Quantum Mechanics Notes

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These are my notes following graduate-level quantum mechanics coursework. The main sources are:

- J. J. Sakurai and J. Napolitano, *Modern Quantum Mechanics*, 3rd ed. (2021).
- R. Shankar, *Principles of quantum mechanics*, 2nd ed. (1994).
- S. Todadri, Quantum Theory I (MIT OCW, 2017).
- L. D. Landau and E. M. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory*, 3rd ed. (1977).

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1. Fundamental Concepts

1.1 Vector Spaces and Hilbert Spaces

1.1.1 Inner Product Spaces

Recall that a **vector space** $(V, +, \cdot, \mathbb{F})$ is an Abelian group with respect to addition equipped with a scalar multiplication operation $\cdot : \mathbb{F} \times V \to V$. Scalar multiplication obeys properties

$$\begin{aligned}\alpha(\beta v) &= (\alpha\beta)v,\\ \alpha(v+w) &= \alpha v + \alpha w,\\ (\alpha+\beta)v &= \alpha v + \beta v,\\ 1_{\mathbb{F}} \cdot v &= v,\end{aligned}$$

for $\alpha, \beta \in \mathbb{F}$ and $v, w \in V$ with $1_{\mathbb{F}}$ the multiplicative identity of $\mathbb{F}$. Unless specified otherwise, we will be working exclusively in the case where our field is of the complex numbers, that is, $\mathbb{F} = \mathbb{C}$. A routine example of a vector space is $\mathbb{C}^n$ itself.

We can upgrade a vector space to an **inner product space** by introducing an operation

$$\langle \cdot, \cdot \rangle : V \times V \to \mathbb{C}$$

with properties for $u, v \in V$ and $\alpha \in \mathbb{C}$,

$$\begin{aligned}\langle u, v\rangle &= \langle v, u\rangle^*,\\ \langle u, v + \alpha w\rangle &= \langle u, v\rangle + \alpha\langle u, w\rangle,\\ u \neq 0 &\implies \langle u, u\rangle > 0.\end{aligned}$$

That is, the inner product is an operation that is (up to complex conjugation) symmetric, linear in its second argument, and is positive definite. An important property is that

$$\langle \alpha u, v\rangle = \langle v, \alpha u\rangle^* = (\alpha\langle v, u\rangle)^* = \alpha^*\langle u, v\rangle.$$

Example 1.1. Examples of inner product spaces.

- Let $V = \mathbb{C}^n$ and attach $\langle u, v\rangle = \sum_i u_i^* v_i$.
- A more interesting example is allowing $V = L^2$:[1] The set of square-integrable functions on some fixed domain U,

  $$\int_U \mathrm{d}x\, |f(x)|^2 < \infty.$$

  Its inner product is given by

  $$\langle f, g\rangle = \int_U \mathrm{d}x\, f^*(x) g(x).$$

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[1] More rigorously, we take this set to be square integrable function equivalence classes where $f \sim g$ iff $f = g$ *almost everywhere*. We will see this to be necessary so that the distance between two functions is zero iff those two functions are the same.

1.1.2 Hilbert Spaces

We may interpret any inner product space as a metric space by defining a norm

$$\|u\| := \sqrt{\langle u, u\rangle}.$$

This gives us a distance function $d(u, v) := \|u - v\|$. A metric space is said to be **complete** if every Cauchy sequence converges: Intuitively this means there are no "holes" between values in the vector space. A **Hilbert space** is a vector space whose induced metric is complete.

Example 1.2. Complete and incomplete metrics.

- $\mathbb{Q}^n$ (over the field $\mathbb{Q}$) provides a simple example of a vector space whose induced metric is incomplete. This is because Cauchy sequence may approach arbitrarily close to an irrational number without actually converging to it, making $\mathbb{Q}^n$ not a Hilbert space.
- $\mathbb{C}^n$ and L^2 both are Hilbert spaces — ones we will be using frequently.

