Chapter 3: Formalism

Quantum Mechanics

1 Operators

Definition 1.1 (Hilbert Space). [def:hilbert-space] **TODO**

Definition 1.2 (Operator Type). [def:operator-type] **TODO**

2 Commutators

Definition 2.1 (Commutator). [def:commutator] $\operatorname{comm}\left(\hat{A},\, \hat{B}\right) := \hat{A}\hat{B} - \hat{B}\hat{A}$.

Remark 2.1 (Notation). [rem:commutator-notation] Others usually write commutators as $[\hat{A}, \hat{B}]$.

Theorem 2.1 (Commuting Operators Share Eigenvectors). [thm:commuting-share-eigenvectors] *If* $\operatorname{comm}\left(\hat{A},\, \hat{B}\right) = 0$*, then* $\hat{A}$ *and* $\hat{B}$ *share a common eigenbasis.*

Proof. **TODO** □

Theorem 2.2 (Distributive Law for Commutators). [thm:commutator-distributive] *For any operators* $\hat{A}, \hat{B}, \hat{C}$*,*

$$\operatorname{comm}\left(\hat{A} + \hat{B},\, \hat{C}\right) = \operatorname{comm}\left(\hat{A},\, \hat{C}\right) + \operatorname{comm}\left(\hat{B},\, \hat{C}\right).$$

Proof. **TODO** □

Theorem 2.3 (Leibniz Rule for the Commutator). [thm:commutator-leibniz] *For any operators* $\hat{A}, \hat{B}, \hat{C}$*,*

$$\operatorname{comm}\left(\hat{A}\hat{B},\, \hat{C}\right) = \hat{A}\,\operatorname{comm}\left(\hat{B},\, \hat{C}\right) + \operatorname{comm}\left(\hat{A},\, \hat{C}\right)\,\hat{B}.$$

Proof. **TODO** □

Theorem 2.4 (Canonical Commutation Relation). [thm:canonical-commutation] *For the position and momentum operators,*

$$\operatorname{comm}(\hat{x},\, \hat{p}) = i\hbar.$$

Proof. **TODO** □

Theorem 2.5 (Hamiltonian Commutators). [thm:hamiltonian-commutators] *For a 1D Hamiltonian* $\hat{H} = \dfrac{\hat{p}^2}{2m} + V(\hat{x})$ *(definition hamiltonian 1d),*

$$\operatorname{comm}\left(\hat{H},\, \hat{x}\right) = -\frac{i\hbar}{m}\,\hat{p}, \qquad \operatorname{comm}\left(\hat{H},\, \hat{p}\right) = i\hbar\, V'(\hat{x}).$$

Proof. **TODO** □

3 Hermitian Operators

Definition 3.1 (Hermition Conjugate)**.** [def:hermition-conjugate] The *Hermitian conjugate* of an operator $\hat{O}$ is denoted $\hat{O}^\dagger$ and is defined by the property

$$\forall f, g, \langle f|\hat{O}g\rangle = \langle \hat{O}^\dagger f|g\rangle$$

Remark 3.1 (Hermitian Conjugate as Matrix Transpose)*.* [rem:hermitian-conjugate-as-matrix-transpose] If $\hat{O}$ is represented as a matrix, then the Hermitian conjugate is the complex conjugate transpose of that matrix. ie,

$$H^\dagger = \left(H^{\mathrm{T}}\right)^*$$

Definition 3.2 (Hermitian Operator)**.** [def:hermitian-operator] An operator $\hat{O}$ is *Hermitian* if it is equal to its Hermitian conjugate, i.e. $\hat{O}^\dagger = \hat{O}$.

4 Unitary Operators

Definition 4.1 (Unitary Operator)**.** [def:unitary-operator] An operator $\hat{U}$ is *unitary* if it satisfies the property $\hat{U}^\dagger\hat{U} = \hat{U}\hat{U}^\dagger = \hat{I}$, where $\hat{I}$ is the identity operator.

