

ADVANCED QUANTUM MECHANICS



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Advanced Quantum Mechanics

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CHAPTER OVERVIEW

1: Linear Vector Spaces and Hilbert Space

The modern version of quantum mechanics was formulated in 1932 by John von Neumann in his famous book *Mathematical Foundations of Quantum Mechanics*, and it unifies Schrödingers wave theory with the matrix mechanics of Heisenberg, Born, and Jordan. The theory is framed in terms of linear vector spaces, so the first couple of lectures we have to remind ourselves of the relevant mathematics.

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1.1: Linear Vector Spaces

Consider a set of vectors, denoted by $|\psi\rangle, |\phi\rangle$, etc., and the complex numbers a, b, c , etc. A linear vector space $\mathcal{V}$ is a mathematical structure of vectors and numbers that obeys the following rules:

1. $|\psi\rangle + |\phi\rangle = |\phi\rangle + |\psi\rangle$ (commutativity),
2. $|\psi\rangle + (|\phi\rangle + |\chi\rangle) = (|\psi\rangle + |\phi\rangle) + |\chi\rangle$ (associativity),
3. $a(|\psi\rangle + |\phi\rangle) = a|\psi\rangle + a|\phi\rangle$ (linearity),
4. $(a + b)|\psi\rangle = a|\psi\rangle + b|\psi\rangle$ (linearity),
5. $a(b|\phi\rangle) = (ab)|\phi\rangle$.

There is also a null vector 0 such that $|\psi\rangle + 0 = |\psi\rangle$, and for every $|\psi\rangle$ there is a vector $|\phi\rangle$ such that $|\psi\rangle + |\phi\rangle = 0$.

For each vector $|\phi\rangle$ there is a dual vector $\langle\phi|$, and the set of dual vectors also form a linear vector space $\mathcal{V}^*$. There is an inner product between vectors from $\mathcal{V}$ and $\mathcal{V}^*$ denoted by $\langle\psi|\phi\rangle$. The inner product has the following properties:

1. $\langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*$,
2. $\langle\psi|\psi\rangle \geq 0$,
3. $\langle\psi|\psi\rangle = 0 \Leftrightarrow |\psi\rangle = 0$,
4. $|\psi\rangle = c_1|\psi_1\rangle + c_2|\psi_2\rangle \Rightarrow \langle\phi|\psi\rangle = c_1\langle\phi|\psi_1\rangle + c_2\langle\phi|\psi_2\rangle$,
5. $\|\phi\| \equiv \sqrt{\langle\phi|\phi\rangle}$ is the norm of $|\phi\rangle$.

If $\|\phi\| = 1$, the vector $|\phi\rangle$ is a unit vector. The set of unit vectors $\{e^{i\varphi}|\psi\rangle\}$ with $\varphi \in [0, 2\pi)$ form a so-called ray in the linear vector space. A linear vector space that has a norm $\|\cdot\|$ (there are many different ways we can define a norm) is called a Hilbert space. We will always assume that the linear vector spaces are Hilbert spaces.

For linear vector spaces with an inner product we can derive the Cauchy-Schwarz inequality, also known as the Schwarz inequality:

$$|\langle\phi|\psi\rangle|^2 \leq \langle\psi|\psi\rangle\langle\phi|\phi\rangle \quad (1.1)$$

This is a very important relation, since it requires only the inner product structure. Relations that are based on this inequality, such as the Heisenberg uncertainty relation between observables, therefore have a very general validity.

If two vectors have an inner product equal to zero, then these vectors are called orthogonal. This is the definition of orthogonality. When these vectors are also unit vectors, they are called orthonormal. A set of vectors $|\phi_1\rangle, |\phi_2\rangle, \dots, |\phi_N\rangle$ are linearly independent if

$$\sum_j a_j |\phi_j\rangle = 0 \quad (1.2)$$

implies that all $a_j = 0$. The maximum number of linearly independent vectors in $\mathcal{V}$ is the dimension of $\mathcal{V}$. Orthonormal vectors form a complete orthonormal basis for $\mathcal{V}$ if any vector can be written as

$$|\psi\rangle = \sum_{k=1}^N c_k |\phi_k\rangle \quad (1.3)$$

and $\langle\phi_j|\phi_k\rangle = \delta_{jk}$. We can take the inner product of $|\psi\rangle$ with any of the basis vectors $|\phi_j\rangle$ to obtain

$$\langle\phi_j|\psi\rangle = \sum_{k=1}^N c_k \langle\phi_j|\phi_k\rangle = \sum_{k=1}^N c_k \delta_{jk} = c_j \quad (1.4)$$