1.1.3 Dual Spaces and Dirac Notation

Given a vector space V, we may define its **dual space** V^* as the set of continuous linear forms

$$f : V \to \mathbb{C}.$$

If V is an inner product space, then we may correspond any vector $v \in V$ with a natural dual vector as the map $w \mapsto \langle v, w\rangle$. Dirac defined a simple notation to represent vectors and dual vectors for use in quantum mechanics, dubbed "bra-ket" notation. A vector $v \in V$ is denoted $|v\rangle$ and its corresponding dual vector is denoted $\langle v|$. By the definition of dual vector, this means applying $\langle v|$ to a vector $|w\rangle$ gives:

$$\langle v|(|w\rangle) = \langle v, w\rangle,$$

the inner product of $|v\rangle$ and $|w\rangle$. This motivates the notation

$$\langle v|w\rangle := \langle v|(|w\rangle) = \langle v, w\rangle.$$

Example 1.3. Interpretation of dual vectors.

- In the case $V = \mathbb{C}^n$, we see that $|v\rangle$ corresponds to a column vector,

$$|v\rangle = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix},$$

while $\langle v|$ corresponds to a row vector,

$$\langle v| = \begin{bmatrix} v_1^* & v_2^* & \cdots & v_n^* \end{bmatrix}.$$

In this case, it is easy to see that $\langle v|w\rangle = \langle v, w\rangle$.

- If $V = L^2$, then $|f\rangle$ corresponds to a square integrable function while $\langle f|$ is an operator on another function $|g\rangle$ that integrates f^*g over the domain.

1.2 Linear Operators

A linear operator $T : V \to V$ is a function such that

$$T|v + \alpha w\rangle = T|v\rangle + \alpha T|w\rangle.$$

This map induces a dual operator $T^* : V^* \to V^*$ that maps $\langle \phi| \in V^*$ as

$$\langle \phi| \mapsto \langle \phi|T.$$

This gives the conjugate-linearity of T on dual vectors,

$$\langle v + \alpha w|T = \langle v|T + \alpha^*\langle w|T.$$

Example 1.4. Let $\{|e_j\rangle\}$ be the standard basis of $\mathbb{C}^n$, then we may represent a linear operator T by an $n \times n$ matrix. Its elements are found by considering how T acts on the standard basis:

$$\langle e_i|T|e_j\rangle = T_{ij}.$$

In fact, if V is any finite-dimensional vector space with $\dim V = n$ then a matrix representation of a linear operator T in basis $\{|b_j\rangle\}$ is

$$T_{ij} = \langle b_i|T|b_j\rangle.$$

1.2.1 Adjoint of an Operator

The **adjoint** $T^\dagger : V \to V$, if exists, of an operator T is defined such that

$$\langle v|Tw\rangle = \langle T^\dagger v|w\rangle.$$

It turns out that such an operator $T^\dagger$ exists and is unique for all operators we will be considering.[2] Thus we formulate how T transforms bras and kets as

$$T|v\rangle = |Tv\rangle,$$
$$\langle v|T = \langle T^\dagger v|.$$

[2] Turns out that if V is a Hilbert space, then $T^\dagger$ always exists uniquely according to the Riesz representation theorem.

An operator T is said to be **Hermitian** if $\langle v|Tw\rangle = \langle Tv|w\rangle$ for all $v, w \in V$.[3]

Some useful properties of the adjoint are

$$\begin{aligned} A^\dagger + B^\dagger &= (A+B)^\dagger, \\ (AB)^\dagger &= B^\dagger A^\dagger, \\ (A^\dagger)^\dagger &= A. \end{aligned} \tag{1}$$

Example 1.5. In $\mathbb{C}^n$, if we represent an operator as a matrix, then its adjoint is just the conjugate transpose of that matrix.

