|a^{(j)}\right\rangle, \qquad \boldsymbol{c} = \begin{pmatrix} c_{a^{(1)}} \\ \vdots \\ c_{a^{(N)}} \end{pmatrix}, \tag{1.112}$$

the action of $\hat{X}$ yields

$$\hat{X}\,|\psi\rangle \;=\; \sum_{i=1}^{N}\sum_{j=1}^{N} X_{ij}\,c_{a^{(j)}}\,\left|a^{(i)}\right\rangle, \qquad \Longleftrightarrow \qquad \boldsymbol{c}' \;=\; \boldsymbol{X}\,\boldsymbol{c}. \tag{1.113}$$

Thus there are $\mathbf{N}^2$ matrix elements X_{ij}, one for each ordered pair (i, j).

Reminder – Orthonormality

$\langle a^{(i)} \mid a^{(j)}\rangle = \delta_{ij}$, and $\hat{I} = \sum_i \left|a^{(i)}\right\rangle\left\langle a^{(i)}\right|$ as in (1.109).

1.3.8. Matrix Representations: Hermitian Adjoint

Adjoint and its matrix The **Hermitian adjoint** $\hat{X}^\dagger$ is characterized by

$$\langle \beta \mid \hat{X} \mid \alpha\rangle \;=\; \big(\langle \alpha \mid \hat{X}^\dagger \mid \beta\rangle\big)^* \quad \text{for all } |\alpha\rangle\,, |\beta\rangle \in \mathcal{H}. \tag{1.114}$$

In the basis $\{\left|a^{(i)}\right\rangle\}$, the matrix of $\hat{X}^\dagger$ is the complex-conjugate transpose of $\boldsymbol{X}$:

$$\big[\hat{X}^\dagger\big]_{ij} \;=\; X_{ji}^*, \qquad \boldsymbol{X}^\dagger \;=\; (\boldsymbol{X}^T)^*. \tag{1.115}$$

Remark 1.7 – Hermitian

Hermitian: $\hat{X} = \hat{X}^\dagger \iff \boldsymbol{X} = \boldsymbol{X}^\dagger$, i.e. $X_{ij} = \overline{X_{ji}}$ (not necessarily real).
Unitary: $\hat{U}^\dagger \hat{U} = \hat{I} \iff \boldsymbol{U}^\dagger \boldsymbol{U} = \boldsymbol{I}$.
Eigenbasis: If the basis is formed by eigenkets of a Hermitian $\hat{X}$, then $\boldsymbol{X} = \mathrm{diag}(a^{(1)}, \ldots, a^{(N)})$ with real $a^{(i)}$.

Reminder – Reality vs. Hermiticity

A Hermitian matrix satisfies $X_{ij} = \overline{X_{ji}}$. It is **real and symmetric** only when all entries are real.

Worked derivations

Example 1.13 – Building $\boldsymbol{X}$ from completeness

Starting from (1.109),

$$\hat{X} = \hat{I}\hat{X}\hat{I} = \sum_{i,j} \left|a^{(i)}\right\rangle \underbrace{\left\langle a^{(i)}\middle|\hat{X}\middle|a^{(j)}\right\rangle}_{X_{ij}} \left\langle a^{(j)}\right| = \sum_{i,j} X_{ij} \left|a^{(i)}\right\rangle\left\langle a^{(j)}\right|,$$

which is (1.110)–(1.111). Acting on $|\psi\rangle = \sum_j c_{a^{(j)}} \left|a^{(j)}\right\rangle$ yields (1.113).

Example 1.14 – Adjoint matrix elements

Using (1.114) with $|\alpha\rangle = \left|a^{(i)}\right\rangle$, $|\beta\rangle = \left|a^{(j)}\right\rangle$,

$$X_{ij} = \langle a^{(i)} \mid \hat{X} \mid a^{(j)}\rangle = \left(\langle a^{(j)} \mid \hat{X}^\dagger \mid a^{(i)}\rangle\right)^* = \left([\hat{X}^\dagger]_{ji}\right)^*,$$

hence $[\hat{X}^\dagger]_{ji} = X_{ij}^*$ and so $[\hat{X}^\dagger]_{ij} = X_{ji}^*$, which is (1.115).

Reminder – Composition in coordinates

With $\boldsymbol{Y} = [Y_{ij}]$: $[\hat{X}\hat{Y}]_{ij} = \sum_k X_{ik} Y_{kj}$ and $[\hat{X}\hat{Y}]^\dagger = \boldsymbol{Y}^\dagger \boldsymbol{X}^\dagger$ (cf. (1.94)).