Substitute this back into the expansion of $|\psi\rangle$, and we find

$$|\psi\rangle = \sum_{k=1}^N |\phi_k\rangle \langle\phi_k|\psi\rangle \quad (1.5)$$

Therefore $\sum_k |\phi_k\rangle \langle\phi_k|$ must act like the identity. In fact, this gives us an important clue that operators of states must take the general form of sums over objects like $|\phi\rangle\langle\chi|$.

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1.2: Operators in Hilbert Space

The objects $|\psi\rangle$ are vectors in a Hilbert space. We can imagine applying rotations of the vectors, rescaling, permutations of vectors in a basis, and so on. These are described mathematically as operators, and we denote them by capital letters A, B, C, etc. In general we write

$$A|\phi\rangle = |\psi\rangle \quad (1.6)$$

for some $|\phi\rangle, |\psi\rangle \in \mathcal{V}$. It is important to remember that operators act on all the vectors in Hilbert space. Let $\{|\phi_j\rangle\}_j$ be an orthonormal basis. We can calculate the inner product between the vectors $|\phi_j\rangle$ and $A|\phi_k\rangle$:

$$\langle\phi_j| (A|\phi_k\rangle) = \langle\phi_j|A|\phi_k\rangle \equiv A_{jk} \quad (1.7)$$

The two indices indicate that operators are matrices.

As an example, consider two vectors, written as two-dimensional column vectors

$$|\phi_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\phi_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (1.8)$$

and suppose that

$$A = \begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix} \quad (1.9)$$

We calculate

$$A_{11} = \langle\phi_1|A|\phi_1\rangle = (1, 0) \cdot \begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = (1, 0) \cdot \begin{pmatrix} 2 \\ 0 \end{pmatrix} = 2 \quad (1.10)$$

Similarly, we can calculate that $A_{22} = 3$, and $A_{12} = A_{21} = 0$ (check this). We therefore have that $A|\phi_1\rangle = 2|\phi_1\rangle$ and $A|\phi_2\rangle = 3|\phi_2\rangle$.

Complex numbers a have complex conjugates a^* and vectors $|\psi\rangle$ have dual vectors $\langle\phi|$. Is there an equivalent for operators? The answer is yes, and it is called the adjoint, or Hermitian conjugate, and is denoted by a dagger $\dagger$. The natural way to define it is according to the rule

$$\langle\psi|A|\phi\rangle^* = \langle\phi|A^\dagger|\psi\rangle \quad (1.11)$$

for any $|\phi\rangle$ and $|\psi\rangle$. In matrix notation, and given an orthonormal basis $\{|\phi_j\rangle\}_j$, this becomes

$$\langle\phi_j|A|\phi_k\rangle^* = A_{jk}^* = \langle\phi_k|A^\dagger|\phi_j\rangle = A_{kj}^\dagger \quad (1.12)$$

So the matrix representation of the adjoint $A^\dagger$ is the transpose and the complex conjugate of the matrix A, as given by $(A^\dagger)_{jk} = A_{kj}^*$. The adjoint has the following properties:

1. $(cA)^\dagger = c^*A^\dagger$,
2. $(AB)^\dagger = B^\dagger A^\dagger$,
3. $(|\phi\rangle)^\dagger = \langle\phi|$.