1.2.2 The Eigenvalue Problem

Recall the eigenvalue problem, where we want to find eigenvalues v and $|v\rangle$ such that

$$A|v\rangle = v|v\rangle.$$

The dual of this equation is given as

$$\langle v|A^\dagger = v^*\langle v|.$$

As in the above, we will often abuse notation by using the same symbol for an eigenvalue and its eigenvector. This technically is ill-defined since anytime $|v\rangle$ is a solution, then any vector in the span of $|v\rangle$ will also be a solution. This can be fixed by taking a convention to always normalize $|v\rangle$, but that doesn't solve the problem when v has a degeneracy greater than 1 (that is, when there exists multiple linearly independent eigenvectors for a given eigenvalue).

Theorem 1.6. *If A is a Hermitian operator, then its eigenvalues are real and its eigenvectors corresponding to different eigenvalues are orthogonal.*

Proof. Let $|v\rangle, |w\rangle$ be eigenvectors of A with corresponding eigenvalues v and w. Then,

$$v\langle v|v\rangle = \langle v|Av\rangle = \langle Av|v\rangle = v^*\langle v|v\rangle,$$

so $v \in \mathbb{R}$. In addition if $v \neq w$,

$$w\langle w|v\rangle = \langle Aw|v\rangle = \langle w|Av\rangle = v\langle w|v\rangle,$$

so $\langle w|v\rangle = 0$, showing orthogonality. □

[3] It turns out that being self-adjoint and Hermitian are not always the same if you allow T to be an unbounded linear operator, but this is a common abuse of terminology.

Many important operators in quantum mechanics are Hermitian. If V is finite dimensional, the space decomposes as the direct sum,

$$V = \bigoplus_{\alpha} V_\alpha,$$

where $V_\alpha = \{|x\rangle \neq 0 : A|x\rangle = \alpha|x\rangle\}$ is the eigenspace for eigenvalue α, whose dimension defines the degeneracy of α. By Theorem 1.6 these eigenspaces are mutually orthogonal, and choosing orthonormal bases in each V_α yields an orthonormal eigenbasis for V.

For now, we will consider the case where V is finite-dimensional. Consider a Hermitian A with eigenbasis $|a_i\rangle$. We may write any vector $|\alpha\rangle$ as

$$|\alpha\rangle = \sum_i c_i |a_i\rangle.$$

By multiplying both sides by $\langle a_i|$, we see that $c_i = \langle a_i|\alpha\rangle$, so

$$|\alpha\rangle = \sum_i |a_i\rangle\langle a_i|\alpha\rangle,$$

which gives identity

$$1 = \sum_i |a_i\rangle\langle a_i|. \tag{2}$$

Intuitively, $|a_i\rangle\langle a_i|$ is a projection operator that projects any state onto basis vector a_i, so the identity is the result of projecting onto each basis vector and summing—this leads to no change as expected.

In none of this discussion did we *require* that V is finite-dimensional or even of countable dimension. Let us have a continuous spectrum of eigenvectors $|x\rangle$ as in

$$A|x\rangle = x|x\rangle.$$

The orthonormality condition is given by $\langle y|x\rangle = \delta(y-x)$ for two eigenvectors $|x\rangle$ and $|y\rangle$. Then any arbitrary vector may be represented by

$$|\alpha\rangle = \int \mathrm{d}x\, \langle x|\alpha\rangle |x\rangle,$$

and we may recover the useful property

$$1 = \int \mathrm{d}x\, |x\rangle\langle x|.$$

One may have noticed that $\delta(y-x) \notin \mathbb{C}$ if $x = y$, so this inner product cannot be well-defined between these eigenvectors $|x\rangle$ and $|y\rangle$. This means that operating using $|x\rangle$ seems ill-defined as an eigenbasis for the Hilbert space. Strictly speaking, it in fact does not form a basis for any Hilbert space and will instead serve as a convenient tool that physicists use for calculations.[4] That is, we may recognize any vector $|\psi\rangle$ in our Hilbert space V as a continuous combination of such "eigenvectors" $|x\rangle$,

$$|\psi\rangle = \int \mathrm{d}x\, \psi(x)|x\rangle,$$

but we should not ever view these $|x\rangle$ as members of our Hilbert space themselves. As a result, we will often adopt the notation $\psi(x) = \langle x|\psi\rangle$ to emphasize that x acts only as a parameterization of vectors.

