

QUANTUM MECHANICS: LECTURE 2

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Abstract

In this lecture, a revision of basic concepts of vector spaces, and vector spaces with a norm. Then a formal definition of a Hilbert spaces is made, with some examples.

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ABSTRACT VECTOR SPACES

In previous courses, the notion of a **vector** was introduced as being an n -tuple of ordered numbers (either real or complex). However, one can have a more general definition for a vector as being an element of a **vector space**. A vector space is a set that satisfies the following property

Let \mathcal{V} be a vector space, and $|\psi\rangle$ and $|\phi\rangle$ are elements of it . Then :

$$\alpha|\psi\rangle + \beta|\phi\rangle, \quad (1)$$

is also an element of that vector space, where α and β are complex or real numbers. The expression (1) is called the **superposition** of the vectors $|\psi\rangle$ and $|\phi\rangle$.

The dimension of \mathcal{V} could either be finite , countably infinite or uncountably infinite (see next section). For finite dimensional- or countably infinite- vector spaces. It is possible to represent a vector $|\psi\rangle$ as a column matrix :

$$|f\rangle \Leftrightarrow \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \end{pmatrix} \quad (2)$$

We can represent the components of the above vector in what-so-called a **spike diagram** representing the magnitude of each component of the vector $|\psi\rangle$.

FUNCTIONS AS VECTORS

It may seem unfamiliar to most readers that functions could be considered as vectors of an uncountably infinite dimensional vector space. In order to see



Figure 1: Spike diagram of a vector in 3 dimensional vector space, and 30 dimensional one.

this, we use the spike diagrams discussed above. This time using a continuous parameter x taking real-number values instead of the discrete index i . The spike diagram for such vector would look like: In fact, this spike diagram looks

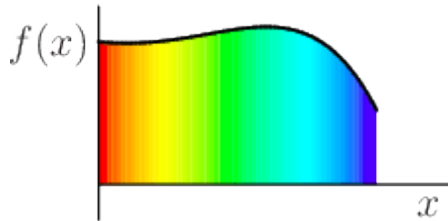


Figure 2: Spike diagram of a vector having infinite components

familiar to the classical graph of a real-valued function $f(x)$: in this way, a

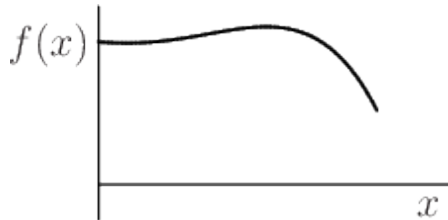


Figure 3: Classical graph of a function $f(x)$

function is just a single vector in an infinite dimensional space. It should be noted that to make the transition to infinite dimensions mathematically meaningful, you need to impose some smoothness constraints on the function. Typically, it is required that the function is continuous, or at least integrable in some sense. These details are not important for our purpose, thus we shant discuss them further.

DUAL SPACES AND INNER PRODUCT

One may define a map $\langle f|$ that sends a vector $|\phi\rangle$ in \mathcal{V} to the real or complex numbers. Defined as - for finite dimensional vector spaces or countably infinite ones:

$$\langle f|\phi\rangle = \sum_i f_i \phi_i \quad (3)$$

or for functions :

$$\langle f|\phi\rangle = \int dx f(x)^* \phi(x) \quad (4)$$

We can easily show that the set of such maps form a vector space themselves, which we call the **dual** vector space and denoted by \mathcal{V}^* . Moreover, the operation between a vector and a (dual) vector is called **inner product** .

The star resembles the complex conjugation $f(x)^$ sometimes they are called linear functionals*

The Bra-Ket notation

Every vector space has its dual. In the notation adopted in quantum mechanics, and invented by Paul Dirac. A member of a vector space is called

a **Ket** and denoted by $|\psi\rangle$, as we have seen, for discrete components it is represented as a column matrix. On the other hand, the elements of the dual space are denoted by a **Bra** $\langle f|$ in Dirac notation. And represented as a row matrix:

$$\langle f| \Leftrightarrow (f_1^* \quad f_2^* \quad f_3^* \quad \dots) \quad (5)$$

The inner product is carried like matrix multiplication between a row and a column

The notation adopted is known as the **Bra-Ket notation**. Since for every vector space there is a dual space. One may turn a Ket vector into a Bra vector, by a one-to-one map. Hence defining the inner product in the vector space itself, calling it an **inner-product space**.

Two vectors $|\psi\rangle$ and $|\phi\rangle$ are called **orthogonal** if and only if :

$$\langle \phi | \psi \rangle = 0$$

Normed spaces

In a similar sense to the magnitude of a vector in the space (like velocity), we can extend this notion to *any* vector with the norm function. $\| \cdot \|$. There are many ways one can define the norm of a vector. However, we are only interested in the norm defined by the inner product:

$$\| \psi \| \equiv \sqrt{\langle \psi | \psi \rangle} \quad (6)$$

Note that the norm is always a **real number**. Vectors with a unit norm is called **normal vectors**.

