Physics 731 Lecture Notes 1

Summary: Mathematical Introduction

These notes summarize several of the background-level mathematical ideas that are relevant for quantum mechanics, including linear vector spaces, dual spaces, Dirac notation, orthonormal basis sets, linear operators, the eigenvalue problem, and the spectral representation of operators. References for this material include **S1r**, **S2**, **S3** Chapter 1, and Shankar Ch 1.

Definition. A *field* F is a set of scalars $\{a, b, c, \ldots\}$ along with two operations, addition and multiplication. Examples: (i) real numbers ($F = \mathbb{R}$), (ii) complex numbers ($F = \mathbb{C}$).

Definition. A *vector space* $V(F)$ consists of a set of quantities called vectors $\{\alpha, \beta, \gamma, \ldots\}$ and a field F, together with two operations, vector addition and scalar multiplication, that satisfy the following criteria:

- $\alpha + \beta \in V$ (closure).
- $\alpha + \beta = \beta + \alpha$ (commutative).
- $(\alpha + \beta) + \gamma = \alpha + (\beta + \gamma)$ (associative).
- There exists a unique 0 such that $\alpha + 0 = 0 + \alpha = \alpha$.
- For all vectors $\alpha \in V$, there exists a unique inverse $-\alpha \in V$ that satisfies $\alpha + (-\alpha) = 0$.
- $c\,\alpha \in V$.
- $c(\alpha + \beta) = c\,\alpha + c\,\beta$.
- $(a + b)\alpha = a\,\alpha + b\,\alpha$.
- $a(b\gamma) = (ab)\gamma$.

Examples: n-dimensional Cartesian vectors $V^n(\mathbb{R})$, n-dimensional complex vectors $V^n(\mathbb{C})$, the set of nth order real polynomials (example of a function space).

Dirac Notation:

- *Ket* vector space: $\alpha \leftrightarrow |\alpha\rangle$. Properties: $|\alpha\rangle + |\beta\rangle = |\alpha + \beta\rangle$, $c|\alpha\rangle = |c\,\alpha\rangle$.
- Dual (*bra*) vector space: $\alpha \to \alpha^\dagger$, $|\alpha\rangle \to \langle\alpha|$. Properties: $\langle\alpha| + \langle\beta| = \langle\alpha + \beta|$, $\langle c\,\alpha| = c^*\langle\alpha|$.

Definition. A set of vectors $\{\alpha_1, \ldots, \alpha_n\}$ in $V(F)$ is a *linearly independent* (LI) set if $\sum_{i=1}^n c_i\alpha_i = 0$ implies that all $\{c_i\} = 0$. Otherwise, the set is *linearly dependent* (LD).

Definition. If the the largest number of LI vectors in the vector space $V(F)$ is n, the *dimension* of the space is n, and it is said to be n-dimensional (then often labeled as $V^n(F)$). The dimension of the space can be finite, countably infinite, or uncountably infinite.

Theorem: If $\{\alpha_1, \ldots \alpha_n\}$ is a LI set in space $V^n(F)$, any $\alpha \in V^N$ can be written as $\alpha = \sum_{i=1}^n c_i\alpha_i$, where the c_i are unique. The $\{\alpha_i\}$ form a *basis* for V^n, and the c_i are the components of α in that basis.

Definition: An *inner product space* (IPS) is a vector space $V(F)$ with an additional operation, the *inner product* (IP). The inner product, denoted by $\langle\alpha|\beta\rangle$, is a bilinear mapping of a vector and a dual vector to the space of scalars, that satisfies the following criteria:

- $\langle\beta|\beta\rangle$ real and ≥ 0.
- $\langle\beta|\beta\rangle = 0$ if and only if $\beta = 0$.
- $\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^*$.
- $\langle\alpha|c_1\beta + c_2\gamma\rangle = c_1\langle\alpha|\beta\rangle + c_2\langle\alpha|\gamma\rangle$.
- $\langle c_1\beta + c_2\gamma|\alpha\rangle = c_1^*\langle\beta|\alpha\rangle + c_2^*\langle\gamma|\alpha\rangle$.

