Lecture #3

Linear spaces

Definition

A linear (or vector) space is a set of elements (called vectors), with an operation of vector addition and an operation of scalar multiplication

Addition rule:

- if Ψ and φ are vectors (elements) of a space $\Rightarrow$ their sum is also a vector of the same space
- commutativity: $\Psi + \varphi = \varphi + \Psi$
- associativity: $(\Psi + \varphi) + \chi = \Psi + (\varphi + \chi)$
- existence of a zero vector 0 such that $0 + \Psi = \Psi + 0 = \Psi$

- Existence of an inverse vector $-\psi$ such that $\psi + (-\psi) = (-\psi) + \psi = 0$

<u>Multiplication rule</u>:

- the product of a scalar with a vector gives another vector. If φ and ψ are vectors, a and b are scalars, $\Rightarrow a\varphi + b\psi$ is also a vector of the same space
- Distibutivity; $a(\psi + \varphi) = a\psi + a\varphi$
  $(a+b)\psi = a\psi + b\psi$
- associativity; $a(b\psi) = (ab)\psi$
- for each element ψ there must exist a unitary element I and a zero scalar such that $I \cdot \psi = \psi \cdot I = \psi$
  $0 \cdot \psi = \psi \cdot 0 = 0$

The vector space is called <u>complex</u> or <u>real</u>, depending on whether complex or <u>only</u> real numbers are used as scalars.

Examples of linear spaces

1) If $\psi = (x_1, x_2, \dots, x_n)$
$\varphi = (y_1, y_2, \dots, y_n)$

(x_i, y_i - numbers)
with addition defined by
$$\psi + \varphi = (x_1 + y_1, x_2 + y_2, \dots, x_n + y_n)$$
and multiplication defined by $\underset{\text{scalar}}{a}\psi = (ax_1, ax_2, \dots ax_n)$

$\Downarrow$

n-dimensional Euclidean space (R^n)

2) The set of all infinite sequences of numbers $(x_1, x_2, \dots, x_k, \dots)$ such that $\sum_{k=1}^{\infty} |x_k|^2$ is finite with addition and scalar multiplication defined as in the previous example $\Rightarrow$ ℓ^2-space

3) The set of all continuous functions of a real variable x with an addition of two vectors ψ and φ defined by $(\psi + \varphi)(x) = \psi(x) + \varphi(x)$

and multiplication $(a\psi)(x) = a\psi(x)$

4) The set of all functions ψ of a real varia-
x for which an integral $\int |\psi(x)|^2 dx$ is finite, with addition and scalar multiplication defined as in the previous example $\Rightarrow$ L^2-space

What about a "wave function space" (let's call it $\mathcal{E}$)? $\Rightarrow$ $\mathcal{E}$ is a subspace of L^2, which in turn is a subspace of Hilbert space.

· Formal definition of the Hilbert space:

– it's a linear space

– there is a so-called scalar product (also called "inner product") defined as:
- (ψ, φ) = complex number
- $(\psi, \varphi) = (\varphi, \psi)^*$
- $(\psi, a\varphi_1 + b\varphi_2) = a(\psi, \varphi_1) + b(\psi, \varphi_2)$
- $(\psi, \psi) = \|\psi\|^2 \geq 0$ (equality only for $\psi = 0$

- it's separable
- it's complete

we won't go into heavy mathematical details to see where this comes from

So, each quantum state of a particle is characterized by a state vector $|\psi\rangle$, belonging to an abstract space $\mathcal{E}$ (which is a subspace of Hilbert space), called the state space of a particle, i.e. $|\psi\rangle \in \mathcal{E}$.

Dimension and basis of a vector space

A set of N vectors $\varphi_1, \varphi_2, \ldots, \varphi_N$ is said to be linearly independent if and only if the solution of the equation $\sum_{i=1}^{N} a_i \varphi_i = 0$ is $a_1 = a_2 = \ldots = a_N = 0$.

If not all a's are zero $\Rightarrow$ one of the vectors can be expressed as a linear combination of the others $\Rightarrow \varphi = \sum_{i=1}^{N} a_i \varphi_i \Rightarrow$ the set $\{\varphi_i\}$ is linearly dependent.

