Part III: Operator and Matrix Analysis

In quantum mechanics and quantum statistics (quantum statistical mechanics) as well as in certain other areas of physics, physical quantities are represented by linear operators on a vector (Hilbert) space. This makes possible the development of these subject areas by use of rigorous mathematical procedures.

Mathematical operations involving linear operators are often carried out by use of matrices. A knowledge of vector space, linear operators, and matrix analysis is required in many areas of physics.

This part of the lecture will cover:

- A brief discussion of vector spaces and linear operators;
- Matrix analysis.

Definition of a Vector Space

A set of objects (vectors) $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, $\cdots$ are said to form a linear space V if

1. the set is closed under commutative and associative addition, so that

$$\mathbf{a} + \mathbf{b} = \mathbf{b} + \mathbf{a}$$

$$(\mathbf{a} + \mathbf{b}) + \mathbf{c} = \mathbf{a} + (\mathbf{b} + \mathbf{c})$$

2. the set is closed under multiplication by a scalar (any complex number) to form a new vector $\lambda\mathbf{a}$, the operation being both distributive and associative so that

$$\lambda(\mathbf{a} + \mathbf{b}) = \lambda\mathbf{a} + \lambda\mathbf{b}$$

$$\lambda(\mu\mathbf{a}) = (\lambda\mu)\mathbf{a}$$

$$(\lambda + \mu)\mathbf{a} = \lambda\mathbf{a} + \mu\mathbf{a}$$

   where λ and μ are arbitrary scalars;

Definition of a Vector Space (cont.)

3. there exists a null vector $\mathbf{0}$ such that for all $\mathbf{a}$

$$\mathbf{a} + \mathbf{0} = \mathbf{a};$$

4. multiplication by unity leaves any vector unchanged, i.e.

$$1\mathbf{a} = \mathbf{a};$$

5. for every $\mathbf{a}$, a vector $-\mathbf{a}$ exists such that

$$\mathbf{a} + (-\mathbf{a}) = \mathbf{0}$$

Linear Dependence & Dimensionality

A set of vectors **a**, **b**, $\cdots$, **u** is said to be *linearly independent* provided no equation

$$\lambda \mathbf{a} + \mu \mathbf{b} + \cdots + \sigma \mathbf{u} = \mathbf{0}$$

holds except the trivial one with $\lambda = \mu = \cdots = \sigma = 0$.

If in a particular vector space there exist n linearly independent vectors but no set of $n+1$ linearly independent ones, the space is said to be n-dimensional.

3D:

$$\lambda \vec{A} + \mu \vec{B} + \nu \vec{C} = 0$$

If $\vec{A}$, $\vec{B}$ and $\vec{C}$ are along the x, y and z directions respectively, then $\lambda = \mu = \nu = 0$.

Completeness

Let $\mathbf{e}_1$, $\mathbf{e}_2$, $\cdots$, $\mathbf{e}_n$ be a set of n linearly independent vectors in an n-dimensional vector space. The if $\mathbf{x}$ is an arbitrary vector in the space, there exists a relation

$$\lambda \mathbf{e}_1 + \mu \mathbf{e}_2 + \cdots + \sigma \mathbf{e}_n + \tau \mathbf{x} = \mathbf{0}$$

with not all the constants equal to zero, and in particular $\tau \neq 0$. Thus $\mathbf{x}$ can be written as a linear combination of the $\mathbf{e}_i$:

$$\mathbf{x} = \sum_{i=1}^{n} x_i \mathbf{e}_i \quad \left(\text{3D:} \vec{A} = A_x \hat{i} + A_y \hat{j} + A_z \hat{k}\right)$$

The vectors $\mathbf{e}_i$ are said to form a *basis*, or *coordinate system*, and the numbers x_i are the *components* of $\mathbf{x}$ in this system. The $\mathbf{e}_i$ are called *base vectors*.

The fact that an arbitrary vector $\mathbf{x}$ can be written as a linear combination of the $\mathbf{e}_i$ is often expressed as: The set of base vector $\mathbf{e}_i$ is *complete*.

Inner Product

Scalar product in 3D: $\vec{A} \cdot \vec{B} = AB \cos\theta$

The **inner product** of two vectors **a** and **b** is denoted by (**a**,**b**).

In quantum mechanics, a vector in Hilbert space is denoted by $|\psi\rangle$, and the innor product (ψ, ϕ) is written as $\langle\psi|\phi\rangle$ where $\langle\psi|$ and $|\phi\rangle$ are called **bra** and **ket** vectors, respectively.

The following properties are valid for the inner product:

$$\langle\psi|\phi + \chi\rangle = \langle\psi|\phi\rangle + \langle\psi|\chi\rangle$$
$$\langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*$$
$$\langle\psi|\lambda\phi\rangle = \lambda\langle\psi|\phi\rangle$$
$$\langle\lambda\psi|\phi\rangle = \lambda^*\langle\psi|\phi\rangle$$

An **Euclidean space** E_n is a vector space on which an inner (scalar) product is defined.

Norm and Orthogonality

3D space:

$$\vec{A} \cdot \vec{B} = \vec{0} \quad \Longrightarrow \quad \vec{A} \perp \vec{B}$$

$$A = |\vec{A}| = \sqrt{\vec{A} \cdot \vec{A}}$$

The **norm** (length), $||\psi||$, of a vector ψ is defined as

$$||\psi|| = (\psi, \psi)^{1/2}$$

If the inner product of two vectors equals zero $(\psi, \phi) = 0$ the two vectors are said to be orthogonal to each other.

If the inner product of any two vectors in a set is zero,

$$(\psi_i, \psi_k) = 0 \quad \text{for} \left\{ \begin{array}{ll} i \neq j & i, j = 1, 2, \cdots, n \\ \psi_i \neq 0 & \text{and } \psi_k \neq 0 \end{array} \right.$$

the vectors are said to form an **orthogonal set**.

If the norm within an orthogonal set is unity

$$||\psi_i|| = 1$$

the set is called **orthonormal**.