A complex IPS is often denoted as a Hilbert space. (Note that the Hilbert space terminology is sometimes reserved for the case of a complete infinite-dimensional space, which we will discuss in greater detail a bit later in this course. Here, following typical practices in physics, the Hilbert space designation will include finite-dimensional spaces.) Examples of inner products include:

- For $V^n(\mathbb{R})$, $\langle\beta|\alpha\rangle = \beta^T\alpha = \sum_{i=1}^n b_i a_i$, where a_i and b_i are the components of α and β, respectively.
- For $V^n(\mathbb{R})$, another valid IP is $\langle\beta|\alpha\rangle_M = \beta^T M\alpha = \sum_{i,j=1}^n b_i M_{ij} a_j$, in which M is a real symmetric matrix ($M_{ij} = M_{ji}$) with positive eigenvalues.
- For $V^n(\mathbb{C})$, $\langle\beta|\alpha\rangle = \beta^\dagger\alpha = \sum_{i=1}^n b_i^* a_i$ is an IP, as is $\langle\beta|\alpha\rangle_M = \beta^\dagger M\alpha = \sum_{i,j=1}^n b_i^* M_{ij} a_j$, in which M is a Hermitian matrix ($M_{ij} = M_{ji}^*$) with positive eigenvalues.
- For the space of real nth order polynomials of a real variable $x \in [A, B]$, $\langle P|Q\rangle = \int_A^B P(x)F(x)Q(x)dx$ is an IP if $F(x)$ is a real and positive function of x over the interval $x \in [A, B]$.

In quantum mechanics, the IPS $V^d(\mathbb{C})$ is what we use to describe finite-dimensional systems with dimension d, while certain function spaces with inner products will be used when describing infinite-dimensional systems. Further discussion of function spaces will take place shortly in this course (in Lecture Notes 2).

Definition. The *norm* of a vector α in an inner product space is $|\alpha| = \sqrt{\langle\alpha|\alpha\rangle}$.

Definition. In $V^n(F)$ IPS, a set of vectors $\{\alpha_1, \ldots \alpha_m\}$ ($m \leq n$) is *orthogonal* if $\langle\alpha_i|\alpha_j\rangle = 0$ for $i \neq j$, and *orthonormal* (ON) if $\langle\alpha_i|\alpha_j\rangle = \delta_{ij}$.

An *orthonormal basis* satisfies the following criteria:

- $\langle i|j\rangle = \delta_{ij}$ (orthonormality),
- $\sum_i |i\rangle\langle i| = \sum_i \Lambda_i = \mathbb{1}$ (completeness), where $\Lambda_i \equiv |i\rangle\langle i|$ is the *projection operator* onto the state i.

For an orthonormal basis, we can write

$$|\beta\rangle = \sum_i |i\rangle\langle i|\beta\rangle = \sum_i \Lambda_i|\beta\rangle, \quad \langle\beta| = \sum_i \langle\beta|i\rangle\langle i| = \sum_i \langle\beta|\Lambda_i.$$

An ON basis $\{\alpha_1, \ldots \alpha_n\}$ can be constructed from a LI set $\{\beta_1, \ldots \beta_n\}$ using the *Gram-Schmidt* procedure. This consists first of computing an orthogonal set $\{\alpha'_1, \ldots \alpha'_n\}$ using

$$|\alpha'_j\rangle = |\beta_j\rangle - \sum_{i=1}^{j-1} |\alpha'_i\rangle \frac{\langle \alpha'_i|\beta_j\rangle}{\langle \alpha'_i|\alpha'_i\rangle},$$

then normalizing:

$$|\alpha_i\rangle = \frac{|\alpha'_i\rangle}{\sqrt{\langle \alpha'_i|\alpha'_i\rangle}}.$$

Definition: A *linear operator* A is a linear mapping of V onto itself: $A|\alpha\rangle = |\alpha'\rangle$, which obeys the property:

$$A|a\alpha + b\beta\rangle = A(a|\alpha\rangle + b|\beta\rangle) = aA|\alpha\rangle + bA|\beta\rangle.$$

The product of two operators A and B generally depends on the order of operation. More precisely, $AB = BA$ only if the *commutator* $[A, B] \equiv AB - BA$ vanishes. The properties of the commutator are:

- $[A, B] = -[B, A]$.
- $[A, B + C] = [A, B] + [A, C]$.
- $[A, BC] = B[A, C] + [A, B]C$.
- $[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$.

The *anticommutator* is given by $\{A, B\} = AB + BA$.

Given the ON basis $\{|i\rangle\}$, the *matrix elements* of A in this basis are $A_{ij} = \langle i|A|j\rangle$, and the *matrix representation* of A in this basis is

$$A = \sum_{i,j} A_{ij}|i\rangle\langle j|.$$

Therefore, $A|\alpha\rangle = |\alpha'\rangle$ in matrix form is

$$\langle j|\alpha'\rangle = \sum_i \langle j|A|i\rangle\langle i|\alpha\rangle = \sum_i A_{ji}\langle i|\alpha\rangle.$$

This means we can write

$$a'_j = \sum_i A_{ji}a_i,$$

where a_i and a'_i are the components of $|\alpha\rangle$ and $|\alpha'\rangle$ in the $\{|i\rangle\}$ basis. Examples: rotation operator in $V^n(\mathbb{R})$; differentiation/multiplication in the space of nth order polynomials ($n \to \infty$).