HILBERT SPACE

An inner product vector space \mathcal{H} , with a norm defined in (6), in addition to another property called *completeness* is called a **Hilbert space**. Hilbert spaces are extremely important in quantum mechanics. They replace the phase spaces of classical mechanics. Hilbert spaces can be finite dimensional or infinite dimensional (both cases we call it **separable** Hilbert spaces), the latter infinite dimensional space might have either continuous and discrete *representations*.

complete vectro space is a space that all Cauchy sequences converge

Basis of a Hilbert space

We can express any vector in the Hilbert space as a linear superposition of $\dim \mathcal{H}$ other vectors. Hence, it is possible to construct orthonormal basis for a Hilbert space. You need as many of them as the dimension of the vector space itself. Given a vector $|\psi\rangle$ in the Hilbert space having a set of orthonormal basis $S = \{|e_i\rangle\}_i$, $|\psi\rangle$ is uniquely expressed in terms of the basis S :

$$|\psi\rangle = \sum_i \langle e_i | \psi \rangle |e_i\rangle \quad (7)$$

The coefficients $c_j = \langle e_j | \psi \rangle$ is sometimes called **Fourier coefficients**. We can have the same argument for the Bra-vectors:

$$\langle \psi | = \sum_i \langle \psi | e_i \rangle \langle e_i | \quad (8)$$

The basis satisfy:

$$\langle e_i | e_j \rangle = \delta_{ij} \quad (9)$$

For function spaces, the basis have continuous parameter x instead of a discrete index the basis therefore are denoted by $|x\rangle$, for all x a real number. A function ϕ is written as :

$$\phi(x) = \langle x | \phi \rangle$$

There is a fundamental difference by what we mean by basis here and the conventional basis taught in Classical mechanics The basis we use are called Schauder basis, whilst the latter is known as Hamel basis

Instead of using the Bra-Ket notation for functions, we shall only denote them by $\phi(x)$.

Note that we need some-sort of structure in the Hilbert space to insure that (7) converges if the sum is infinite. We call the Hilbert space in with the series of this type the ℓ^2 space, or the space of square-summable sequences. Moreover, the integrals used in this course - and in quantum mechanics in general- are known as the *Lebesgue integrals*, they are different from Riemann integrals defined in calculus courses.

Here, we have illustrated the most relevant properties of Hilbert spaces that concern us in the study of introductory quantum mechanics. A lot of mathematical details and rigor has been spared in this lecture. It is urged from the reader to conduct a further reading in the theory of Hilbert space; please consult: *Functional Analysis* by M. Reed and B. Simon.

THE SPACE L^2

Functions form a vector space, as we have seen previously, nevertheless, we need to imply an additional restriction on functions in order to form a Hilbert space. Let $\phi(x)$ be a function defined on the interval $[a, b]$, the norm of this function is defined to be - in accordance to the formal definition of the norm- :

$$\|\phi(x)\| = \sqrt{\int_a^b \phi(x)^* \phi(x) dx} \quad (10)$$

For the norm to exist, the function $\phi(x)$ needs to be **square integrable** on the interval $[a, b]$. It is not hard to show that the set of square-integrable functions on the same interval form a Hilbert space. This Hilbert space is known as the $L^2(R; d\mu)$ space. It reads; the space of square-integrable function on the interval/Region R , with respect to the measure $d\mu$. By measure we mean the volume element that we integrate over. In 1-D case $d\mu = dx$. Sometimes, one wishes to define a *weight* $w(x)$ for the space, but this is out of the scope of this course.

Functions of L^2 could be of several variables, real or complex-valued

The space L^2 can have basis of orthogonal, and normalised functions $(u_1(x), u_2(x), \dots)$ depending on the interval of interest. For example the classical orthogonal polynomials including:

- Hermite polynomials:

$$H_n(x) = K_n^{-1} e^{x^2} \frac{d^n}{dx^n} (e^{-x^2}). \quad (11)$$

They could form basis for the space $L^2(-\infty, +\infty; dx)$.

- Legendre polynomials:

$$L_n^v = K_n^{-1} x^{-v} e^x \frac{d^n}{dx^n} (x^{v+1} e^x). \quad (12)$$

They could form basis for the space $L^2(0, +\infty; dx)$.

- Legendre polynomials (of the first kind):

$$P_n = K_n^{-1} \frac{d^n}{dx^n} (1 - x^2) \quad (13)$$

They could form basis for the space $L^2(0, 1; dx)$.

The second example of L^2 spaces, are the ones used in Fourier analysis. Where $\cos(nkx)$ and $\sin(nkx)$ form an orthonormal basis for a given L^2 space with an interval L . Recall that we can expand any function in a Fourier series

:

$$f(x) = \sum_{n=0}^{\infty} A_n \cos\left(\frac{n\pi x}{L}\right) + B_n \sin\left(\frac{n\pi x}{L}\right) \quad (14)$$

Where :

$$A_n = \int_0^L f(x) \cos\left(\frac{n\pi x}{L}\right) dx \quad (15)$$

$$B_n = \int_0^L f(x) \sin\left(\frac{n\pi x}{L}\right) dx \quad (16)$$

Or expanding the function in a continuous basis (Fourier integral).

NOTE

Advanced readers might not find the discussion in this lecture formal neither accurate enough, as discussing mathematical rigor of Hilbert spaces is very distant from the course aims.

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