Advanced Quantum Mechanics

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Linear Algebra: Vector space

DEFINITION 1.1 A vector space V is a set with the following properties;

(0-1) For any $u, v \in V$, their sum $u + v \in V$.

(0-2) For any $u \in V$ and $c \in K$, their scalar multiple $cu \in V$.

(1-1) $(u + v) + w = u + (v + w)$ for any $u, v, w \in V$.

(1-2) $u + v = v + u$ for any $u, v \in V$.

(1-3) There exists an element $0 \in V$ such that $u + 0 = u$ for any $u \in V$. This element 0 is called the **zero-vector**.

(1-4) For any element $u \in V$, there exists an element $v \in V$ such that $u+v = 0$. The vector v is called the **inverse** of u and denoted by $-u$.

(2-1) $c(x + y) = cx + cy$ for any $c \in K, u, v \in V$.

(2-2) $(c + d)u = cu + du$ for any $c, d \in K, u \in V$.

(2-3) $(cd)u = c(du)$ for any $c, d \in K, u \in V$.

(2-4) Let 1 be the unit element of K. Then $1u = u$ for any $u \in V$.

Fundamental property: vectors can be stretched and added.

The usual rules of addition and multiplication hold.

There is a null vector.

In QM: K = $\mathbb{C}$ (complex vector space)

Notation

Vectors will be denoted as follows

Dirac notation: **ket** ←

$$|x\rangle = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}, \quad x_i \in \mathbb{C}$$

→ Usual notation

Therefore we have:

$$|x\rangle = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}, \ |y\rangle = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} \Rightarrow |x\rangle + |y\rangle = \begin{pmatrix} x_1 + y_1 \\ x_2 + y_2 \\ \vdots \\ x_n + y_n \end{pmatrix}, \ a|x\rangle = \begin{pmatrix} ax_1 \\ ax_2 \\ \vdots \\ ax_n \end{pmatrix}$$

Linear (in-)dependence, basis, dimension

Linear combination $c_1|x\rangle + c_2|y\rangle$

Linear independent vectors: a set of vectors is linearly independent iff their only linear combination resulting in the null vector can be obtained with all coefficients equal to 0. Otherwise there are called **linearly dependent**.

$$\sum_{i=1}^{k} c_i|x_i\rangle = |\omega\rangle \quad \Leftrightarrow \quad c_i = 0 \; (1 \leq i \leq k)$$

Null vector

Basis: a set of linear independent vectors such that *any other vector* can be written as linear combination of those vectors.

Dimension: number of basis vectors (n), always **finite** for us. Then, V = $\mathbb{C}^n$

Examples

EXERCISE 1.1 Find the condition under which two vectors

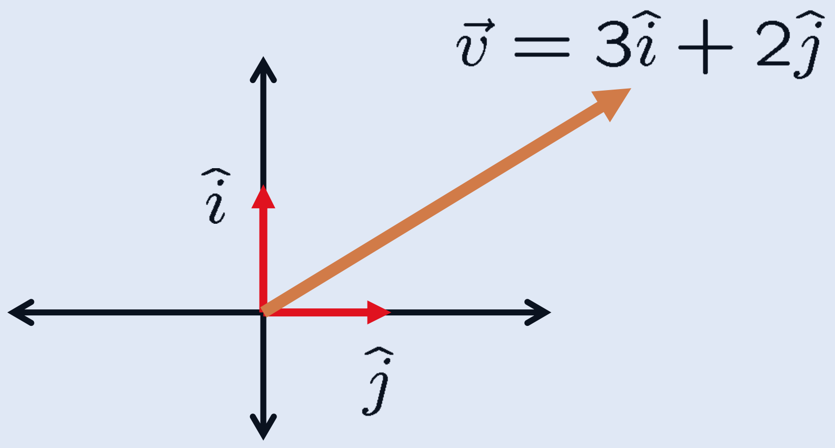
$$|v_1\rangle = \begin{pmatrix} x \\ y \\ 3 \end{pmatrix}, \ |v_2\rangle = \begin{pmatrix} 2 \\ x - y \\ 1 \end{pmatrix} \in \mathbb{R}^3$$

are linearly independent.

EXERCISE 1.2 Show that a set of vectors

$$|v_1\rangle = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad |v_2\rangle = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad |v_3\rangle = \begin{pmatrix} 1 \\ -1 \\ -1 \end{pmatrix}$$

is a basis of $\mathbb{C}^3$.



Geometric representation of vectors and basis (V = $\mathbb{R}^2$)

Inner product

It is a function

$< . \mid . >: \quad V \times V \;\rightarrow\; \mathbb{C}$

With the following properties:

1. $\langle x|[\alpha|y\rangle + \beta|z\rangle] = \alpha\langle x|y\rangle + \beta\langle x|z\rangle$
2. $\langle x|y\rangle = \langle y|x\rangle^*$
3. $\langle x|x\rangle \geq 0$ and is null iff $|x\rangle = |\omega\rangle$

Usual definition

$$|x\rangle = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}, \quad |y\rangle = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

Then

$$\langle x|y\rangle = \sum_{i=1}^{n} x_i^* y_i$$

Norm and metric. Hilbert spaces

The inner product defines automatically a **norm**

$$\|x\| = \sqrt{\langle x|x\rangle}$$

and a **metric** (distance)

$$d(x,y) = \|x - y\|$$

$$\|x\|^2 = \sqrt{\sum_{i=1}^{n} |x_i|^2}$$

$$\|x - y\|^2 = \sqrt{\sum_{i=1}^{n} |x_i - y_i|^2}$$

Hilbert space ($\mathcal{H}$): a vector space with a inner product (simple definition because we are working with vector spaces of finite dimension)