The dimension of the space is given by the maximum number of linearly independent vectors the space can have. If the vectors $(\varphi_1, \varphi_2, \dots, \varphi_N)$ are linearly independent $\Rightarrow$ the space is N-dimensional. In this case, any vector ψ of the vector space can be expressed as a linear combination

$$\psi = \sum_{i=1}^{N} a_i \varphi_i \qquad (1)$$

set of vectors $\{\varphi_i\} \Rightarrow$ base vectors

If the scalar products $(\varphi_i, \varphi_j) = \delta_{ij} \Rightarrow$ the basis is orthonormal

Kronecker

If the basis spans entire space $\Rightarrow$ it is complete

The expansion coefficients a_i in (1) are called the components of the vector ψ in the basis. Each component $a_j = (\varphi_j, \psi)$.

Examples

1) Are functions $f(x) = 4$, $g(x) = x^2$, $h(x) = e^{2x}$ linearly independent?

Consider $a_1 f(x) + a_2 g(x) + a_3 h(x) =$

$= 4a_1 + a_2 x^2 + a_3 e^{2x} = 0 \Rightarrow$ only if $a_1 = a_2 = a_3 = 0$

$\Downarrow$

f, g, h are linearly independent

2) $f(x) = x$, $g(x) = 5x$, $h(x) = x^2 \Rightarrow$? linearly independent or dependent!

$\Downarrow$

$a_1 x + a_2 \cdot 5x + a_3 \cdot x^2 = 0$

is it valid only if $a_1 = a_2 = a_3 = 0$?

$\Downarrow$

not really $\Rightarrow x(a_1 + 5a_2 + a_3 x) = 0 \Rightarrow$

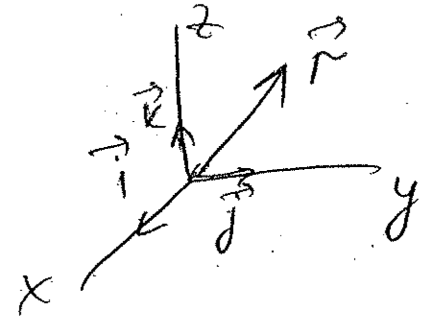
can be if $a_3 = 0$, $a_1 = -5a_2 \neq 0$!

$\Downarrow$

linearly dependent

Is the choice of the basis unique? ⇒ no! (8)

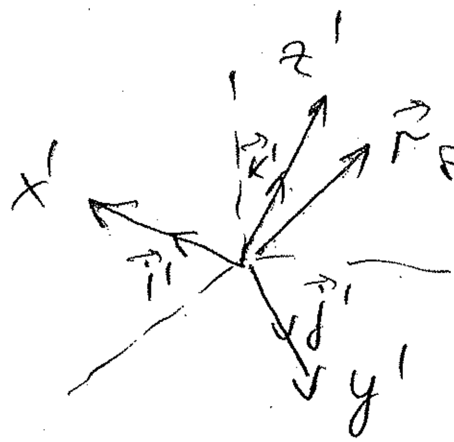
Consider



$\vec r = x\vec i + y\vec j + z$

⇓

expansion of $\vec r$ in the $\vec i, \vec j, \vec k$ - basis



← same vector $\vec r$

$\vec r = x'\vec i' + y'\vec j' + z'\vec k'$

⇓

expansion of $\vec r$ in the $\vec i', \vec j', \vec k'$ - basis

note that expansion coefficients are different in different bases! ⇐

Let's go back to wave functions ⇒

we are used to coordinate representation of the wave function ⇒ $\Psi(\vec r, t)$ ⇒ what if we don't want to use a coordinate-related basis? ⇒ to free state vectors from coordinate meaning ⇒ Dirac introduced a notation, in which he denoted the state

vector $\Psi \Rightarrow$ by a ket vector $|\Psi\rangle$ (9)
its complex conjugate $\Psi^* \Rightarrow$ by a bra $\langle\Psi|$, and the scalar product (φ,Ψ) (which is one of the attributes of Hilbert space, to which state vectors belong!) – by a bra-ket $\langle\varphi|\Psi\rangle$

~~For every ket $|\Psi\rangle$ there exists a unique bra~~ $\langle\Psi|$ and vice versa. If $|\Psi\rangle \in \mathcal{E} \Rightarrow$ $\langle\Psi| \in \mathcal{E}^* \Leftarrow$ dual space of $\mathcal{E}$.

