Vector spaces and operators

Sourendu Gupta

TIFR Graduate School

Quantum Mechanics 1
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Vectors

Take vectors such as $\mathbf{x} = (x_1, x_2, x_3)$ and $\mathbf{y} = (y_1, y_2, y_3)$. Let a, b, c, *etc.*, be scalars. Then, the following are true—

1. A vector multiplied by a scalar is a vector: $a\mathbf{x} = (ax_1, ax_2, ax_3)$. Addition of scalars is distributive over multiplication by a vector. Multiplication of scalars is compatible with multiplication by a vector.
2. Two vectors can be added to give a new vector: $\mathbf{x} + \mathbf{y} = x_1 + y_1, x_2 + y_2, x_3 + y_3$. Vector addition is commutative: $\mathbf{x} + \mathbf{y} = \mathbf{y} + \mathbf{x}$, and associative: $(\mathbf{x} + \mathbf{y}) + \mathbf{z} = \mathbf{x} + (\mathbf{y} + \mathbf{z})$. Multiplication by scalars is distributive over vector addition: $a(\mathbf{x} + \mathbf{y}) = a\mathbf{x} + a\mathbf{y}$.
3. There exists a zero vector: $\mathbf{0}$ such that $\mathbf{x} + \mathbf{0} = \mathbf{x}$ for any vector $\mathbf{x}$. Every vector has a negative; a vector and its negative add up to $\mathbf{0}$.
4. There is an inner product (dot product): $\mathbf{x} \cdot \mathbf{y} = x_1 y_1 + x_2 y_2 + x_3 y_3$.

Transformations of bases

Using the operations that are allowed in a vector space, we can form operators on vector spaces, *i.e.*, operations which take any basis $\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_D\}$ and creates a new set of vectors

$$\begin{aligned} \mathbf{y}_1 &= a_{11}\mathbf{x}_1 + a_{12}\mathbf{x}_2 + \cdots + a_{1D}\mathbf{x}_D, \\ \mathbf{y}_2 &= a_{21}\mathbf{x}_1 + a_{22}\mathbf{x}_2 + \cdots + a_{2D}\mathbf{x}_D, \quad \cdots \\ \mathbf{y}_D &= a_{D1}\mathbf{x}_1 + a_{D2}\mathbf{x}_2 + \cdots + a_{DD}\mathbf{x}_D. \end{aligned}$$

The scalar coefficients in this linear transformation can be collected together into the matrix

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1D} \\ a_{21} & a_{22} & \cdots & a_{2D} \\ \vdots & \vdots & \cdots & \vdots \\ a_{D1} & a_{D2} & \cdots & a_{DD} \end{pmatrix}.$$

Linear transformations

- If the new set $\{\mathbf{y}_i\}$ is to be a basis, then the vectors must be linearly independent. This implies that for the new set to be a basis, one must have $\mathrm{Det}\, A \neq 0$. (**Prove this**).
- Usually, linear operations are introduced as linear transformations of the components of a vector through the equation $\widetilde{\mathbf{v}} = A\mathbf{v}$. (**Show that this follows from the transformation of bases**)
- Given that we have defined addition of vectors and multiplication by scalars as the only way to generate new vectors out of those at hand, the transformation of bases are the only operations we are allowed. Thus, linear transformations of vector spaces are the only transformations that we can deal with.
- Every linear operator on a vector space clearly has a representation as a matrix. Any linear operator that takes an orthonormal basis into another orthonormal basis is an orthogonal transformation. (**Prove this**)

Dirac Bra and Ket notation

An inner product of a vector, $\mathbf{v}$, with itself is usually denoted by $\mathbf{v}\cdot\mathbf{v}$. When the vector is represented by a column of components, then this notation actually means $\mathbf{v}^T\mathbf{v}$, where $\mathbf{v}^T$ is the transpose, *i.e.*, a row of components. Then, using the usual rules of matrix multiplication, $\mathbf{v}\cdot\mathbf{v} = v_1^2 + v_2^2 + \cdots + v_3^2$. For a vector with complex components, $\mathbf{v}\cdot\mathbf{v} \equiv \mathbf{v}^\dagger\mathbf{v}$, where the Hermitean conjugate, $\mathbf{v}^\dagger$ is the row vector with each component being the complex conjugate of the column vector's component.