Linear functionals

It is a function $f : \mathcal{H} \to \mathbb{C}$

such that $f(\alpha x + \beta y) = \alpha f(x) + \beta f(y)$

It naturally defines a vector space $\boldsymbol{\mathcal{H}}^*$, called the **(algebraic) dual** of $\boldsymbol{\mathcal{H}}$.

$$(f_1 + f_2)(x) = f_1(x) + f_2(x)$$

$$(\alpha f)(x) = \alpha f(x)$$

Linear functionals

Let $\{\hat{e}_i\}$ with i = 1,…n be a basis of $\mathcal{H}$. Then for any vector x:

$$f(x) = f\left(\sum_{i=1}^{n} x_i \hat{e}_i\right) = \sum_{i=1}^{n} x_i f(\hat{e}_i) = \sum_{i=1}^{n} x_i \xi_i \qquad \text{with} \qquad \xi_i = f(\hat{e}_i) \in \mathbb{C}$$

Therefore f is uniquely identified by the numbers $(\xi_1, \xi_2, \ldots \xi_n)$, which are the values of f at the basis vectors. In particular let us consider the functionals

$(\xi_1, \xi_2, \ldots \xi_n)$

$(1,0, \ldots 0) \quad \leftrightarrow \quad \hat{e}^*_1$

$(0,1, \ldots 0) \quad \leftrightarrow \quad \hat{e}^*_2$

…

$(0,0, \ldots 1) \quad \leftrightarrow \quad \hat{e}^*_n$

By construction: $\hat{e}^*_i (\hat{e}_j) = \delta_{ij}$

It can be shown that $\{\hat{e}^*_i\}$ forms a basis of $\mathcal{H}^*$ called the **dual basis**

Riesz's representation theorem

Every functional on $\mathcal{H}$ can be represented in terms of an inner product

$$f(x) = \langle z|x\rangle$$

where z depends on f, and is uniquely determined by it. Therefore

$f \quad \leftrightarrow \quad z$ such that $f(\cdot) = \langle z|\cdot\rangle$

There is a **1-to-1 correspondence between vectors and functionals.**

Dirac notation

$$|z\rangle \quad \leftrightarrow \quad \langle z|$$

ket the vector

bra the functional

Given a basis |1>, |2> … |n> in $\mathcal{H}$, we will always consider the dual basis of $\mathcal{H}^*$, which we will denote as <1|, <2| … <n|. Then

<i|j> = δ_{ij}.

Also

$$|x\rangle = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \mapsto \langle x| = (x_1^*, \ldots, x_n^*)$$

so that

functional Riesz's theorem coefficient ξ_i

$$\langle x|(|y\rangle) = \langle x|y\rangle = \sum_{i=1}^{n} x_i^* y_i$$

This gives a **clear mathematical meaning to the Dirac bra-ket notation**

Example

EXERCISE 1.3 Let

$$|x\rangle = \begin{pmatrix} 1 \\ i \\ 2+i \end{pmatrix}, \quad |y\rangle = \begin{pmatrix} 2-i \\ 1 \\ 2+i \end{pmatrix}$$

Find $\| |x\rangle \|$, $\langle x|y\rangle$ and $\langle y|x\rangle$.

Basis

$\langle e_i | e_j \rangle = \delta_{ij}$

Let $|x\rangle = \sum_{i=1}^{n} c_i |e_i\rangle$. The inner product of $|x\rangle$ and $\langle e_j|$ yields

$$\langle e_j | x \rangle = \sum_{i=1}^{n} c_i \langle e_j | e_i \rangle = \sum_{i=1}^{n} c_i \delta_{ji} = c_j \rightarrow c_j = \langle e_j | x \rangle.$$

Linear Operator

A map $A : \mathbb{C}^n \to \mathbb{C}^n$ is a **linear operator** if

$$A(c_1|x\rangle + c_2|y\rangle) = c_1 A|x\rangle + c_2 A|y\rangle$$

is satified for arbitrary $|x\rangle, |y\rangle \in \mathbb{C}^n$ and $c_k \in \mathbb{C}$. Let us choose an arbitrary orthonormal basis $\{|e_k\rangle\}$. It is shown below that A is expressed as an $n \times n$ matrix.

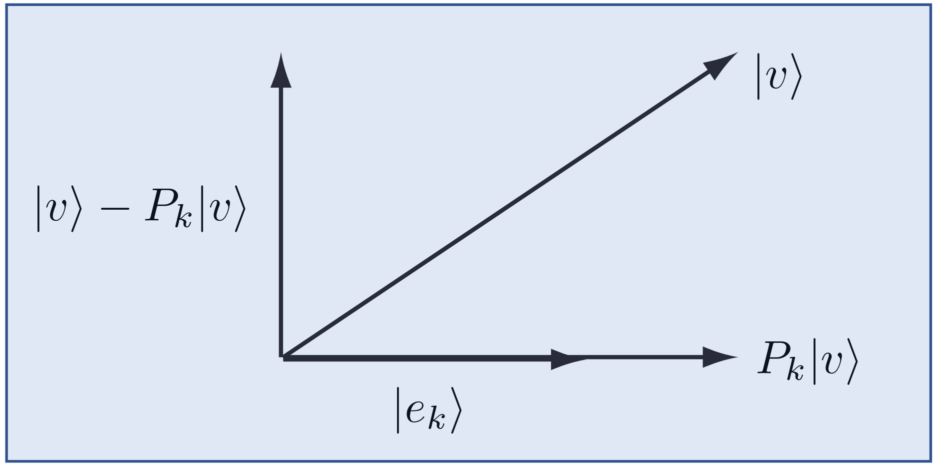
$$A|e_k\rangle = \sum_{i=1}^{n} |e_i\rangle A_{ik}. \qquad A_{jk} = \langle e_j|A|e_k\rangle. \qquad A = \sum_{j,k} A_{jk}|e_j\rangle\langle e_k|$$