5 Conjugation and Similarity Transforms

Definition 5.1 (Conjugation Action)**.** [def:conjugation-action] The *conjugation action* of an operator $\hat{U}$ on another operator $\hat{A}$ is defined as

$$\hat{A} \;\longmapsto\; \hat{U}^\dagger\,\hat{A}\,\hat{U}$$

After applying the operator $\hat{U}$ to $|\psi\rangle$, the expected value of $\hat{A}$ becomes

$$\langle \hat{U}\psi|\,\hat{A}\,|\hat{U}\psi\rangle = \langle\psi|\,\hat{U}^\dagger\hat{A}\hat{U}\,|\psi\rangle\,.$$

So the conjugation action gives the transformed operator $\hat{U}^\dagger\hat{A}\hat{U}$ whose expected value on the original state $|\psi\rangle$ matches $\hat{A}$'s expected value on the transformed state $\hat{U}\,|\psi\rangle$.

6 Functions of Operators

Definition 6.1 (Holomorphic Functional Calculus)**.** [def:operator-function] For every function f analytic in a neighborhood of some center $c \in \mathbb{C}$, with Taylor expansion

$$f(z) \;=\; \sum_{n=0}^{\infty} \frac{f^{(n)}(c)}{n!}\,(z-c)^n,$$

and every operator $\hat{A}$, define

$$f(\hat{A}) \;:=\; \sum_{n=0}^{\infty} \frac{f^{(n)}(c)}{n!}\,(\hat{A} - c\,\hat{I})^n$$

(subject to convergence; $\hat{I}$ is the identity operator). This blanket recipe defines a canonical map $f \longmapsto f(\hat{A})$ from analytic scalar functions to operators, known as the *holomorphic functional calculus*.

Example 6.1 (Operator Exponential)**.** [eg:operator-exponential] Take $f(z) = e^z$ with center $c = 0$. Since $(e^z)^{(n)} = e^z$ and $e^0 = 1$, we have $f^{(n)}(0) = 1$ for all n, so the scalar Taylor series reads

$$e^z \;=\; \sum_{n=0}^{\infty} \frac{z^n}{n!}.$$

Feed this into the operator recipe. With $c = 0$, the shift $\hat{A} - c\hat{I} = \hat{A}$, giving

$$e^{\hat{A}} \;:=\; \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!}\, \hat{A}^n \;=\; \sum_{n=0}^{\infty} \frac{\hat{A}^n}{n!}.$$

Remark 6.1 ($f(\hat{A})$ Is a Constructed Operator). [rem:operator-function-meaning] $f(\hat{A})$ is not literal function application: $\hat{A}$ is an operator, not a scalar. The symbol names a *new operator* built from f's Taylor coefficients (scalars) and $\hat{A}$'s powers, using only operations that operators support (powers, scalar multiplication, addition).

Remark 6.2 ($f(\hat{A})$ Is a First-Class Operator). [rem:operator-function-first-class]

- Once built, $f(\hat{A})$ is an ordinary operator: add, compose, conjugate, or nest as usual. Commutes with $\hat{A}$ and any $g(\hat{A})$; may not commute with operators outside $\{\hat{A}\}$'s commutant.
- The choice of center c is a computational convenience only — $f(\hat{A})$ is intrinsic, and different centers give the same operator where their series converge.

Theorem 6.1 (Action on Eigenvectors)**.** [thm:operator-function-eigenvector] *If* $\hat{A}\,|\lambda\rangle = \lambda\,|\lambda\rangle$*, then* $f(\hat{A})\,|\lambda\rangle = f(\lambda)\,|\lambda\rangle$.

Proof. Since $\hat{A}^n\,|\lambda\rangle = \lambda^n\,|\lambda\rangle$, we have $(\hat{A} - c\hat{I})^n\,|\lambda\rangle = (\lambda - c)^n\,|\lambda\rangle$, so

$$f(\hat{A})\,|\lambda\rangle = \sum_{n=0}^{\infty} \frac{f^{(n)}(c)}{n!}(\lambda - c)^n\,|\lambda\rangle = f(\lambda)\,|\lambda\rangle\,.$$

□

7 Ehrenfest's Theorem

Theorem 7.1 (Generalized Ehrenfest's Theorem)**.** [thm:ehrenfest] *For any observable* $\hat{A}$*,*

$$\frac{d}{dt}\langle\hat{A}\rangle = \frac{1}{i\hbar}\langle \mathrm{comm}\Big(\hat{A},\, \hat{H}\Big)\rangle + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle.$$