Note the order of the operators in 2: AB is generally not the same as BA. The difference between the two is called the commutator, denoted by

$$[A, B] = AB - BA \quad (1.13)$$

For example, we can choose

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (1.14)$$

which leads to

$$\begin{aligned} [A, B] &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & -2 \\ 2 & 0 \end{pmatrix} \neq 0. \end{aligned} \quad (1.15)$$

Many, but not all, operators have an inverse. Let $A|\phi\rangle = |\psi\rangle$ and $B|\psi\rangle = |\phi\rangle$. Then we have

$$BA|\phi\rangle = |\phi\rangle \quad \text{and} \quad AB|\psi\rangle = |\psi\rangle \quad (1.16)$$

If Eq. (1.16) holds true for all $|\phi\rangle$ and $|\psi\rangle$, then B is the inverse of A , and we write $B = A^{-1}$. An operator that has an inverse is called invertible. Another important property that an operator may possess is positivity. An operator is positive if

$$\langle\phi|A|\phi\rangle \geq 0 \quad \text{for all } |\phi\rangle \quad (1.17)$$

We also write this as $A \geq 0$.

From the matrix representation of operators you can easily see that the operators themselves form a linear vector space:

1. $A + B = B + A$,
2. $A + (B + C) = (A + B) + C$,
3. $a(A + B) = aA + aB$,
4. $(a + b)A = aA + bA$,
5. $a(bA) = (ab)A$.

We can also define the operator norm $\|A\|$ according to

$$\|A\| = \sqrt{\text{Tr}(A^\dagger A)} \equiv \sqrt{\sum_{ij} A_{ij}^* A_{ji}}, \quad (1.18)$$

which means that the linear vector space of operators is again a Hilbert space. The symbol $\text{Tr}(\cdot)$ denotes the trace of an operator, and we will return to this special operator property later in this section.

Every operator has a set of vectors for which

$$A|a_j\rangle = a_j|a_j\rangle, \quad \text{with } a_j \in \mathbb{C} \quad (1.19)$$

This is called the eigenvalue equation (or eigenequation) for A , and the vectors $|a_j\rangle$ are the eigenvectors. The complex numbers a_j are eigenvalues. In the basis of eigenvectors, the matrix representation of A becomes

$$A = \begin{pmatrix} a_1 & 0 & \cdots & 0 \\ 0 & a_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_N \end{pmatrix} \quad (1.20)$$

When some of the a_j s are the same, we speak of degenerate eigenvalues. When there are n identical eigenvalues, we have n -fold degeneracy. The eigenvectors corresponding to this eigenvalue then span an n -dimensional subspace of the vector space. We will return to subspaces shortly, when we introduce projection operators.

For any orthonormal basis $\{|\phi_j\rangle\}_j$ we have

$$\langle\phi_j|A|\phi_k\rangle = A_{jk} \quad (1.21)$$

which can be written in the form

$$A = \sum_{jk} A_{jk} |\phi_j\rangle \langle\phi_k| \quad (1.22)$$

For the special case where $|\phi_j\rangle = |a_j\rangle$ this reduces to

$$A = \sum_j a_j |a_j\rangle \langle a_j| \quad (1.23)$$

This is the spectral decomposition of A . When all a_j are equal, we have complete degeneracy over the full vector space, and the operator becomes proportional (up to a factor a_j) to the identity $\mathbb{I}$.

Note that this is independent of the basis $\{|a_j\rangle\}$. As a consequence, for any orthonormal basis $\{|\phi_j\rangle\}$ we have

$$\mathbb{I} = \sum_j |\phi_j\rangle \langle\phi_j| \quad (1.24)$$

This is the completeness relation, and we will use this many times in our calculations.

Lemma

If two non-degenerate operators commute ($[A, B] = 0$), then they have a common set of eigenvectors.

Proof

Let $A = \sum_k a_k |a_k\rangle \langle a_k|$ and $B = \sum_{jk} B_{jk} |a_j\rangle \langle a_k|$. We can choose this without loss of generality: we write both operators in the eigenbasis of A . Furthermore, $[A, B] = 0$ implies that $AB = BA$.

$$\begin{aligned} AB &= \sum_{klm} a_k B_{lm} |a_k\rangle \langle a_l| \langle a_m| = \sum_{lm} a_l B_{lm} |a_l\rangle \langle a_m| \\ BA &= \sum_{klm} a_k B_{lm} |a_l\rangle \langle a_m| \langle a_k| \langle a_k| = \sum_{lm} a_m B_{lm} |a_l\rangle \langle a_m| \end{aligned} \quad (1.25)$$

Therefore

$$[A, B] = \sum_{lm} (a_l - a_m) B_{lm} |a_l\rangle \langle a_m| = 0 \quad (1.26)$$

If $a_l \neq a_m$ for $l \neq m$, then $B_{lm} = 0$, and $B_{lm} \propto \delta_{lm}$. Therefore $\{|a_j\rangle\}$ is an eigenbasis for B .