Projection Operator

$$P_k \equiv |e_k\rangle\langle e_k|$$

The set $\{P_k = |e_k\rangle\langle e_k|\}$ satisfies the conditions

$$\text{(i)} \qquad P_k^2 = P_k,$$
$$\text{(ii)} \qquad P_k P_j = 0 \quad (k \neq j),$$
$$\text{(iii)} \qquad \sum_k P_k = I \quad \text{(completeness relation)}.$$



EXAMPLE 1.1 Let

$$|e_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, |e_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

They define an orthonormal basis as is easily verified. Projection operators are

$$P_1 = |e_1\rangle\langle e_1| = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad P_2 = |e_2\rangle\langle e_2| = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

They satisfy the completeness relation

$$\sum_k P_k = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$$

and the orthogonality condition

$$P_1 P_2 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

The reader should verify that $P_k^2 = P_k$.

Hermitian Conjugate – Hermitian operator

DEFINITION 1.2 (Hermitian conjugate) Given a linear operator A : $\mathbb{C}^n \to \mathbb{C}^n$, its Hermitian conjugate $A^\dagger$ is defined by

$$\langle u|A|v\rangle \equiv \langle A^\dagger u|v\rangle = \langle v|A^\dagger|u\rangle^*,$$

where $|u\rangle, |v\rangle$ are arbitrary vectors in $\mathbb{C}^n$.

The above definition shows that $\langle e_j|A|e_k\rangle = \langle e_k|A^\dagger|e_j\rangle^*$. Therefore, we find the relation $A_{jk} = (A^\dagger)^*_{kj}$, namely

$$(A^\dagger)_{jk} = A^*_{kj}.$$

$$(cA)^\dagger = c^* A^\dagger, \quad (A+B)^\dagger = A^\dagger + B^\dagger, \quad (AB)^\dagger = B^\dagger A^\dagger.$$

DEFINITION 1.3 (Hermitian matrix) A matrix $A : \mathbb{C}^n \to \mathbb{C}^n$ is said to be a **Hermitian matrix** if it satisifies $A^\dagger = A$.

Unitary operator

DEFINITION 1.4 (**Unitary matrix**) Let $U : \mathbb{C}^n \to \mathbb{C}^n$ be a matrix which satisfies $U^\dagger = U^{-1}$. Then U is called a **unitary matrix**. Moreover, if U is unimodular, namely $\det U = 1$, U is said to be a **special unitary matrix**.

The set of unitary matrices is a group called the **unitary group**, while that of the special unitary matrices is a group called the **special unitary group**. They are denoted by $\mathrm{U}(n)$ and $\mathrm{SU}(n)$, respectively.

Let $\{|e_1\rangle, \ldots, |e_n\rangle\}$ be an orthonormal basis in $\mathbb{C}^n$. Suppose a matrix $U : \mathbb{C}^n \to \mathbb{C}^n$ satisifes $U^\dagger U = I$. By operating U on $\{|e_k\rangle\}$, we obtain a vector $|f_k\rangle = U|e_k\rangle$. These vectors are again orthonormal since

$$\langle f_j|f_k\rangle = \langle e_j|U^\dagger U|e_k\rangle = \langle e_j|e_k\rangle = \delta_{jk}. \tag{1.26}$$

Note that $|\det U| = 1$ since $\det U^\dagger U = \det U^\dagger \det U = |\det U|^2 = 1$.

Eigenvalues & Eigenvectors

$$A|v\rangle = \lambda|v\rangle, \quad \lambda \in \mathbb{C}.$$

Then λ is called an **eigenvalue** of A, while $|v\rangle$ is called the corresponding **eigenvector**. The above equation being a linear equation, the norm of the eigenvector cannot be fixed. Of course, it is always possible to normalize $|v\rangle$ such that $\||v\rangle\| = 1$. We often use the symbol $|\lambda\rangle$ for an eigenvector corresponding to an eigenvalue λ to save symbols.

Let us find the eigenvalue λ next. Note first that the eigenvalue equation is rewritten as

$$\sum_j (A - \lambda I)_{ij} v_j = 0.$$

This equation in v_j has nontrivial solutions if and only if the matrix $A - \lambda I$ has no inverse, namely

$$D(\lambda) \equiv \det(A - \lambda I) = 0.$$

characteristic equation

Eigenvalues & Eigenvectors of Hermitian operators

THEOREM 1.2 All the eigenvalues of a Hermitian matrix are real numbers. Moreover, two eigenvectors corresponding to different eigenvalues are orthogonal.

Proof. Let A be a Hermitian matrix and let $A|\lambda\rangle = \lambda|\lambda\rangle$. The Hermitian conjugate of this equation is $\langle\lambda|A = \lambda^*\langle\lambda|$. From these equations we obtain $\langle\lambda|A|\lambda\rangle = \lambda\langle\lambda|\lambda\rangle = \lambda^*\langle\lambda|\lambda\rangle$, which proves $\lambda = \lambda^*$ since $\langle\lambda|\lambda\rangle \neq 0$.