1.2.3 Change of Basis

Let V be finite-dimensional. If A is Hermitian, then we've already shown that we can form a basis from eigenvectors of A. This is to say that A is *diagonalized* under this basis. That is, if we can perform a change of basis using

$$U = [|a_1\rangle \cdots |a_n\rangle]$$

by the transformation $A \to U^{-1}AU$. Now, since the base vectors $\{|a_i\rangle\}$ are orthonormal, U is actually **unitary**, which means that

$$UU^\dagger = U^\dagger U = 1.$$

Thus our change of basis transformation can be written as

$$A \to U^\dagger AU. \tag{3}$$

Now if A was the matrix used to form these eigenvectors then

$$\langle e_j|U^\dagger AU|e_i\rangle = \langle a_j|A|a_i\rangle = a_i\delta_{ij},$$

so it is diagonal under this basis.

Theorem 1.7. *Let $\{|a_i\rangle\}$ and $\{|b_i\rangle\}$ both be orthonormal bases. Then there exists a unitary operator U that can transform between these. The form of U is*

$$U = \sum_i |b_i\rangle\langle a_i|.$$

Proof. The U shown is unitary since

$$U^\dagger U = \sum_{k,l} |a_k\rangle\langle b_k|b_l\rangle\langle a_l| = \sum_k |a_k\rangle\langle a_k| = 1,$$

where we have used the fact that $|\alpha\rangle\langle\beta|^\dagger = |\beta\rangle\langle\alpha|$. Now, clearly U transforms us from $\{|a_i\rangle\}$ to $\{|b_i\rangle\}$:

$$U|a_k\rangle = \sum_i |b_i\rangle\langle a_i|a_k\rangle = |b_k\rangle.$$

□

[4] There do, however, exist formalisms to include distributions like the delta function within an extension of a Hilbert space. Such a space is called a *rigged Hilbert space*.

Thus any set of eigenvectors can be transformed to any other set of eigenvectors. In fact, it turns out that such a unitary change of basis does not even alter eigenvalues: Suppose A and B are Hermitian with eigenbases $\{a_i\}$ and $\{b_i\}$ related by a unitary transformation U. Then we have

$$UAU^\dagger|b_i\rangle = UAU^\dagger U|a_i\rangle = UA|a_i\rangle = a_i U|a_i\rangle = a_i|b_i\rangle.$$

That is $UAU^\dagger$ shares eigenvalues with A.

Remark:

It turns out that quite a lot of interesting cases are such that $B = UAU^\dagger$. Consider for example spin angular momentum S_x and S_z. They share eigenvalues $\pm\hbar/2$ and turn out to be related by a unitary rotation operator.

We may also consider change of bases in the continuous case. Suppose we have two continuous spectra $\{|x\rangle\}$ and $\{|y\rangle\}$. Then

$$|\psi\rangle = \int \mathrm{d}x\, \psi(x)|x\rangle = \int \mathrm{d}y\, \tilde{\psi}(y)|y\rangle,$$

where $\tilde{\psi}(y) = \langle y|\psi\rangle$. If we know $\langle x|y\rangle$ (recall, here $|x\rangle$ and $|y\rangle$ are understood to be drawn for different bases), then we may arrive at a change-of-basis using

$$\begin{aligned} \psi(x) &= \int \mathrm{d}y\, \tilde{\psi}(y)\langle x|y\rangle, \\ \tilde{\psi}(y) &= \int \mathrm{d}x\, \psi(x)\langle y|x\rangle. \end{aligned} \tag{4}$$

Example 1.8. Consider two continuous spectra on Hilbert space L^2: $\{|x\rangle\}$ and $\{|p\rangle\}$. These will later correspond to position and momentum states. Their parameterizations $\psi(x) = \langle x|\psi\rangle$ and $\tilde{\psi}(p) = \langle p|\psi\rangle$ of a state $\psi \in L^2$ are called *wavefunctions*. It will turn out that

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

so the position-space wavefunctions and momentum-space wavefunctions are related by Equation 4 as

$$\begin{aligned} \psi(x) &= \frac{1}{\sqrt{2\pi\hbar}} \int \mathrm{d}p\, \tilde{\psi}(p) e^{ixp/\hbar}, \\ \tilde{\psi}(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int \mathrm{d}x\, \psi(x) e^{-ixp/\hbar}. \end{aligned}$$

That is, these wavefunctions are related by the Fourier transform, so position-space and momentum-space are Fourier duals of each other.