1.3.9. Matrix Multiplication and Operator Representations

Reminder – Dimension compatibility

If $A \in \mathbb{C}^{m\times n}$ and $B \in \mathbb{C}^{n\times p}$, then the product $C = AB$ exists and $C \in \mathbb{C}^{m\times p}$. The inner dimensions n must match.

Matrix multiplication

For $A = (a_{ik}) \in \mathbb{C}^{m\times n}$ and $B = (b_{kj}) \in \mathbb{C}^{n\times p}$, the product $C = AB$ is defined entrywise by

$$c_{ij} = \sum_{k=1}^{n} a_{ik}\, b_{kj}, \qquad 1 \le i \le m, \quad 1 \le j \le p. \tag{1.116}$$

Example 1.15 – 2×2 multiplication

Let $A = \left(\begin{smallmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{smallmatrix}\right)$, $B = \left(\begin{smallmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{smallmatrix}\right)$. Then $C = AB$ has entries

$$\begin{aligned} c_{11} &= a_{11}b_{11} + a_{12}b_{21}, & c_{12} &= a_{11}b_{12} + a_{12}b_{22}, \\ c_{21} &= a_{21}b_{11} + a_{22}b_{21}, & c_{22} &= a_{21}b_{12} + a_{22}b_{22}, \end{aligned} \tag{1.117}$$

i.e. $C = \left(\begin{smallmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{smallmatrix}\right)$ with entries given by (1.117).

Reminder – Algebraic rules

Associativity: $(AB)C = A(BC)$; Distributivity: $A(B + C) = AB + AC$ and $(B+C)A = BA+CA$; Non-commutativity in general: $AB \neq BA$.

Operator composition and matrix product

Fix an orthonormal basis $\{|a^{(i)}\rangle\}_{i=1}^{N}$. For operators $\hat{X}, \hat{Y}$ define

$$X_{ik} \coloneqq \langle a^{(i)} \mid \hat{X} \mid a^{(k)}\rangle, \qquad Y_{kj} \coloneqq \langle a^{(k)} \mid \hat{Y} \mid a^{(j)}\rangle. \tag{1.118}$$

Then for the composite $\hat{Z} = \hat{X}\hat{Y}$,

$$Z_{ij} \;\coloneqq\; \langle a^{(i)} \mid \hat{Z} \mid a^{(j)}\rangle \;=\; \sum_{k=1}^{N} X_{ik}\, Y_{kj}, \tag{1.119}$$

i.e. the matrix of $\hat{Z}$ equals the matrix product of $\hat{X}$ and $\hat{Y}$:

$$[\hat{Z}] \;=\; [\hat{X}]\,[\hat{Y}]. \tag{1.120}$$

Theorem 1.12 – Derivation of (1.119) from completeness

Using the completeness relation $\hat{I} = \sum_{k=1}^{N} |a^{(k)}\rangle\langle a^{(k)}|$ (cf. (1.109)),

$$\langle a^{(i)} \mid \hat{X}\hat{Y} \mid a^{(j)}\rangle = \sum_{k=1}^{N} \langle a^{(i)} \mid \hat{X} \mid a^{(k)}\rangle\langle a^{(k)} \mid \hat{Y} \mid a^{(j)}\rangle,$$

which is exactly (1.119).

Example 1.16 – Spin-$\frac{1}{2}$: non-commutativity via Pauli matrices

With $\sigma_x = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$, $\sigma_y = \left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right)$, $\sigma_z = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$, one computes

$$\sigma_x\sigma_y = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)\left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right) = \left(\begin{smallmatrix} i & 0 \\ 0 & -i \end{smallmatrix}\right) = i\,\sigma_z, \qquad \sigma_y\sigma_x = -\,i\,\sigma_z, \tag{1.121}$$

hence $\sigma_x\sigma_y = -\sigma_y\sigma_x$. This exhibits non-commutativity while preserving associativity.

Matrix adjoint and products

If $\boldsymbol{X} = [X_{ij}]$ and $\boldsymbol{Y} = [Y_{ij}]$ are the matrices of $\hat{X}$ and $\hat{Y}$ in the fixed basis, then

$$(\boldsymbol{XY})^\dagger \;=\; \boldsymbol{Y}^\dagger\boldsymbol{X}^\dagger, \qquad \text{equivalently} \quad (\hat{X}\hat{Y})^\dagger \;=\; \hat{Y}^\dagger\hat{X}^\dagger, \tag{1.122}$$

consistent with (1.115).