Let $A|\mu\rangle = \mu|\mu\rangle$ $(\mu \neq \lambda)$, next. Then $\langle\mu|A = \mu\langle\mu|$ since $\mu \in \mathbb{R}$. From $\langle\mu|A|\lambda\rangle = \lambda\langle\mu|\lambda\rangle$ and $\langle\mu|A|\lambda\rangle = \mu\langle\mu|\lambda\rangle$, we obtain $0 = (\lambda - \mu)\langle\mu|\lambda\rangle$. Since $\mu \neq \lambda$, we must have $\langle\mu|\lambda\rangle = 0$. ∎

Therefore, the set of eigenvectors $\{|\lambda_k\rangle\}$ of a Hermitian matrix A may be made into a complete set

$$I = \sum_{i=1}^{n} |\lambda_i\rangle\langle\lambda_i|$$

$$A = \sum_i \lambda_i |\lambda_i\rangle\langle\lambda_i|,$$

spectral decomposition of A

Exercises

EXERCISE 1.9 Let

$$A = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1+i \\ 1-i & 0 \end{pmatrix}.$$

Find the eigenvalues and the corresponding normalized eigenvectors. Show that the eigenvectors are mutually orthogonal and that they satisfy the completeness relation. Find a unitary matrix which diagonalizes A.

EXERCISE 1.10 (1) Suppose A is skew-Hermitian, namely $A^\dagger = -A$. Show that all the eigenvalues are pure imaginary.

(2) Let U be a unitary matrix. Show that all the eigenvalues are unimodular, namely $|\lambda_j| = 1$.

(3) Let A be a normal matrix. Show that A is Hermitian if and only if all the eigenvalues of A are real.

A matrix A is **normal** if it satisfies $AA^\dagger = A^\dagger A$

Exercises

Exercise 2.12: Prove that the matrix

$$\begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}$$

is not diagonalizable.

Exercise 2.13: If $|w\rangle$ and $|v\rangle$ are any two vectors, show that $(|w\rangle\langle v|)^\dagger = |v\rangle\langle w|$

Exercise 2.20: (Basis changes) Suppose A' and A'' are matrix representations of an operator A on a vector space V with respect to two different orthonormal bases, $|v_i\rangle$ and $|w_i\rangle$. Then the elements of A' and A'' are $A'_{ij} = \langle v_i|A|v_j\rangle$ and $A''_{ij} = \langle w_i|A|w_j\rangle$. Characterize the relationship between A' and A''.

Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Product of Pauli matrices

$$\{\sigma_i, \sigma_j\} = \sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij}I.$$

$$[\sigma_i, \sigma_j] = \sigma_i\sigma_j - \sigma_j\sigma_i = 2i\sum_k \varepsilon_{ijk}\sigma_k,$$

$$\varepsilon_{ijk} = \begin{cases} 1, & (i,j,k) = (1,2,3), (2,3,1), (3,1,2) \\ -1 & (i,j,k) = (2,1,3), (1,3,2), (3,2,1) \\ 0 & \text{otherwise.} \end{cases}$$

$$\sigma_i\sigma_j = i\sum_{k=1}^{3} \varepsilon_{ijk}\sigma_k + \delta_{ij}I\,.$$

Pauli matrices

The spin-flip ("ladder") operators are defined by

$$\sigma_+ = \frac{1}{2}(\sigma_x + i\sigma_y) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \sigma_- = \frac{1}{2}(\sigma_x - i\sigma_y) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$ **Eigenstates of σ_z**

Verify that $\sigma_+|\uparrow\rangle = \sigma_-|\downarrow\rangle = 0, \quad \sigma_+|\downarrow\rangle = |\uparrow\rangle, \quad \sigma_-|\uparrow\rangle = |\downarrow\rangle$. The projection operators to the eigenspaces of σ_z with the eigenvalues ± 1 are

$$P_+ = |\uparrow\rangle\langle\uparrow| = \tfrac{1}{2}(I + \sigma_z) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

$$P_- = |\downarrow\rangle\langle\downarrow| = \tfrac{1}{2}(I - \sigma_z) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

$$\sigma_\pm^2 = 0, \quad P_\pm^2 = P_\pm, \quad P_+ P_- = 0.$$

Function of an operator

PROPOSITION 1.1 Let A be Hermitian matrix in the above theorem. Then for an arbitrary $n \in \mathbb{N}$, we obtain

$$A^n = \sum_\alpha \lambda_\alpha^n P_\alpha.$$

If, furthermore, A^{-1} exists, the above formula may be extended to $n \in \mathbb{Z}$ by noting that λ_α^{-1} is an eigenvalue of A^{-1}.

Proof. Let $n \in \mathbb{N}$. Then

$$A^n P_\alpha = \lambda_\alpha A^{n-1} P_\alpha = \ldots = \lambda_\alpha^{n-1} A P_\alpha = \lambda_\alpha^n P_\alpha,$$

from which we obtain

$$A^n = A^n \sum_\alpha P_\alpha = \sum_\alpha A^n P_\alpha = \sum_\alpha \lambda_\alpha^n P_\alpha.$$

To prove the second half of the proposition, we only need to show that A^{-1} has an eigenvalue λ_α^{-1}, provided that A^{-1} exists (and hence $\lambda_\alpha \neq 0$), and the corresponding projection operator is P_α. We find

$$|\lambda_{\alpha,p}\rangle = A^{-1} A |\lambda_{\alpha,p}\rangle = \lambda_\alpha A^{-1} |\lambda_{\alpha,p}\rangle \to A^{-1} |\lambda_{\alpha,p}\rangle = \lambda_\alpha^{-1} |\lambda_{\alpha,p}\rangle.$$

