QUANTUM MECHANICS: LECTURE 3

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Abstract

An introduction to linear operators in Hilbert space.

CONTENTS

OUTER PRODUCT

For a finite-dimensional vector space, the outer product can be understood as simple matrix multiplication:

$$|\phi\rangle\langle\psi| \doteq \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{pmatrix} \begin{pmatrix} \psi_1^* & \psi_2^* & \cdots & \psi_N^* \end{pmatrix} = \begin{pmatrix} \phi_1\psi_1^* & \phi_1\psi_2^* & \cdots & \phi_1\psi_N^* \\ \phi_2\psi_1^* & \phi_2\psi_2^* & \cdots & \phi_2\psi_N^* \\ \vdots & \vdots & \ddots & \vdots \\ \phi_N\psi_1^* & \phi_N\psi_2^* & \cdots & \phi_N\psi_N^* \end{pmatrix}$$

The outer product is an N×N matrix.

LINEAR OPERATORS

The term 'linear operator' is used in many contexts, in quantum mechanics however, we are interested -mainly- in linear operators, acting on a Hilbert space. Linear operators are maps from a Hilbert space to itself (known mathematically as Endomorphisms). In simple words, they send 'kets' to 'kets'. Operators are represented as square matrices (for finite dimensional or countably infinite dimensional Hilbert spaces). Hence, all the algebra of matrices will apply to operators. Such as :

we shall always mean linear operator when we use the term operator from now on

The algebra of operators

1. Linearity:
   Let $\hat{A}$ and $\hat{B}$ be operators acting on the Hilbert space $\mathcal{H}$,α and β are

scalars, and $|\psi\rangle$ and $|\phi\rangle$ be vectors in $\mathcal{H}$. Then the following properties hold:

$$(\alpha\hat{A}+\beta\hat{B})|\psi\rangle = \alpha(\hat{A}|\psi\rangle) + \beta(\hat{B}|\psi\rangle) \tag{1}$$

Moreover:

$$\hat{A}(\alpha|\psi\rangle + \beta|\phi\rangle) = \alpha(\hat{A}|\psi\rangle) + \beta(\hat{A}|\phi\rangle) \tag{2}$$

A result from above :

$$\hat{A}|\psi\rangle = \sum_i \langle i|\psi\rangle \left(\hat{A}|i\rangle\right) \tag{3}$$

2. Eigenvalue:
A scalar λ is called an **eigenvalue** if it satisfied the equation:

$$\hat{A}|\psi\rangle = \lambda|\psi\rangle \tag{4}$$

Called the **eigenvalue equation,** and the vector $|\psi\rangle$ is called an **eigenket/ eigenvector**. This equation is equivalent to :

$$\det\left(\hat{A} - \lambda\hat{I}\right) = 0 \tag{5}$$

For $\hat{I}$ or just I being the identity operator. An important result from this property is the spectral decomposition, that we shall discuss later in this lecture.

3. Self-adjointness (Hermitian operators)
Let $\hat{A}$ be an operator, then $\hat{A}^\dagger$ is the **hermitian conjugate** of this operator It is simply the hermitian matrix in the matrix representation of $\hat{A}$. The hermitian conjugate acts on the dual space of $\mathcal{H}$ (acts on the Bras). The following properties for the hermitian conjugation are listed below (for reminding)

   - $\left(\hat{A}^\dagger\right)^\dagger = \hat{A}$ involutiveness

   - If an inverse for the operator exists then:

   $$\left(\hat{A}^{-1}\right)^\dagger = \left(\hat{A}^\dagger\right)^{-1}$$

   - Antilinearity:

   $$\left(\alpha\hat{A}+\beta\hat{B}\right)^\dagger = \alpha^*\hat{A}^\dagger + \beta^*\hat{B}^\dagger$$

   - $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger$.