The ket $|\Psi\rangle$ represents the system completely, i.e. knowing $|\Psi\rangle$ means knowing all amplitudes in all possible representations!!
If we need to find the probability of finding the particle at some position in space $\Rightarrow$ work with the coordinate representation: the state vector is given by $\Psi(\vec{r},t) = \langle\vec{r},t|\Psi\rangle$

In the coordinate representation, the scalar product

$$\langle \varphi | \psi \rangle = \int \varphi^*(\vec{r},t)\,\psi(\vec{r},t)\,d^3r$$

If we are concerned with momentum of the particle $\vec{p}$ $\Rightarrow$ it's more convenient to use momentum representation $\Rightarrow$ $\psi(\vec{p},t) = \langle \vec{p},t|\psi\rangle$

Scalar product $\Rightarrow$ $\langle \varphi | \psi \rangle = \int \varphi^*(\vec{p},t) \cdot \psi(\vec{p},t)\,d^3p$

momentum space wave function

Later we will consider cases when it saves a lot of time and effort to choose a more suitable representation!

Properties of kets, bras and brakets

- Every ket has a corresponding bra $\Rightarrow$

$$(|\psi\rangle)^* = \langle \psi | \qquad\qquad |a\psi\rangle = a|\psi\rangle$$

$$(a|\psi\rangle)^* = a^*\langle\psi| \quad ; \quad \langle a\psi| = a^*\langle\psi|$$

complex number

- Scalar product

$\langle \varphi | \psi \rangle \neq \langle \psi | \varphi \rangle$ in general case! $\Rightarrow$

$\langle \varphi | \psi \rangle^* = \langle \psi | \varphi \rangle$

$\Updownarrow$

$$\langle \varphi | \psi \rangle^* = \left(\int \varphi^*(\vec{r},t)\, \psi(\vec{r},t)\, d^3r \right)^* =$$

$$= \int \psi^*(\vec{r},t)\, \varphi(\vec{r},t)\, d^3r = \langle \psi | \varphi \rangle$$

$\langle \varphi | \psi \rangle = \langle \psi | \varphi \rangle$ <u>only</u> if $|\psi\rangle, |\varphi\rangle$ are real!

- The norm $\langle \psi | \psi \rangle$ is real and positive

If $|\psi\rangle$ is <u>normalized</u> $\Rightarrow \langle \psi | \psi \rangle = 1$

- Schwarz inequality

$$|\langle \psi | \varphi \rangle|^2 \leq \langle \psi | \psi \rangle \langle \varphi | \varphi \rangle$$

if $|\psi\rangle$ and $|\varphi\rangle$ are linearly dependent (i.e. $|\psi\rangle = a|\varphi\rangle$) $\Rightarrow$ equality.

- Triangle inequality

$$\sqrt{\langle \psi + \varphi | \psi + \varphi \rangle} \leq \sqrt{\langle \psi | \psi \rangle} + \sqrt{\langle \varphi | \varphi \rangle}$$

if $|\varphi\rangle, |\psi\rangle$ are linearly dependent $\Rightarrow$ equality

- Orthogonality

$|\psi\rangle$ and $|\varphi\rangle$ are orthogonal if $\langle\psi|\varphi\rangle = 0$

- Orthonormality

$|\psi\rangle$ and $|\varphi\rangle$ are orthonormal if they are orthogonal and each has a unit norm:

$\langle\psi|\varphi\rangle = 0$, $\langle\psi|\psi\rangle = 1$, $\langle\varphi|\varphi\rangle = 1$

- Forbidden quantities $\Rightarrow$ $|\psi\rangle|\varphi\rangle$ or $\langle\psi|\langle\varphi|$

unless they belong to different spaces, e.g. $|\psi\rangle \in \mathcal{E}_x$, $|\varphi\rangle \in \mathcal{E}_y$ $\Rightarrow$

$$|\psi\rangle \otimes |\varphi\rangle \in \mathcal{E}_x \otimes \mathcal{E}_y$$

$\uparrow$ tensor product

Physical meaning of the scalar product

1) $\langle\varphi|\psi\rangle$ represents a projection of $|\psi\rangle$ onto $|\varphi\rangle$

2) $\langle\varphi|\psi\rangle$ represents the probability amplitude that the system's state $|\psi\rangle$ will be found in the state $|\varphi\rangle$ after a measurement