Lecture 2. Introduction to Quantum Mechanics - additional

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Math: Basis

In linear algebra, a basis *B* of a finite-dimensional vector space *V* over a field *F* is a linearly-independent subset of *V* that **spans** *V*. If $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n$ are basis vectors of *V*, then

$$c_1\mathbf{v}_1 + \cdots + c_n\mathbf{v}_n = 0 \text{ implies } c_1 = \cdots = c_n = 0$$

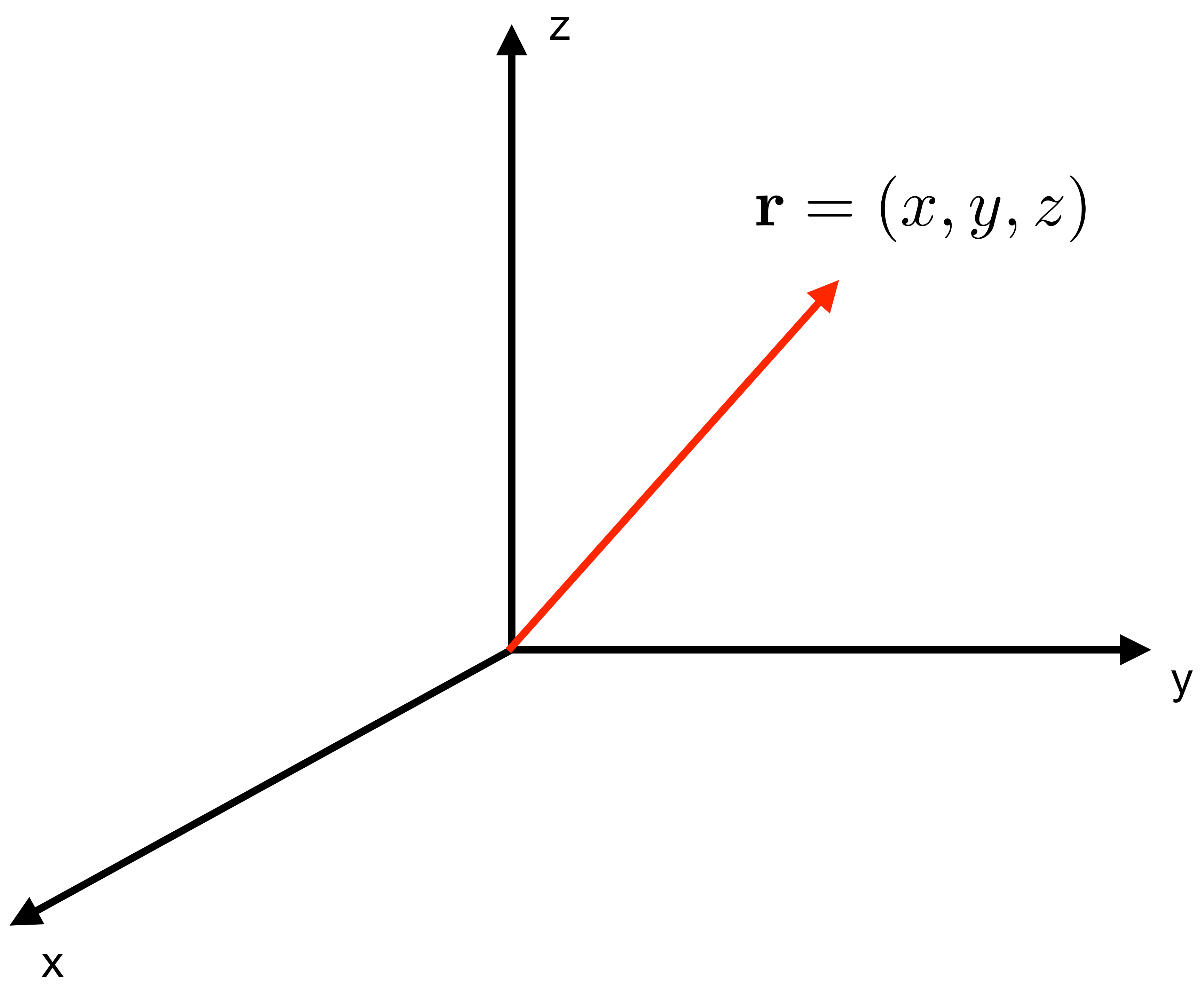
$$\forall \mathbf{w} \in V,\ \exists a_1, \cdots, a_n \text{ such that } \mathbf{w} = a_1\mathbf{v}_1 + \cdots + a_n\mathbf{v}_n$$

This concept can be expanded to *functions*.