The proof of the converse is left as an exercise. It turns out that this is also true when A and/or B are degenerate.

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1.3: Hermitian and Unitary Operators

Next, we will consider two special types of operators, namely Hermitian and unitary operators. An operator A is Hermitian if and only if $A^\dagger = A$.

Lemma

An operator is Hermitian if and only if it has real eigenvalues: $A^\dagger = A \Leftrightarrow a_j \in \mathbb{R}$.

Proof

The eigenvalue equation of A implies that

$$A|a_j\rangle = a_j|a_j\rangle \Rightarrow \langle a_j|A^\dagger = a_j^* \langle a_j|, \quad (1.27)$$

which means that $\langle a_j|A|a_j\rangle = a_j$ and $\langle a_j|A^\dagger|a_j\rangle = a_j^*$. It is now straightforward to show that $A = A^\dagger$ implies $a_j = a_j^*$, or $a_j \in \mathbb{R}$. Conversely, $a_j \in \mathbb{R}$ implies $a_j = a_j^*$, and

$$\langle a_j|A|a_j\rangle = \langle a_j|A^\dagger|a_j\rangle \quad (1.28)$$

Let $|\psi\rangle = \sum_k c_k |a_k\rangle$. Then

$$\begin{aligned} \langle \psi|A|\psi\rangle &= \sum_j |c_j|^2 \langle a_j|A|a_j\rangle = \sum_j |c_j|^2 \langle a_j|A^\dagger|a_j\rangle = \sum_j |c_j|^2 \langle a_j|A^\dagger|a_j\rangle \\ &= \langle \psi|A^\dagger|\psi\rangle \end{aligned} \quad (1.29)$$

for all $|\psi\rangle$, and therefore $A = A^\dagger$.

Next, we construct the exponent of an operator A according to $U = \exp(icA)$. We have included the complex number c for completeness. At first sight, you may wonder what it means to take the exponent of an operator. Recall, however, that the exponent has a power expansion:

$$U = \exp(icA) = \sum_{n=0}^{\infty} \frac{(ic)^n}{n!} A^n \quad (1.30)$$

The n^{th} power of an operator is straightforward: just multiply A n times with itself. The expression in Eq. (1.30) is then well defined, and the exponent is taken as an abbreviation of the power expansion. In general, we can construct any function of operators, as long as we can define the function in terms of a power expansion:

$$f(A) = \sum_{n=0}^{\infty} f_n A^n \quad (1.31)$$

This can also be extended to functions of multiple operators, but now we have to be very careful in the case where these operators do not commute. Familiar rules for combining normal functions no longer apply (see exercise 4b).

We can construct the adjoint of the operator U according to

$$U^\dagger = \left(\sum_{n=0}^{\infty} \frac{(ic)^n}{n!} A^n \right)^\dagger = \sum_{n=0}^{\infty} \frac{(-ic^*)^n}{n!} A^{\dagger n} = \exp(-ic^* A^\dagger) \quad (1.32)$$

In the special case where $A = A^\dagger$ and c is real, we calculate

$$UU^\dagger = \exp(icA) \exp(-ic^* A^\dagger) = \exp(icA) \exp(-icA) = \exp[ic(A - A)] = \mathbb{I}, \quad (1.33)$$

since A commutes with itself. Similarly, $U^\dagger U = \mathbb{I}$. Therefore, $U^\dagger = U^{-1}$, and an operator with this property is called unitary. Each unitary operator can be generated by a Hermitian (self-adjoint) operator A and a real number c . A is called the generator of U . We often write $U = U_A(c)$. Unitary operators are basis transformations.