Therefore the projection operator corresponding to the eivengalue λ_α^{-1} is P_α. The case $n = 0$, $I = \sum_\alpha P_\alpha$, is nothing but the completeness relation. Now we have proved that Eq. (1.42) applies to an arbitrary $n \in \mathbb{Z}$. ∎

Exercises

EXAMPLE 1.6 Let us consider σ_y again. It follows directly from Example 1.5 that

$$\exp(i\alpha\sigma_y) \equiv \sum_{k=0}^{\infty} \frac{(i\alpha\sigma_y)^k}{k!} = e^{i\alpha}P_1 + e^{-i\alpha}P_2 = \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix}.$$

EXERCISE 1.13 Suppose a 2×2 matrix A has eigenvalues $-1, 3$ and the corresponding eigenvectors

$$|e_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ i \end{pmatrix}, \quad |e_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix},$$

respectively. Find A.

EXERCISE 1.14 Let

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}.$$

(1) Find the eigenvalues and the corresponding normalized eigenvectors of A.
(2) Write down the spectral decomposition of A.
(3) Find $\exp(i\alpha A)$.

Exercises

EXERCISE 1.15 Let

$$A = \begin{pmatrix} 5 & -2 & -4 \\ -2 & 2 & 2 \\ -4 & 2 & 5 \end{pmatrix}.$$

(1) Find the eigenvalues and the corresponding eigenvectors of A.
(2) Find the spectral decomposition of A.
(3) Find the inverse of A by making use of the spectral decomposition.

PROPOSITION 1.2 Let $\hat{\boldsymbol{n}} \in \mathbb{R}^3$ be a unit vector and $\alpha \in \mathbb{R}$. Then

$$\exp\left(i\alpha\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma}\right) = \cos\alpha I + i(\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma})\sin\alpha,$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$.

Exercises

Exercise 2.34: Find the square root and logarithm of the matrix

$$\begin{bmatrix} 4 & 3 \\ 3 & 4 \end{bmatrix}.$$

Tensor product

DEFINITION 1.5 Let A be an $m \times n$ matrix and let B be a $p \times q$ matrix. Then

$$A \otimes B = \begin{pmatrix} a_{11}B, a_{12}B, \ldots, a_{1n}B \\ a_{21}B, a_{22}B, \ldots, a_{2n}B \\ \cdots \\ a_{m1}B, a_{m2}B, \ldots, a_{mn}B \end{pmatrix} \tag{1.47}$$

is an $(mp) \times (nq)$ matrix called the **tensor product (Kronecker product)** of A and B.

It should be noted that not all $(mp) \times (nq)$ matrices are tensor products of an $m \times n$ matrix and a $p \times q$ matrix. In fact, an $(mp) \times (np)$ matrix has $mnpq$ degrees of freedom, while $m \times n$ and $p \times q$ matrices have $mn + pq$ in total. Observe that $mnpq \gg mn + pq$ for large enough m, n, p and q. This fact is ultimately related to the power of quantum computing compared to its classical counterpart.

Exercises

EXAMPLE 1.8

$$\sigma_x \otimes \sigma_z = \begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}.$$

EXAMPLE 1.9 We can also apply the tensor product to vectors as a special case. Let

$$|u\rangle = \begin{pmatrix} a \\ b \end{pmatrix}, \quad |v\rangle = \begin{pmatrix} c \\ d \end{pmatrix}.$$

Then we obtain

$$|u\rangle \otimes |v\rangle = \begin{pmatrix} a|v\rangle \\ b|v\rangle \end{pmatrix} = \begin{pmatrix} ac \\ ad \\ bc \\ bd \end{pmatrix}.$$

The tensor product $|u\rangle \otimes |v\rangle$ is often abbreviated as $|u\rangle|v\rangle$ or $|uv\rangle$ when it does not cause confusion.

Exercises

$$\begin{bmatrix} 1 \\ 2 \end{bmatrix} \otimes \begin{bmatrix} 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 1 \times 2 \\ 1 \times 3 \\ 2 \times 2 \\ 2 \times 3 \end{bmatrix} = \begin{bmatrix} 2 \\ 3 \\ 4 \\ 6 \end{bmatrix}$$

$$X \otimes Y = \begin{bmatrix} 0 \cdot Y & 1 \cdot Y \\ 1 \cdot Y & 0 \cdot Y \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix}$$

Exercise 2.26: Let $|\psi\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$. Write out $|\psi\rangle^{\otimes 2}$ and $|\psi\rangle^{\otimes 3}$ explicitly, both in terms of tensor products like $|0\rangle|1\rangle$, and using the Kronecker product.

Exercise 2.27: Calculate the matrix representation of the tensor products of the Pauli operators (a) X and Z; (b) I and X; (c) X and I. Is the tensor product commutative?

Exercises

EXERCISE 1.18 Let A and B be as above and let C be an $n \times r$ matrix and D be a $q \times s$ matrix. Show that

$$(A \otimes B)(C \otimes D) = (AC) \otimes (BD).$$

It similarly holds that

$$(A_1 \otimes B_1)(A_2 \otimes B_2)(A_3 \otimes B_3) = (A_1 A_2 A_3) \otimes (B_1 B_2 B_3),$$

and its generalizations whenever the dimensions of the matrices match so that the products make sense.