Dirac introduced the notation $|v\rangle$ (called **ket**) for the column vector $\mathbf{v}$ and the notation $\langle v|$ (called **bra**) for the Hermitean conjugate $\mathbf{v}^\dagger$. An inner product $\langle w|v\rangle$ is called a **bracket**, and is a complex number (**c-number**).

Measurements are Hermitean operators

- A measurement on a quantum state gives a single number (scalar, c-number). Since a quantum state is a vector, $|v\rangle$, there is only one way to form a scalar from it, and that is to take an inner product.
- Since the result of a measurement on a single quantum state, $|v\rangle$, cannot involve some other quantum state, $|w\rangle$. Hence, inner products such as $\langle w|v\rangle$ seem to be ruled out.
- Is $\langle v|v\rangle$ the only possible representation of a measurement? No, because it is possible to represent every measurement by an appropriate operator A so that the result of the measurement is $\langle v|A|v\rangle$.
- Dynamical measurements ($\mathbf{q}$, $\mathbf{p}$, H, $\mathbf{L}$, *etc.*) must all yield real numbers. If A is the operator that describes a dynamical measurement, then one must have $\langle v|A|v\rangle^* = \langle v|A|v\rangle$. But by definition $\langle v|A|v\rangle^* = \langle v|A^\dagger|v\rangle$. Hence one has $A^\dagger = A$ for a dynamical measurement. Such operators are called Hermitean operators.

Independent measurements and ensembles (1)

- An **ensemble of quantum systems** is a collection of identical systems which have no definite phase correlations with each other. Thus the same measurement made on different members of the ensemble are totally uncorrelated with each other.
- An ensemble is specified by a **density matrix**, ρ. This is a Hermitean operator with unit trace.
- If one of the eigenvalues of ρ is unity (and the remainder, therefore, zero), then in the diagonal basis one has $\rho = |v\rangle\langle v|$, and each member of the ensemble is said to be in the **pure state** $|v\rangle$. Otherwise the ensemble is said to be in a **mixed state**.
- A mixed state is not a coherent superposition of quantum states. A mixed state density matrix describes an ensemble in which different members are in different states.

Independent measurements and ensembles (2)

- The expectation value of any operator in the ensemble is $\mathrm{Tr}\,\rho A$. If the ensemble corresponds to a pure state, *i.e.*, $\rho = |v\rangle\langle v|$, then the expectation value $\mathrm{Tr}\,\rho A = \langle v|A|v\rangle$, as expected. If $|v\rangle$ is an eigenstate of A, then every measurement yields the same eigenvalue. Otherwise, a measurement on different members of the pure state ensemble yield different eigenvalues and the average of these measurements is the expectation value.
- **By computing the variance of measurements in different members of the ensemble, is it possible to check whether one has a pure state or a mixed state?**

Eigenbases of Hermitean operators

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- **Eigenvectors of Hermitean operators are orthogonal to each other**. Let $|\lambda\rangle$ and $|\mu\rangle$ be two distinct eigenvectors of a Hermitean operator A with eigenvalues λ and μ respectively. Now $\langle\mu|A|\lambda\rangle = \lambda\langle\mu|\lambda\rangle$ where A acts to the right. Also, $\langle\lambda|A|\mu\rangle = \mu\langle\lambda|\mu\rangle$. But $\langle\lambda|A|\mu\rangle^* = \langle\mu|A^\dagger|\lambda\rangle = \langle\mu|A|\lambda\rangle$. Hence, if $\mu \neq \lambda$, one has $\langle\mu|\lambda\rangle = 0$.

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- When the two eigenvalues are equal, the eigenvectors need not be orthogonal. However, one can always construct two linear combinations which are orthogonal to each other (by the **Gram-Schmidt process**).

A problem

Consider the matrix

$$M = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

1. Is this matrix Hermitean?
2. What are the eigenvalues and eigenvectors of this matrix?
3. Are there linear combinations of eigenvectors which are also eigenvectors?
4. Is the unitary transformation that diagonalizes M unique?

