

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} , \dots 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 $\mathbf{a}, \mathbf{b}, \dots, \mathbf{u}$ is said to be *linearly independent* provided no equation

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

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

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:

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

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

Completeness

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

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

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 inner 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:

$$\vec{A} \cdot \vec{B} = \vec{0} \implies \vec{A} \perp \vec{B}$$

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

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,

$$(\psi_i, \psi_k) = 0 \quad \text{for} \quad \begin{cases} i \neq j & i, j = 1, 2, \dots, n \\ \psi_i \neq 0 & \text{and } \psi_k \neq 0 \end{cases}$$

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**.