1.4: Projection Operators and Tensor Products

We can combine two linear vector spaces $\mathcal{U}$ and $\mathcal{V}$ into a new linear vector space $\mathcal{W} = \mathcal{U} \oplus \mathcal{V}$. The symbol $\oplus$ is called the direct sum. The dimension of $\mathcal{W}$ is the sum of the dimensions of $\mathcal{U}$ and $\mathcal{V}$:

$$\dim \mathcal{W} = \dim \mathcal{U} + \dim \mathcal{V} \quad (1.34)$$

A vector in $\mathcal{W}$ can be written as

$$|\Psi\rangle_{\mathcal{W}} = |\psi\rangle_{\mathcal{U}} + |\phi\rangle_{\mathcal{V}}, \quad (1.35)$$

where $|\psi\rangle_{\mathcal{U}}$ and $|\phi\rangle_{\mathcal{V}}$ are typically not normalized (i.e., they are not unit vectors). The spaces $\mathcal{U}$ and $\mathcal{V}$ are so-called subspaces of $\mathcal{W}$.

As an example, consider the three-dimensional Euclidean space spanned by the Cartesian axes x , y , and z . The xy -plane is a two-dimensional subspace of the full space, and the z -axis is a one-dimensional subspace. Any three-dimensional form can be projected onto the xy -plane by setting the z component to zero. Similarly, we can project onto the z -axis by setting the x and y coordinates to zero. A projector is therefore associated with a subspace. It acts on a vector in the full space, and forces all components to zero, except those of the subspace it projects onto.

The formal definition of a projector $P_{\mathcal{U}}$ on $\mathcal{U}$ is given by

$$P_{\mathcal{U}}|\Psi\rangle_{\mathcal{W}} = |\psi\rangle_{\mathcal{U}} \quad (1.36)$$

This is equivalent to requiring that $P_{\mathcal{U}}^2 = P_{\mathcal{U}}$, $P_{\mathcal{U}}^2 = P_{\mathcal{U}}$, or $P_{\mathcal{U}}$ is idempotent. One-dimensional projectors can be written as

$$P_j = |\phi_j\rangle \langle \phi_j| \quad (1.37)$$

Two projectors P_1 and P_2 are orthogonal is $P_1 P_2 = 0$. If $P_1 P_2 = 0$, then $P_1 + P_2$ is another projector:

$$(P_1 + P_2)^2 = P_1^2 + P_1 P_2 + P_2 P_1 + P_2^2 = P_1^2 + P_2^2 = P_1 + P_2 \quad (1.38)$$

When P_1 and P_2 commute but are non-orthogonal (i.e., they overlap), the general projector onto their combined subspace is

$$P_{1+2} = P_1 + P_2 - P_1 P_2 \quad (1.39)$$

(Prove this.) The orthocomplement of P is $\mathbb{I} - P$, which is also a projector:

$$P(\mathbb{I} - P) = P - P^2 = P - P = 0 \quad \text{and} \quad (\mathbb{I} - P)^2 = \mathbb{I} - 2P + P^2 = \mathbb{I} - P \quad (1.40)$$

Another way to combine two vector spaces $\mathcal{U}$ and $\mathcal{V}$ is via the tensor product: $\mathcal{W} = \mathcal{U} \otimes \mathcal{V}$, where the symbol $\otimes$ is called the direct product or tensor product. The dimension of the space $\mathcal{W}$ is then

$$\dim \mathcal{W} = \dim \mathcal{U} \cdot \dim \mathcal{V} \quad (1.41)$$

Let $|\psi\rangle \in \mathcal{U}$ and $|\phi\rangle \in \mathcal{V}$. Then

$$|\psi\rangle \otimes |\phi\rangle \in \mathcal{W} = \mathcal{U} \otimes \mathcal{V} \quad (1.42)$$