EXERCISE 1.19 Show that

$$\begin{aligned} A \otimes (B + C) &= A \otimes B + A \otimes C \\ (A \otimes B)^{\dagger} &= A^{\dagger} \otimes B^{\dagger} \\ (A \otimes B)^{-1} &= A^{-1} \otimes B^{-1} \end{aligned}$$

whenever the matrix operations are well-defined.

Show, from the above observations, that the tensor product of two unitary matrices is also unitary and that the tensor product of two Hermitian matrices is also Hermitian.

EXERCISE 1.20 Let A and B be an $m \times m$ matrix and a $p \times p$ matrix, respectively. Show that

$$\begin{aligned} \mathrm{tr}(A \otimes B) &= (\mathrm{tr}A)(\mathrm{tr}B), \\ \det(A \otimes B) &= (\det A)^p (\det B)^m. \end{aligned}$$

Exercises

EXERCISE 1.21 Let $|a\rangle, |b\rangle, |c\rangle, |d\rangle \in \mathbb{C}^n$. Show that

$$(|a\rangle\langle b|) \otimes (|c\rangle\langle d|) = (|a\rangle \otimes |c\rangle)(\langle b| \otimes \langle d|) = |ac\rangle\langle bd|.$$

THEOREM 1.6 Let A be an $m \times m$ matrix and B be a $p \times p$ matrix. Let A have the eigenvalues $\lambda_1, \ldots, \lambda_m$ with the corresponding eigenvectors $|u_1\rangle, \ldots, |u_m\rangle$ and let B have the eigenvalues $\mu_1, \ldots, \mu_p$ with the corresponding eigenvectors $|v_1\rangle, \ldots, |v_p\rangle$. Then $A \otimes B$ has mp eigenvalues $\{\lambda_j \mu_k\}$ with the corresponding eigenvectors $\{|u_j v_k\rangle\}$.

Proof. We show that $|u_j v_k\rangle$ is an eigenvector. In fact,

$$\begin{aligned}(A \otimes B)(|u_j v_k\rangle) &= (A|u_j\rangle) \otimes (B|v_k\rangle) = (\lambda_j |u_j\rangle) \otimes (\mu_k |v_k\rangle) \\ &= \lambda_j \mu_k (|u_j v_k\rangle) \ .\end{aligned}$$

Therefore, the eigenvalue is $\lambda_j \mu_k$ with the corresponding eigenvector $|u_j v_k\rangle$. Since there are mp eigenvectors, the vectors $|u_j v_k\rangle$ exhaust all of them. ∎

EXERCISE 1.22 Let A and B be as above. Show that $A \otimes I_p + I_m \otimes B$ has the eigenvalues $\{\lambda_j + \mu_k\}$ with the corresponding eigenvectors $\{|u_j v_k\rangle\}$, where I_p is the $p \times p$ unit matrix.

Quantum Mechanics

1. **The state** of a physical system is represented by a normalized vector |ψ> of a suitable Hilbert space.
2. **Observables** (like position, momentum, spin…) are represented by suitable Hermitian operators.
3. The state evolved according to the **Schrödinger equation**

$$i\hbar\frac{\partial|\psi\rangle}{\partial t} = H|\psi\rangle,$$

It is a linear equation, and implies the **superposition principle:** the linear combination of two possible states is still a possible state of the system.

Quantum Mechanics

4. In a **measurement**, the only possible outcomes are the **eigenvalues** of the Hermitian operator associated to the observable. The outcomes are **random** and distributed with the **Born rule**

$$\mathbb{P}[c_i] = |\langle c_i|\psi\rangle|^2$$

where $|c_i\rangle$ is the eigenstate associated to the eigenvalue c_i and $|\psi\rangle$ is the state of the system at the time of the measurement.

5. After the measurement, the state collapses to the eigenstate associated to the measured observable (**von Neumann collapse**)

$$|\psi\rangle \quad \longrightarrow \quad |a_n\rangle$$

Comments

In Axiom 1, the phase of the vector may be chosen arbitrarily; $|\psi\rangle$ in fact represents the "ray" $\{e^{i\alpha}|\psi\rangle \; |\alpha \in \mathbb{R}\}$. This is called the **ray representation**. In other words, we can totally igonore the phase of a vector since it has no observable consequence. Note, however, that the *relative* phase of two different states is meaningful. Although $|\langle\phi|e^{i\alpha}\psi\rangle|^2$ is independent of α, $|\langle\phi|\psi_1 + e^{i\alpha}\psi_2\rangle|^2$ does depend on α.

Axiom 4 may be formulated in a different but equivalent way as follows. Suppose we would like to measure an observable a. Let $A = \sum_i \lambda_i |\lambda_i\rangle\langle\lambda_i|$ be the corresponding operator, where $A|\lambda_i\rangle = \lambda_i|\lambda_i\rangle$. Then the expectation value $\langle A\rangle$ of a after measurements with respect to many copies of a state $|\psi\rangle$ is

$$\langle A\rangle = \langle\psi|A|\psi\rangle. \tag{2.2}$$

Let us expand $|\psi\rangle$ in terms of $|\lambda_i\rangle$ as $|\psi\rangle = \sum_i c_i|\lambda_i\rangle$ to show the equivalence between two formalisms. According to A 2, the probability of observing λ_i upon measurement of a is $|c_i|^2$, and therefore the expectation value after many measurements is $\sum_i \lambda_i |c_i|^2$. If, conversely, Eq. (2.2) is employed, we will obtain the same result since

$$\langle\psi|A|\psi\rangle = \sum_{i,j} c_j^* c_i \langle\lambda_j|A|\lambda_i\rangle = \sum_{i,j} c_j^* c_i \lambda_i \delta_{ij} = \sum_i \lambda_i |c_i|^2.$$

This measurement is called the **projective measurement**. Any particular outcome λ_i will be found with the probability

$$|c_i|^2 = \langle\psi|P_i|\psi\rangle, \tag{2.3}$$

where $P_i = |\lambda_i\rangle\langle\lambda_i|$ is the projection operator, and the state immediately after the measurement is $|\lambda_i\rangle$ or equivalently

$$\frac{P_i|\psi\rangle}{\sqrt{\langle\psi|P_i|\psi\rangle}}, \tag{2.4}$$

where the overall phase has been ignored.