1.2.4 Commuting Operators

Two operators A and B commute if $AB = BA$. To encode this information, we define the **commutator**

$$[A, B] := AB - BA.$$

We also define the **anti-commutator**

$$\{A, B\} := AB + BA.$$

Then operators A and B commute iff $[A, B] = 0$. We should state a few useful properties of the commutator:

$$\begin{gathered}
[A, B] = -[B, A], \\
[A + \alpha B,\, C] = [A, C] + \alpha[B, C], \\
[A, BC] = [A, B]C + B[A, C], \\
[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0, \\
[A, B]^\dagger = [B^\dagger, A^\dagger].
\end{gathered} \tag{5}$$

Theorem 1.9. *If A and B are Hermitian and commute then B is block diagonal in the eigenbasis of A.*

Proof. We have,

$$0 = \langle a_i|[A, B]|a_j\rangle = (a_i - a_j)\langle a_i|B|a_j\rangle,$$

so if $a_i \neq a_j$ then $\langle a_i|B|a_j\rangle = 0$. If $a_i = a_j$ then we may have an eigenspace of dimension d corresponding to this eigenvalue. We cannot guarantee these are diagonal for B, but this guarantees block diagonality. □

From Theorem 1.9, if A is non-degenerate we have that the eigenvectors of A are also eigenvectors of B:

$$\begin{aligned}
B|a_i\rangle &= \sum_{j,k} |a_j\rangle\langle a_j|B|a_k\rangle\langle a_k|a_i\rangle \\
&= \sum_j |a_j\rangle\langle a_j|B|a_i\rangle \\
&= \langle a_i|B|a_i\rangle|a_i\rangle,
\end{aligned}$$

so $|a_i\rangle$ is an eigenvector of B with eigenvalue $\langle a_i|B|a_i\rangle$. In fact, this remains true even in the presence of degeneracy, but to do this we must diagonalize B which amounts to starting with the block-diagonal form that Theorem 1.9 provides and diagonalizing each block matrix. Since A is diagonal in its own basis, it is possible to diagonalize the block matrices within B without affecting A.

1.2.5 Functions of Operators

Recall that if A is Hermitian, then

$$A = \sum_i a_i|a_i\rangle\langle a_i|,$$

or in continuous case,

$$A = \int \mathrm{d}a\, a|a\rangle\langle a|.$$

Let $f : \mathbb{R} \to \mathbb{R}$ be defined for the set of eigenvalues of any operator A. Then we define

$$f(A) := \sum_i f(a_i)|a_i\rangle\langle a_i|,$$

and in continuous case

$$f(A) := \int \mathrm{d}a\, f(a)|a\rangle\langle a|.$$

Example 1.10. Examples of using functions of operators.

- Recall that if A can be diagonalized as $A = U^{-1}DU$ with $D = \mathrm{diag}(a_i)$ and $U = [u_i]$, then

  $$A^n = U^{-1}D^nU.$$

  This means A^n has eigenvalues a_i^n. Our definition of functions on operators with $f(\cdot) = (\cdot)^n$ agrees here.

- If f has Taylor series

  $$f(x) = \sum_{k=0}^{\infty} \frac{f^{(k)}(0)}{k!} x^k,$$

  then our definition provides

  $$f(A) = \sum_i \sum_{k=0}^{\infty} \frac{f^{(k)}(0)}{k!} a_i^k |a_i\rangle\langle a_i| = \sum_{k=0}^{\infty} \frac{f^{(k)}(0)}{k!} A^k.$$

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