If $|\psi\rangle = \sum_j a_j |\psi_j\rangle$ and $|\phi\rangle = \sum_j b_j |\phi_j\rangle$, then the tensor product of these vectors can be written as

$$|\psi\rangle \otimes |\phi\rangle = \sum_{jk} a_j b_k |\psi_j\rangle \otimes |\phi_k\rangle = \sum_{jk} a_j b_k |\psi_j\rangle |\phi_k\rangle = \sum_{jk} a_j b_k |\psi_j, \phi_k\rangle, \quad (1.43)$$

where we introduced convenient abbreviations for the tensor product notation. The inner product of two vectors that are tensor products is

$$(\langle \psi_1 | \otimes \langle \phi_1 |) (|\psi_2\rangle \otimes |\phi_2\rangle) = \langle \psi_1 | \psi_2 \rangle \langle \phi_1 | \phi_2 \rangle \quad (1.44)$$

Operators also obey the tensor product structure, with

$$(A \otimes B)|\psi\rangle \otimes |\phi\rangle = (A|\psi\rangle) \otimes (B|\phi\rangle) \quad (1.45)$$

and

$$(A \otimes B)(C \otimes D)|\psi\rangle \otimes |\phi\rangle = (AC|\psi\rangle) \otimes (BD|\phi\rangle) \quad (1.46)$$

General rules for tensor products of operators are

1. $A \otimes 0 = 0$ and $0 \otimes B = 0$,
2. $\mathbb{I} \otimes \mathbb{I} = \mathbb{I}$,
3. $(A_1 + A_2) \otimes B = A_1 \otimes B + A_2 \otimes B$,
4. $aA \otimes bB = (ab)A \otimes B$,
5. $(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$,
6. $(A \otimes B)^\dagger = A^\dagger \otimes B^\dagger$.

Note that the last rule preserves the order of the operators. In other words, operators always act on their own space. Often, it is understood implicitly which operator acts on which subspace, and we will write $A \otimes \mathbb{I} = A$ and $\mathbb{I} \otimes B = B$. Alternatively, we can add subscripts to the operator, e.g., $A_{\mathcal{U}}$ and $B_{\mathcal{V}}$.

As a practical example, consider two two-dimensional operators

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} \quad (1.47)$$

with respect to some orthonormal bases $\{|a_1\rangle, |a_2\rangle\}$ and $\{|b_1\rangle, |b_2\rangle\}$ for A and B , respectively (not necessarily eigenbases). The question is now: what is the matrix representation of $A \otimes B$? Since the dimension of the new vector space is the product of the dimensions of the two vector spaces, we have $\dim \mathcal{W} = 2 \cdot 2 = 4$. A natural basis for $A \otimes B$ is then given by $\{|a_j, b_k\rangle\}_{jk}$, with $j, k = 1, 2$, or

$$|a_1\rangle |b_1\rangle, \quad |a_1\rangle |b_2\rangle, \quad |a_2\rangle |b_1\rangle, \quad |a_2\rangle |b_2\rangle \quad (1.48)$$

We can construct the matrix representation of $A \otimes B$ by applying this operator to the basis vectors in Eq. (1.48), using

$$A |a_j\rangle = A_{1j} |a_1\rangle + A_{2j} |a_2\rangle \quad \text{and} \quad B |b_k\rangle = B_{1k} |b_1\rangle + B_{2k} |b_2\rangle \quad (1.49)$$

which leads to

$$\begin{aligned} A \otimes B |a_1, b_1\rangle &= (A_{11} |a_1\rangle + A_{21} |a_2\rangle) (B_{11} |b_1\rangle + B_{21} |b_2\rangle) \\ A \otimes B |a_1, b_2\rangle &= (A_{11} |a_1\rangle + A_{21} |a_2\rangle) (B_{12} |b_1\rangle + B_{22} |b_2\rangle) \\ A \otimes B |a_2, b_1\rangle &= (A_{12} |a_1\rangle + A_{22} |a_2\rangle) (B_{11} |b_1\rangle + B_{21} |b_2\rangle) \\ A \otimes B |a_2, b_2\rangle &= (A_{12} |a_1\rangle + A_{22} |a_2\rangle) (B_{12} |b_1\rangle + B_{22} |b_2\rangle) \end{aligned} \quad (1.50)$$