Comments

Comments

The Schrödinger equation (2.1) in Axiom A 3 is formally solved to yield

$$|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle, \tag{2.5}$$

if the Hamiltonian H is time-independent, while

$$|\psi(t)\rangle = \mathcal{T} \exp\left[-\frac{i}{\hbar}\int_0^t H(t)dt\right]|\psi(0)\rangle \tag{2.6}$$

if H depends on t, where $\mathcal{T}$ is the time-ordering operator defined by

$$\mathcal{T}[A(t_1)B(t_2)] = \begin{cases} A(t_1)B(t_2), & t_1 > t_2 \\ B(t_2)A(t_1), & t_2 \geq t_1 \end{cases},$$

for a product of two operators. Generalization to products of more than two operators should be obvious. We write Eqs. (2.5) and (2.6) as $|\psi(t)\rangle = U(t)|\psi(0)\rangle$. The operator $U(t) : |\psi(0)\rangle \mapsto |\psi(t)\rangle$, which we call the **time-evolution operator**, is unitary. Unitarity of $U(t)$ guarantees that the norm of $|\psi(t)\rangle$ is conserved:

$$\langle\psi(0)|U^\dagger(t)U(t)|\psi(0)\rangle = \langle\psi(0)|\psi(0)\rangle = 1.$$

Uncertainty principle

EXERCISE 2.1 (Uncertainty Principle)
(1) Let A and B be Hermitian operators and $|\psi\rangle$ be some quantum state on which A and B operate. Show that

$$|\langle\psi|[A, B]|\psi\rangle|^2 + |\langle\psi|\{A, B\}|\psi\rangle|^2 = 4|\langle\psi|AB|\psi\rangle|^2.$$

(2) Prove the Cauchy-Schwarz inequality

$$|\langle\psi|AB|\psi\rangle|^2 \leq \langle\psi|A^2|\psi\rangle\langle\psi|B^2|\psi\rangle.$$

(3) Show that

$$|\langle\psi|[A, B]|\psi\rangle|^2 \leq 4\langle\psi|A^2|\psi\rangle\langle\psi|B^2|\psi\rangle.$$

(4) Show that

$$\Delta(A)\Delta(B) \geq \frac{1}{2}|\langle\psi|[A, B]|\psi\rangle|, \tag{2.7}$$

where $\Delta(A) \equiv \sqrt{\langle\psi|A^2|\psi\rangle - \langle\psi|A|\psi\rangle^2}$.

(5) Suppose $A = Q$ and $B = P \equiv \frac{\hbar}{i}\frac{d}{dQ}$. Deduce from the above arguments that

$$\Delta(Q)\Delta(P) \geq \frac{\hbar}{2}.$$

Example

EXAMPLE 2.1 Let us consider a time-independent Hamiltonian

$$H = -\frac{\hbar}{2}\omega\sigma_x. \tag{2.8}$$

Suppose the system is in the eigenstate of σ_z with the eigenvalue $+1$ at time $t = 0$;

$$|\psi(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

The wave function $|\psi(t)\rangle$ $(t > 0)$ is then found from Eq. (2.5) to be

$$|\psi(t)\rangle = \exp\left(i\frac{\omega}{2}\sigma_x t\right)|\psi(0)\rangle. \tag{2.9}$$

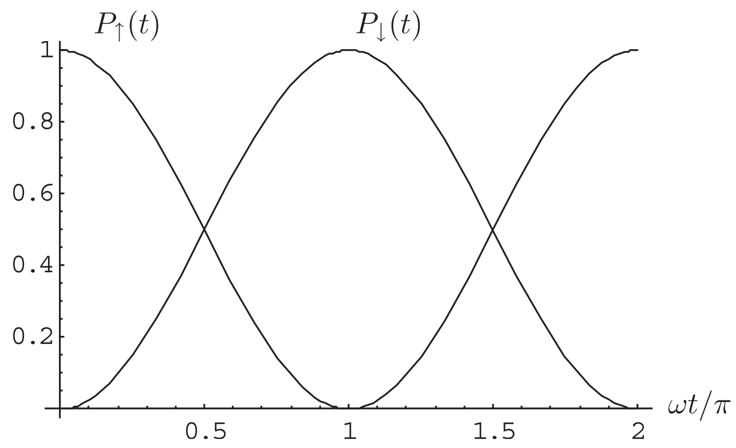
The matrix exponential function in this equation is evaluated with the help of Eq. (1.44) and we find

$$|\psi(t)\rangle = \begin{pmatrix} \cos\omega t/2 & i\sin\omega t/2 \\ i\sin\omega t/2 & \cos\omega t/2 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\omega t/2 \\ i\sin\omega t/2 \end{pmatrix}. \tag{2.10}$$

Suppose we measure the observable σ_z. Note that $|\psi(t)\rangle$ is expanded in terms of the eigenvectors of σ_z as

$$|\psi(t)\rangle = \cos\frac{\omega}{2}t|\sigma_z = +1\rangle + i\sin\frac{\omega}{2}t|\sigma_z = -1\rangle.$$

The state oscillates among the two eigenstates. Why? What should happen to not have the oscillation? What are the probabilities of outcomes of measurements?