Note that two vectors are orthogonal if their inner product is zero.

Math: Basis

For example, let's consider our most familiar "vector space", $\mathbb{R}^3$.



Any point in $\mathbb{R}^3$ can be represented with linear combination of three basis vectors,

$$\hat{e}_1 = [1, 0, 0]^T, \ \hat{e}_2 = [0, 1, 0]^T, \ \hat{e}_3 = [0, 0, 1]^T$$

$$\mathbf{r} = x\hat{e}_1 + y\hat{e}_2 + z\hat{e}_3$$

In other words, basis vectors *span* (or *generate*) all vectors in $\mathbb{R}^3$.

This procedure can be done for the functions.

Math: Dirac Notation

Consider functions as “vectors” - **ket** vectors

$$f(x) \mapsto |f\rangle = [f(x_0), f(x_1), f(x_2), \cdots, f(x_n)]^T$$

Taking *Hermitian conjugate* yields **bra** vectors. We call this Dirac’s bracket notation.

Hermitian conjugate = complex conjugate + transpose.

$$f(x)^* \mapsto \langle f| = [f(x_0)^*, f(x_1)^*, f(x_2)^*, \cdots, f(x_n)^*] = |f\rangle^\dagger$$

In the *function space* - where all functions live - there exists orthogonal basis.

Therefore, we can express a function as a linear combination of such basis functions.

Math: Basis

For example, we can expand certain functions* into the linear combination of sine functions.

$$f(x) = \sum_{n=0}^{\infty} c_n \sin nx$$

Certain set of functions can express *function space*. These are called the basis functions.

In most cases, basis functions are mutually orthogonal. If two functions are orthogonal, their inner product is zero. Inner product of two functions are defined as follows.

$$\langle f, g \rangle = \int f^*(x) g(x)\, dx$$

Math: Hermitian operators

Let's introduce **Dirac notation**.

$$\int f^*(x)g(x)\,dx = \langle f|g\rangle\,, \quad \int f^*(x)\hat{A}g(x)\,dx = \left\langle f\middle|\hat{A}\middle|g\right\rangle$$

An operator is **Hermitian** if

$$\int f^*(x)\hat{A}g(x)\,dx = \int g(x)[\hat{A}f(x)]^*\,dx, \quad \left\langle f\middle|\hat{A}g\right\rangle = \left\langle \hat{A}f\middle|g\right\rangle$$

All operators in quantum mechanics are Hermitian.

Math: Hermitian operators

Hermitian operators have real eigenvalues.

$$\left\langle \psi_n \middle| \hat{A}\psi_n \right\rangle = \langle \psi_n | a_n \psi_n \rangle = a_n$$

By definition, this term should have same value.

$$\left\langle \hat{A}\psi_n \middle| \psi_n \right\rangle = \langle a_n \psi_n | \psi_n \rangle = a_n^*$$

Therefore eigenvalues are real.

Math: Hermitian operators

Theorem. Eigenfunctions of Hermitian operators are orthogonal.

Let's assume that all eigenvalues are different. $\hat{A}\psi_n = a_n\psi_n$

$$\left\langle \psi_m \middle| \hat{A}\psi_n \right\rangle = a_n \left\langle \psi_m | \psi_n \right\rangle$$

$$\left\langle \psi_n \middle| \hat{A}\psi_m \right\rangle = a_m \left\langle \psi_n | \psi_m \right\rangle \implies \left\langle \psi_n \middle| \hat{A}\psi_m \right\rangle^* = a_m \left\langle \psi_m | \psi_n \right\rangle$$

Since *A* is Hermitian, two terms are equivalent.

Eigenvalues a_m and a_n are different unless $m=n$. Therefore

$$\left\langle \psi_m | \psi_n \right\rangle = \delta_{mn}$$

If one includes the normalization condition.

Math: Hermitian operators

Therefore, **eigenfunctions of Hermitian operators constructs orthogonal basis**.

In other words, if we find any solutions of Schrödinger equation, it constructs orthogonal basis.

In other words (again), arbitrary function can be expressed with the linear combination of $\{\psi_n\}_{n=1}^{\infty}$!

Conclusion. Eigenfunctions of quantum-mechanical operators are *complete*.

Digression. If you know linear algebra, …

understanding these arguments can be done in the analogy of **Hermitian matrices**.