Diagonalizing a matrix

- Collect the eigenvectors of A into a matrix U such that every column of U is one of the eigenvectors. Then $U^\dagger U = 1$, since the eigenvectors are orthonormal. Also, $U^\dagger AU$ is diagonal, *i.e.*, **Hermitean matrices can be diagonalized by unitary transformations**.
- **The (normalized) eigenvectors, $|i\rangle$, of A with eigenvalues λ_i (here $1 \le i \le D$) form a basis**. As a result, any normalized state can be written in the form

$$|\psi\rangle = \sum_{i=1}^{D} \psi_i |i\rangle, \qquad \text{where} \qquad \sum_{i=1}^{D} |\psi_i|^2 = 1.$$

- A measurement of A in the quantum state $|i\rangle$ would always give the value λ_i. For a superposition of eigenstates, as above, each measurement could give a different value; but with average

$$\langle\psi|A|\psi\rangle = \sum_{i=1}^{D} |\psi_i|^2 \lambda_i.$$

Commuting operators

- Two operators A and B commute if $AB = BA$.
- The **commutator** of A and B is $[A, B] = AB - BA$. $[A, B] = 0$ when the operators commute.
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$$0 = \sum_k (A_{ik} B_{kj} - B_{ik} A_{kj}) = (\lambda_i - \lambda_j) B_{ij}.$$

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A problem

Consider the matrices

$$A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad \text{and} \qquad B = \frac{1}{3}\begin{pmatrix} 1 & -2 & -2 \\ -2 & 1 & -2 \\ -2 & -2 & 1 \end{pmatrix}.$$

1. Are these matrices simultaneously diagonalizable?
2. What are the eigenvalues and eigenvectors of A?
3. Use the eigenvectors of A to construct an unitary transformation, U. Find $U^\dagger BU$.
4. Construct a one-parameter (θ) set of unitary matrices $V(\theta)$ such that $V(\theta)^\dagger U^\dagger AUV(theta)$ are diagonal for all θ. Find what happens to $V(\theta)^\dagger U^\dagger AUV(theta)$ as a function of θ.
5. Is there an unique set of common eigenvectors of A and B?

Complete set of commuting operators

- If a set of (Hermitean) operators $\{A_1, A_2, \cdots, A_N\}$ all commute with each other, and no other operator can be found in the vector space which commute with this set, then this is called a complete set of commuting operators.
- There may be distinct complete sets of commuting operators in the same vector space.
- Given a complete set of commuting operators, there is an unique unitary transformation which diagonalizes all of them simultaneously. (If the set is not complete, then the unitary transformation may not be unique: see the caviat on the previous page).
- Since, the unitary transformation is unique, each eigenvector is uniquely labelled by the eignvalue of each operator: $|\lambda_1, \lambda_2, \cdots, \lambda_N\rangle$. **A quantum state is completely specified by the eigenvalues of a complete set of commuting operators**.

Who is afraid of Hilbert spaces?

These words will not appear in this course again

1. We have seen how to define complete bases of vectors, and how to use these bases to give the components of an arbitrary vector. All possible vectors in a **vector space** are generated by changing these components. A real vector space has real components; a complex vector space needs complex components.
2. A vector space is **complete** if every (Cauchy) sequence of vectors converges to a point in the space. (Counterexample)
3. Every complete vector space is a Hilbert space. If the components of the vectors are complex, then this is a complex vector space.
4. A separable Hilbert space is one in which a countable set of commuting operators exist, *i.e.*, a countable set of eigenvalues specify each vector.

Summary: the postulates of quantum mechanics

Postulate 1

Starting from the analysis of the double slit experiment, we have uncovered the fact that quantum states are elements of a vector space.

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Postulate 1

Starting from the analysis of the double slit experiment, we have uncovered the fact that quantum states are elements of a vector space.

Postulate 2

The most natural construction on a vector space is of linear operators, and we identified these with physical quantities.

References

1. The Principles of Quantum Mechanics, by P. A. M. Dirac. The material in this lecture is a paraphrasing of parts of this book.
2. Quantum Mechanics (Non-relativistic theory), by L. D. Landau and E. M. Lifschitz. The material in this (and the previous) lecture roughly correspond to the first chapter of this book.
3. The Feynman Lectures in Physics (Vol 3), by R. P. Feynman *et al*. The material in this lecture has a tiny bit of overlap with Chapter 20 of this book.
4. Mathematical Methods for Physicists, by G. Arfken. This book contains chapters on matrices and vector spaces which will be useful throughout this course.