Example

Next let us take the initial state

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix},$$

which is an eigenvector of σ_x (and hence the Hamiltonian) with the eigenvalue $+1$. We find $|\psi(t)\rangle$ in this case as

$$|\psi(t)\rangle = \begin{pmatrix}\cos\omega t/2 & i\sin\omega t/2\\ i\sin\omega t/2 & \cos\omega t/2\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = \frac{e^{i\omega t/2}}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}. \qquad (2.11)$$

Therefore the state remains in its initial state at an arbitrary $t > 0$. This is an expected result since the system at $t = 0$ is an eigenstate of the Hamiltonian.

Exercise

EXERCISE 2.2 Let us consider a Hamiltonian

$$H = -\frac{\hbar}{2}\omega\sigma_y. \tag{2.12}$$

Suppose the initial state of the system is

$$|\psi(0)\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{2.13}$$

(1) Find the wave function $|\psi(t)\rangle$ at later time $t > 0$.
(2) Find the probability for the system to have the outcome $+1$ upon measurement of σ_z at $t > 0$.
(3) Find the probability for the system to have the outcome $+1$ upon measurement of σ_x at $t > 0$.

Exercise: generalization

Now let us formulate Example 2.1 and Exercise 2.2 in the most general form. Consider a Hamiltonian

$$H = -\frac{\hbar}{2}\omega\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma}, \tag{2.14}$$

where $\hat{\boldsymbol{n}}$ is a unit vector in $\mathbb{R}^3$. The time-evolution operator is readily obtained, by making use of the result of Proposition 1.2, as

$$U(t) = \exp(-iHt/\hbar) = \cos\frac{\omega}{2}t\ I + i(\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma})\sin\frac{\omega}{2}t. \tag{2.15}$$

Suppose the initial state is

$$|\psi(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

for example. Then we find

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle = \begin{pmatrix} \cos(\omega t/2) + i n_z \sin(\omega t/2) \\ i(n_x + i n_y)\sin(\omega t/2) \end{pmatrix}. \tag{2.16}$$

The reader should verify that $|\psi(t)\rangle$ is normalized at any instant of time $t > 0$.

Bipartite systems

A system composed of two separate components is called **bipartite**. Then the system as a whole lives in a Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$, whose general vector is written as

$$|\psi\rangle = \sum_{i,j} c_{ij} |e_{1,i}\rangle \otimes |e_{2,j}\rangle, \tag{2.29}$$

where $\{|e_{a,i}\rangle\}$ $(a = 1, 2)$ is an orthonormal basis in $\mathcal{H}_a$ and $\sum_{i,j} |c_{ij}|^2 = 1$.

A state $|\psi\rangle \in \mathcal{H}$ written as a tensor product of two vectors as $|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$, $(|\psi_a\rangle \in \mathcal{H}_a)$ is called a **separable state** or a **tensor product state**. A separable state admits a classical interpretation such as "The first system is in the state $|\psi_1\rangle$, while the second system is in $|\psi_2\rangle$." It is clear that the set of separable states has dimension $\dim\mathcal{H}_1 + \dim\mathcal{H}_2$. Note however that the total space $\mathcal{H}$ has different dimensions since we find, by counting the number of coefficients in (2.29), that $\dim\mathcal{H} = \dim\mathcal{H}_1 \dim\mathcal{H}_2$. This number is considerably larger than the dimension of the sparable states when $\dim\mathcal{H}_a$ $(a = 1, 2)$ are large. What are the missing states then?

Bipartite systems

Such non-separable states are called **entangled** in quantum theory [9]. The fact

$$\dim\mathcal{H}_1 \dim\mathcal{H}_2 \gg \dim\mathcal{H}_1 + \dim\mathcal{H}_2$$

tells us that most states in a Hilbert space of a bipartite system are entangled when the constituent Hilbert spaces are higher dimensional. These entangled states refuse classical descriptions. Entanglement will be used extensively as a powerful computational resource in quantum information processing and quantum computation.

Entanglement is deeply related to quantum nonlocality, the most fascinating lesson of quantum theory

Schmidt decomposition

PROPOSITION 2.1 Let $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ be the Hilbert space of a bipartite system. Then a vector $|\psi\rangle \in \mathcal{H}$ admits the **Schmidt decomposition**

$$|\psi\rangle = \sum_{i=1}^{r} \sqrt{s_i}|f_{1,i}\rangle \otimes |f_{2,i}\rangle \text{ with } \sum_i s_i = 1, \tag{2.31}$$

where $s_i > 0$ are called the **Schmidt coefficients** and $\{|f_{a,i}\rangle\}$ is an orthonormal set of $\mathcal{H}_a$. The number $r \in \mathbb{N}$ is called the **Schmidt number** of $|\psi\rangle$.

The proof will be done in Introduction to Quantum Information Theory

It follows from the above proposition that a bipartite state $|\psi\rangle$ is separable if and only if its Schmidt number r is 1.

Multipartite systems

Generalization to a system with more components, i.e., a **multipartite system**, should be obvious. A system composed of N components has a Hilbert space

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \ldots \otimes \mathcal{H}_N, \tag{2.32}$$

where $\mathcal{H}_a$ is the Hilbert space to which the ath component belongs. Classification of entanglement in a multipartite system is far from obvious, and an analogue of the Schmidt decompostion is not known to date for $N \geq 3$.*