An operator is called **self-adjoint** , if it is equal to its hermitian conjugate:

$$\hat{A}^\dagger = \hat{A}$$

In other words, it acts both on the Kets and on the Bras. An important theorem for self-adjoint operators is stated below:
All the eigenvalues for a self-adjoint operator are real

Other properties of the matrices can be revised from a linear algebra book.

SPECTRAL THEOREM

An important result from linear algebra is the spectral decomposition of an operator in terms of its eigenvalues and eigenvectors. If the set eigenvectors $\{|u_1\rangle, |u_2\rangle, |u_3\rangle \cdots\}$ form a basis for the Hilbert space, and the set of eigenvalues $\{\lambda_i\}$ satisfying:

$$\hat{A}|u_j\rangle = \lambda_j|u_j\rangle \tag{6}$$

Then the operator $\hat{A}$ is decomposed as follows:

$$\hat{A} = \sum_i \lambda_i |u_i\rangle\langle u_i| \tag{7}$$

Note that the outer product $|u_i\rangle\langle u_i|$ is gives the identity matrix / operator I. Hence, we may **diagonalise** the operator $\hat{A}$ if we have found all of its eigenvalues.

If two eigenkets have different eigenvalues they ought to be orthogonal

As for uncountably-infinite dimensional Hilbert spaces , which we refer to by: **inseparable** Hilbert spaces, the spectral theorem reads :

$$\hat{A} = \int d\mu(\lambda)\lambda \tag{8}$$

where, $d\mu(\lambda)$ is the integration measure that depends on the nature of spectrum for the measurement outcomes in the theory. We are not going to go further in the details, as they are beyond the scope of our course.

PROJECTION OPERATORS

The identity operator

From the commutativity of Kets with (complex) scalars now follows that

$$\sum_{i\in\mathbb{N}} |e_i\rangle\langle e_i| = \hat{I} \tag{9}$$

must be the identity operator, which sends each vector to itself. This can be inserted in any expression without affecting its value, for example

$$\langle v|w\rangle = \langle v| \sum_{i\in\mathbb{N}} |e_i\rangle\langle e_i|w\rangle = \langle v| \sum_{i\in\mathbb{N}} |e_i\rangle\langle e_i| \sum_{j\in\mathbb{N}} |e_j\rangle\langle e_j|w\rangle = \langle v|e_i\rangle\langle e_i|e_j\rangle\langle e_j|w\rangle \tag{10}$$

Projection operators

We define the projection operator $\hat{P}_\alpha$ for a normalised vector $|\alpha\rangle$,as :

$$\hat{P}_\alpha \equiv |\alpha\rangle\langle\alpha| \tag{11}$$

. Observe that the projection operator is self-adjoint. and satisfies the identity:

$$\hat{P}_\alpha^2 = |\alpha\rangle\langle\alpha||\alpha\rangle\langle\alpha| = |\alpha\rangle\langle\alpha| = \hat{P}_\alpha \tag{12}$$

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UNITARY OPERATORS

An operator $\hat{U}$ is called **unitary** if it preserves the inner product for two vectors, and thereby the norm . This also can be stated as:

$$\hat{U}^\dagger\hat{U} = \hat{U}\hat{U}^\dagger = \hat{I}. \tag{13}$$

Therefore, a unitary, self-adjoint operator is its own inverse .

EXAMPLES

Rotation in the Euclidean 2-D space

A vector in the 2-D plane is represented by :

$$|r\rangle = \begin{pmatrix} x \\ y \end{pmatrix} \tag{14}$$

The basis vectors are:

$$|e_x\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |e_y\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{15}$$

We can define a rotation operator $\hat{R}(\vartheta)$, that acts on the vector $|r\rangle$ by rotating it with an angle ϑ. This operator has a matrix representation:

$$\hat{R} = \begin{pmatrix} \cos\vartheta & -\sin\vartheta \\ \sin\vartheta & \cos\vartheta \end{pmatrix} \tag{16}$$

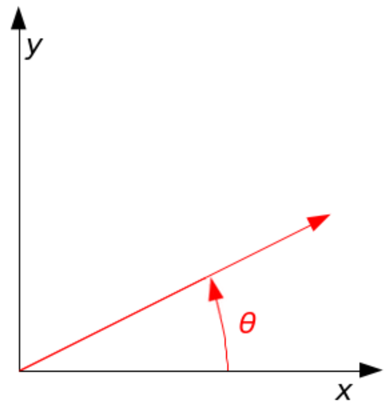

Figure 1: The rotation in 2-D space, carried put by the rotation operator.