Looking at the first line of Eq. (1.50), the basis vector $|a_1, b_1\rangle$ gets mapped to all basis vectors:

$$A \otimes B |a_1, b_1\rangle = A_{11}B_{11} |a_1, b_1\rangle + A_{11}B_{21} |a_1, b_2\rangle + A_{21}B_{11} |a_2, b_1\rangle + A_{21}B_{21} |a_2, b_2\rangle \quad (1.51)$$

Combining this into matrix form leads to

$$A \otimes B = \begin{pmatrix} A_{11}B_{11} & A_{11}B_{12} & A_{12}B_{11} & A_{12}B_{12} \\ A_{11}B_{21} & A_{11}B_{22} & A_{12}B_{21} & A_{12}B_{22} \\ A_{21}B_{11} & A_{21}B_{12} & A_{22}B_{11} & A_{22}B_{12} \\ A_{21}B_{21} & A_{21}B_{22} & A_{22}B_{21} & A_{22}B_{22} \end{pmatrix} = \begin{pmatrix} A_{11}B & A_{12}B \\ A_{21}B & A_{22}B \end{pmatrix} \quad (1.52)$$

Recall that this is dependent on the basis that we have chosen. In particular, $A \otimes B$ may be diagonalized in some other basis.

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1.5: The Trace and Determinant of an Operator

There are two special functions of operators that play a key role in the theory of linear vector spaces. They are the trace and the determinant of an operator, denoted by $\text{Tr}(A)$ and $\det(A)$, respectively. While the trace and determinant are most conveniently evaluated in matrix representation, they are independent of the chosen basis.

When we defined the norm of an operator, we introduced the trace. It is evaluated by adding the diagonal elements of the matrix representation of the operator:

$$\text{Tr}(A) = \sum_j \langle \phi_j | A | \phi_j \rangle, \quad (1.53)$$

where $\{|\phi_j\rangle\}_j$ is any orthonormal basis. This independence means that the trace is an invariant property of the operator. Moreover, the trace has the following important properties:

1. If $A = A^\dagger$, then $\text{Tr}(A)$ is real,
2. $\text{Tr}(aA) = a \text{Tr}(A)$,
3. $\text{Tr}(A + B) = \text{Tr}(A) + \text{Tr}(B)$,
4. $\text{Tr}(AB) = \text{Tr}(BA)$ (the "cyclic property").

The first property follows immediately when we evaluate the trace in the diagonal basis, where it becomes a sum over real eigenvalues. The second and third properties convey the linearity of the trace. The fourth property is extremely useful, and can be shown as follows:

$$\begin{aligned} \text{Tr}(AB) &= \sum_j \langle \phi_j | AB | \phi_j \rangle = \sum_{jk} \langle \phi_j | A | \psi_k \rangle \langle \psi_k | B | \phi_j \rangle \\ &= \sum_{jk} \langle \psi_k | B | \phi_j \rangle \langle \phi_j | A | \psi_k \rangle = \sum_k \langle \psi_k | BA | \psi_k \rangle \\ &= \text{Tr}(BA) \end{aligned} \quad (1.54)$$

This derivation also demonstrates the usefulness of inserting a resolution of the identity in strategic places. In the cyclic property, the operators A and B may be products of two operators, which then leads to

$$\text{Tr}(ABC) = \text{Tr}(BCA) = \text{Tr}(CAB) \quad (1.55)$$

Any cyclic (even) permutation of operators under a trace gives rise to the same value of the trace as the original operator ordering.

Finally, we construct the partial trace of an operator that lives on a tensor product space. Suppose that $A \otimes B$ is an operator in the Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$. We can trace out Hilbert space $\mathcal{H}_1$, denoted by $\text{Tr}_1(\cdot)$:

$$\text{Tr}_1(A \otimes B) = \text{Tr}(A)B, \quad \text{or equivalently} \quad \text{Tr}_1(A_1 B_2) = \text{Tr}(A_1) B_2 \quad (1.56)$$

Taking the partial trace has the effect of removing the entire Hilbert space $\mathcal{H}_1$ from the description. It reduces the total vector space. The partial trace always carries an index, which determines which space is traced over.

