Vector spaces and operators

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Quantum states are vectors

We saw that the state of a quantum particle is specified by a wave function $\psi(\mathbf{x}, t)$. We saw that the probability of finding a particle at position $\mathbf{x}$ at time t is proportional to $|\psi(\mathbf{x}, t)|^2$.

Since the probability that the particle is somewhere is unity, one has

$$\int d^D x \, |\psi(\mathbf{x}, t)|^2 = 1.$$

So the wave function lies in the space of square integrable functions. This is a vector space.

We may try to generalize this and say that the state of a quantum particle, *i.e.*, a quantum state is given by a vector in some space. We will try to find whether this is a meaningful statement.

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).

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 $\{\hat{\mathbf{x}}_1, \hat{\mathbf{x}}_2, \cdots, \hat{\mathbf{x}}_D\}$ and creates a new set of vectors

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

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 $\{\hat{\mathbf{y}}_i\}$ is to be a basis, then the vectors must be linearly independent. This implies that $\det A \neq 0$. (Prove this).
- We have defined addition of vectors and multiplication by scalars as the only way to generate new vectors out of those at hand. So, linear transformations are the only possible operations.
- We can also think of linear operations as linear transformations of the components of a vector through the equation $\widetilde{\mathbf{v}} = A\mathbf{v}$.
- Any linear operator that takes an orthonormal basis into another orthonormal basis is an orthogonal transformation. (Prove this)

Measurements are Hermitean operators

The result of a measurement on a quantum state $|v\rangle$ is a scalar.

- One scalar is $\langle v|v\rangle$; has only a single value, therefore not a general measurement.
- A measurement on $|v\rangle$ cannot generally involve another quantum state, $|w\rangle$. Hence, inner products such as $\langle w|v\rangle$ cannot generally describe a measurement.
- We could try to associte a measurement with a linear operator, *i.e.*, a matrix A. The result of the measurement can be $\langle v|A|v\rangle$.
- Measurements ($\mathbf{q}$, $\mathbf{p}$, H, $\mathbf{L}$, *etc.*) must yield real numbers. If A is a measurement, then $\langle v|A|v\rangle^* = \langle v|A|v\rangle$. But by definition $\langle v|A|v\rangle^* = \langle v|A^\dagger|v\rangle$. Hence $A^\dagger = A$ for a measurement. Such operators are called Hermitean operators.

Quantum states are not exactly vectors

Since we work with only normalized quantum states, $|v\rangle$, it is clear that $|w\rangle = \alpha\,|v\rangle$ is the same state, where α is any complex number. No matter what the value of α, after normalization, $|w\rangle$ reduces to $|v\rangle$.

Furthermore, since $\langle w| = \alpha^*\,\langle v|$, it turns out that $\langle w|\,A\,|w\rangle = |\alpha|^2\,\langle v|\,A\,|v\rangle$. Normalization removes this factor of $|\alpha|^2$. As a result, all physical measurements in the two states give the same result.

As a result, every vector does not specify an unique quantum state. Instead, a quantum state is a ray in a complex vector space. The same thing is meant if we say that a quantum state is a projective vector.

A projective space

Consider a one-dimensional real vector space: the real line. There are an infinite number of vectors, one for every point on the real line. In the projective version of this, every non-zero vector $|v\rangle$ is equivalent to the point unity. So the only two projective vectors are $|0\rangle$ and $|1\rangle$.

Problem 3.1

Consider the two-dimensional real vector space: a plane. We can construct from this the space of two-dimensional real projective vectors. Construct and describe this space.

Problem 3.2

Similarly, construct and describe the space of one-dimensional complex vectors.

Eigenbases of Hermitean operators

- Diagonal elements of Hermitean operators are real.
- Eigenvalues of Hermitean operators are real. If $|\lambda\rangle$ is a (normalized) eigenvector of A with eigenvalue λ, then $\langle\lambda| A |\lambda\rangle = \lambda$. Since $\lambda^* = \langle\lambda| A |\lambda\rangle^* = \langle\lambda| A^\dagger |\lambda\rangle = \lambda$, λ is real.
- 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 $\langle\mu|\lambda\rangle = 0$.
- 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).

Diagonalizing a matrix

- Collect the eigenvectors of A into a matrix U every column of which is one of the eigenvectors. Then $U^\dagger U = 1$, since the eigenvectors are orthonormal. Since, $U^\dagger A U$ is diagonal, unitary matrices diagonalize Hermitean matrices.
- The eigenvectors, $|i\rangle$, of A with eigenvalues λ_i (with $1 \le i \le D$) form a basis. A measurement of A in the state $|i\rangle$ will only give the value λ_i.
- Any state can be written in the form

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

Each measurement of A on $|\psi\rangle$ 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.
- If two operators commute, then they have the same eigenstates (*i.e.*, they are simultaneously diagonalizable). Let $|i\rangle$ be the eigenstates of A with eigenvalues λ_i. The matrix elements of A are $A_{ij} = \langle i|A|j\rangle$ and those of B are B_{ij}. Also, $A_{ij} = \lambda_i \delta_{ij}$. Since the operators commute, one has

$$0 = \sum_k (A_{ik}B_{kj} - B_{ik}A_{kj}) = (\lambda_i - \lambda_j)B_{ij}.$$

When $i \neq j$, the equality demands that $B_{ij} = 0$. Hence B is diagonal in the same basis as A. (There is a small gap in the proof; fix it.)

Problem 3.3

Consider the matrix

$$M = \frac{1}{2}\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}.$$

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?

Problem 3.4

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 $V(\theta)^\dagger U^\dagger BUV(\theta)$ 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. (Of a separable, complex Hilbert space, if you want to be pedantic)

Postulate 2

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

Keywords and References

Keywords

wave function, quantum state, ket. bra, bracket, c-number, linear operators, orthogonal operators, unitary operators, Hermitean operators, ray, projective space, eigenvalues, eigenvectors, Gram-Schmidt process, commutator, vector space, Hilbert space, completeness, Cauchy sequence.

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