The differential operator

There are operators also acting on function space, they have the same properties as the operators discussed above, but with slight modifications. For example, the operators acting on function space cannot have an *explicit* matrix representation.

The most famous operators which act on function space are the differential operators; denoted by $\hat{L}$. There are a variety of differential operators. They play an important rôle in the theory of differential equations. In fact, most of the problems in quantum mechanics are related to the analysis of the differential operators related to dynamical observables; as we shall see.

Take the function $f(x) = e^{\lambda x}$. It is the eigenfunction of the differential operator $\frac{d}{dx}$, with an eigenvalue λ. Hence, we conclude that $e^{\lambda x}$, is a solution to the differential equation:

$$\frac{d}{dx}(f(x) = \lambda f(x) \tag{17}$$

The operator $\frac{d^2}{dx^2}$ has two eigenfunctions $e^{+\lambda x}$ and $e^{-\lambda x}$ they resemble solutions for the differential equation :

$$\frac{d^2}{dx^2}(f(x) = \lambda f(x) \tag{18}$$

And by the superposition principle, a general solution would be:

$$f(x) = Ae^{+\lambda x} + Be^{-\lambda x} \tag{19}$$

COMMUTATORS

Just like ordinary matrix multiplication, the product between operators is generally non-commutative. In fact, this particular property of operator multiplication is behind the unfamiliar phenomena observed in quantum mechanics, thus generally we have :

$$\hat{A}\hat{B} \neq \hat{B}\hat{A} \tag{20}$$

We define the **commutator** between two operators as:

$$[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A} \tag{21}$$

The commutator satisfies the following properties:

$[\alpha A + \beta B, C] = \alpha[A, C] + \beta[B, C]$	linearity in both slots.
$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$	Jacobi Identity
$[AB, C] = [A, C]B + A[B, C]$	Product rule

For the last property, it is a rule of thumb to think of the commutator as a kind of derivative $\mathcal{D}_C = [\cdot, C]$:

$$\mathcal{D}_C\,(AB) = \mathcal{D}_C(A)B + A\mathcal{D}_C(B)$$

function of operator

Just like scalars, one can a function of an operator: $f(\hat{A})$ This is justified because, one can expand the function $f(\hat{A})$ as a series:

$$f(\hat{A}) \approx f_0 I + f_1\hat{A} + \frac{f_2}{2!}\hat{A}\hat{A} + \ldots \tag{22}$$

Since operator product is defined, the function itself is well-defined as well Commutator of a function is given by :

$$[f(\hat{B}), \hat{A}] = \left(\frac{df(\hat{B})}{d\hat{B}}\right)[\hat{B}, \hat{A}] \tag{23}$$

Provided that

$$[[\hat{B}, \hat{A}], \hat{A}] = 0$$

Another important formula to learn is the Hadamard Lemma:

$$e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + [\hat{A}, \hat{B}] + \frac{1}{2!}[\hat{A}, [\hat{A}, \hat{B}]] + \ldots \tag{24}$$

commuting operators

For two commuting operators,

$$[\hat{A}, \hat{B}] = 0 \tag{25}$$

one can find a common set of eigenbasis :

$$\hat{A}|i\rangle = a_i|i\rangle \tag{26}$$

$$\hat{B}|i\rangle = b_i|i\rangle \tag{27}$$

The eigenkets form a mutual eigenbasis for the states $\hat{A}|\psi\rangle$ and $\hat{B}|\psi\rangle$. Hence one can simultaneously diagonalise both operators.

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