1.3.10. Matrix Representations of Kets and Operators

Kets as column vectors

Fix an orthonormal basis $\{|a^{(i)}\rangle\}_{i=1}^{N}$. Every ket admits the expansion

$$|\alpha\rangle \;=\; \sum_{i=1}^{N} c_i \left|a^{(i)}\right\rangle, \qquad c_i \;=\; \langle a^{(i)} \mid \alpha\rangle, \tag{1.123}$$

so that the coordinate (column) vector of $|\alpha\rangle$ in this basis is

$$|\alpha\rangle \;\longleftrightarrow\; \boldsymbol{\alpha} \;=\; \begin{pmatrix} \langle a^{(1)} \mid \alpha\rangle \\ \langle a^{(2)} \mid \alpha\rangle \\ \vdots \\ \langle a^{(N)} \mid \alpha\rangle \end{pmatrix} \in \mathbb{C}^{N\times 1}. \tag{1.124}$$

Reminder – Bras as row vectors

The dual vector is $\langle\alpha| \;=\; \sum_{i=1}^{N} c_i^* \left\langle a^{(i)}\right|$, with row representation $\langle\alpha| \;\longleftrightarrow\; \boldsymbol{\alpha}^\dagger \;=\; (\overline{c_1}, \ldots, \overline{c_N})$. Thus $\langle\beta \mid \alpha\rangle = \boldsymbol{\beta}^\dagger\boldsymbol{\alpha}$.

Action of an operator on a ket

Let $\hat{X} : \mathcal{H} \to \mathcal{H}$ and define its matrix elements in the chosen basis by

$$X_{ij} \;=\; \langle a^{(i)} \mid \hat{X} \mid a^{(j)}\rangle, \qquad 1 \le i, j \le N. \tag{1.125}$$

Then, using (1.123) and completeness $\hat{I} = \sum_j |a^{(j)}\rangle\langle a^{(j)}|$,

$$\hat{X}\,|\alpha\rangle \;=\; \sum_{i=1}^{N} \left(\sum_{j=1}^{N} X_{ij}\, \langle a^{(j)} \mid \alpha\rangle \right) \left|a^{(i)}\right\rangle, \tag{1.126}$$

so the components of $|\beta\rangle \coloneqq \hat{X}\,|\alpha\rangle$ are

$$\langle a^{(i)} \mid \beta\rangle \;=\; \sum_{j=1}^{N} X_{ij}\, \langle a^{(j)} \mid \alpha\rangle \qquad (1 \le i \le N). \tag{1.127}$$

In matrix form,

$$\boldsymbol{\beta} \;=\; \boldsymbol{X}\,\boldsymbol{\alpha}, \qquad \boldsymbol{X} \;=\; [X_{ij}]_{i,j=1}^{N}, \tag{1.128}$$

which is the standard matrix multiplication rule.

Example 1.17 – Explicit coordinate form

With $\boldsymbol{X} = \begin{pmatrix} X_{11} & \cdots & X_{1N} \\ \vdots & \ddots & \vdots \\ X_{N1} & \cdots & X_{NN} \end{pmatrix}$, $\boldsymbol{\alpha} = \begin{pmatrix} \langle a^{(1)}|\alpha\rangle \\ \vdots \\ \langle a^{(N)}|\alpha\rangle \end{pmatrix}$, one has $\boldsymbol{\beta} = \boldsymbol{X}\,\boldsymbol{\alpha} = \begin{pmatrix} \sum_j X_{1j}\langle a^{(j)}|\alpha\rangle \\ \vdots \\ \sum_j X_{Nj}\langle a^{(j)}|\alpha\rangle \end{pmatrix}$, which matches (1.127).

Key properties (coordinate form)

1. **Column vector representation of kets:** $|\alpha\rangle \leftrightarrow \boldsymbol{\alpha} \in \mathbb{C}^{N\times 1}$ as in (1.124).
2. **Matrix representation of operators:** $\hat{X} \leftrightarrow \boldsymbol{X} \in \mathbb{C}^{N\times N}$ with entries (1.125).
3. **Matrix multiplication rule:** $\boldsymbol{\beta} = \boldsymbol{X}\,\boldsymbol{\alpha}$ (see (1.128)).
4. **Completeness and consistency:** Inserting $\hat{I} = \sum_i |a^{(i)}\rangle\langle a^{(i)}|$ reproduces (1.126) and (1.127).