Definition: Given a linear operator A in $V^n(F)$, there may exist an *inverse* operator A^{-1}, such that

$$AA^{-1} = A^{-1}A = 1.$$

(Note that not all operators have inverses, but many do. Example: rotation operator in $V^n(\mathbb{R})$.)

Definition: The *outer product* $|\alpha\rangle\langle\beta|$ denotes an operator which acts on states in $V^n(F)$. The outer product acts on an arbitary ket $|\gamma\rangle$ as follows:

$$(|\alpha\rangle\langle\beta|)|\gamma\rangle = |\alpha\rangle\langle\beta|\gamma\rangle.$$

In the usual vector language, the outer product is given by $\alpha\beta^\dagger$, where α and β are both column vectors. We have already seen examples of the outer product, such as the projection operators $\Lambda_i = |i\rangle\langle i|$, which satisfy $\sum_i \Lambda_i = \mathbb{1}$, and the matrix representation of a linear operator A in an ON basis $\{i\}$, as $A = \sum_{i,j} A_{ij}|i\rangle\langle j|$.

Definition: The dual of $A|\alpha\rangle = |A\alpha\rangle$ is $\langle A\alpha| = \langle\alpha|A^\dagger$, in which $A^\dagger$ is called the *adjoint* of A. $A^\dagger$ is defined as follows: given the linear operator A, for all α, β in $V^n(F)$,

$$\langle\beta|A^\dagger|\alpha\rangle = \langle A\beta|\alpha\rangle = \langle\alpha|A\beta\rangle^* = \langle\alpha|A|\beta\rangle^*.$$

The adjoint operator obeys the following properties:

- $(A^\dagger)^\dagger = A$.
- $(AB)^\dagger = B^\dagger A^\dagger$.
- $(cA)^\dagger = c^* A^\dagger$.

The matrix representation of $A^\dagger$ is

$$A^\dagger = \sum_{i,j} (A^\dagger)_{ij}|i\rangle\langle j| = \sum_{i,j} A^*_{ji}|i\rangle\langle j|.$$

An operator is *self-adjoint* or *Hermitian* if $A = A^\dagger$. An operator is *unitary* if $A^\dagger = A^{-1}$.

Eigenvalue problem. Given an operator A acting in $V^n(F)$, if $A|\omega\rangle = \omega|\omega\rangle$, then $|\omega\rangle$ is an *eigenvector* of A with *eigenvalue* ω. In matrix notation, $\sum_{j=1}^n A_{ij}\omega_j = \omega\omega_i$. The eigenvalues are determined by solving the characteristic equation, which is given by

$$\det(A - \omega\mathbb{1}) = 0.$$

For each distinct eigenvalue, there are one or more LI eigenvectors (there can be at most n of them).

For Hermitian operators A acting in the vector space $V^n(\mathbb{C})$, the following important properties hold:

- The eigenvectors corresponding to distinct eigenvalues are orthogonal, and the eigenvalues are real.
- A has n LI eigenvectors, though not necessarily n distinct eigenvalues.

The eigenvectors of A can be used to form a complete ON basis. In the case that all eigenvalues are distinct and each has a corresponding eigenvector (the non-degenerate case), the eigenvectors are automatically orthogonal, and each is labeled by its corresponding eigenvalue (or a shorthand notation for this eigenvalue). Within quantum mechanics, these labels are often referred to as *quantum numbers*. In the case of degeneracy, orthogonality is not automatic, but an ON set can be constructed within each degenerate subspace, for example by using the Gram-Schmidt procedure.

The Hermitian matrix A is diagonalized by the unitary transformation

$$U^\dagger A U = A_{\text{diag}}.$$

Here U is a unitary matrix with its columns given by the normalized eigenvectors of this ON basis set and A_{diag} is a diagonal matrix with the eigenvalues of A as its diagonal entries, which are ordered according to the (arbitrary) ordering of the columns of U.

The *spectral representation* of a Hermitian operator A, in which $A|\omega_i\rangle = \omega_i|\omega_i\rangle$, is

$$A = \sum_i \omega_i \Lambda_i,$$

in which we recall that $\Lambda_i = |\omega_i\rangle\langle\omega_i|$ (and of course $\langle\omega_i|\omega_j\rangle = \delta_{ij}$). The power of this representation arises in dealing with functions of the operator A, which can be expressed as

$$f(A) = \sum_i f(\omega_i)\Lambda_i.$$

For example, A^{-1}, the inverse operator of A (if it exists), is given by

$$A^{-1} = \sum_i \omega_i^{-1}\Lambda_i,$$

and e^A takes the form

$$e^A = \sum_i e^{\omega_i}\Lambda_i.$$