The determinant of a 2×2 matrix is given by

$$\det(A) = \det \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = A_{11}A_{22} - A_{12}A_{21} \quad (1.57)$$

The determinant of higher-dimensional matrices can be defined recursively as follows: The topleft element of an $n \times n$ matrix defines an $(n-1) \times (n-1)$ matrix by removing the top row and the left column. Similarly, any other element in the left column defines an $(n-1) \times (n-1)$ matrix by removing the left column and the row of the element we chose. The determinant of the $n \times n$ matrix is then given by the top-left element times the determinant of the remaining $(n-1) \times (n-1)$ matrix, minus the product of the second element down in the left column and the remaining $(n-1) \times (n-1)$ matrix, plus the third element times the remaining matrix, etc.

The determinant of the product of matrices is equal to the product of the determinants of the matrices:

$$\det(AB) = \det(A) \det(B) \quad (1.58)$$

Moreover, if A is an invertible matrix, then we have

$$\det(A^{-1}) = \det(A)^{-1} \quad (1.59)$$

This leads to an important relation between similar matrices $A = X^{-1}BX$:

$$\begin{aligned}\det(A) &= \det(X^{-1}BX) = \det(X^{-1}) \det(B) \det(X) \\ &= \det(X)^{-1} \det(B) \det(X) = \det(B)\end{aligned}\quad (1.60)$$

In particular, this means that the determinant is independent of the basis in which the matrix is written, which means that it is an intrinsic property of the operator associated with that matrix.

Finally, here's a fun relation between the trace and the determinant of an operator:

$$\det[\exp(A)] = \exp[\text{Tr}(A)] \quad (1.61)$$

? Exercises

1. Vectors and matrices:

- Are the following three vectors linearly dependent or independent: $a = (2, 3, -1)$, $b = (0, 1, 2)$, and $c = (0, 0, -5)$?
- Consider the vectors $|\psi\rangle = 3i|\phi_1\rangle - 7i|\phi_2\rangle$ and $|\chi\rangle = |\phi_1\rangle + 2|\phi_2\rangle$, with $\{|\phi_i\rangle\}$ an orthonormal basis. Calculate the inner product between $|\psi\rangle$ and $|\chi\rangle$, and show that they satisfy the Cauchy-Schwarz inequality.
- Consider the two matrices

$$A = \begin{pmatrix} 0 & i & 2 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 2 & i & 0 \\ 3 & 1 & 5 \\ 0 & -i & -2 \end{pmatrix} \quad (1.62)$$

Calculate A^{-1} and BA^{-1} . Are they equal?

- Calculate $A \otimes B$ and $B \otimes A$, where $A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $B = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

2. Operators:

- Which of these operators are Hermitian: $A + A^\dagger$, $i(A + A^\dagger)$, $i(A - A^\dagger)$, and $A^\dagger A$?
- Prove that a shared eigenbasis for two operators A and B implies that $[A, B] = 0$.
- Let U be a transformation matrix that maps one complete orthonormal basis to another. Show that U is unitary
- How many real parameters completely determine a $d \times d$ unitary matrix?

3. Properties of the trace and the determinant:

- Calculate the trace and the determinant of the matrices A and B in exercise 1c.
- Show that the expectation value of A can be written as $\text{Tr}(|\psi\rangle\langle\psi|A)$.
- Prove that the trace is independent of the basis.

4. Commutator identities.

- Let $F(t) = e^{At}e^{Bt}$. Calculate dF/dt and use $[e^{At}, B] = (e^{At}Be^{-At} - B)e^{At}$ to simplify your result.
- Let $G(t) = e^{At+Bt+f(t)H}$. Show by calculating dG/dt , and setting $dF/dt = dG/dt$ at $t = 1$, that the following operator identity

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]}, \quad (1.63)$$

holds if A and B both commute with $[A, B]$. Hint: use the Hadamard lemma

$$e^{At}Be^{-At} = B + \frac{t}{1!}[A, B] + \frac{t^2}{2!}[A, [A, B]] + \dots \quad (1.64)$$

- Show that the commutator of two Hermitian operators is anti-Hermitian ($A^\dagger = -A$).
- Prove the commutator analog of the Jacobi identity

$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0 \quad (1.65)$$

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