

# The Mathematics of Quantum Mechanics

# Hilbert spaces of finite dimension

$\mathcal{H} \rightarrow$  a vector space of dimension  $N$  over complex numbers.  $|\phi\rangle, |\chi\rangle, \dots \in \mathcal{H}$

$\lambda, \mu \in \mathbb{C} \Rightarrow$  linear vector space: if  $|\phi\rangle, |\chi\rangle, \dots \in \mathcal{H} \Rightarrow$   
 $\lambda|\phi\rangle \equiv |\lambda\phi\rangle \in \mathcal{H}$   
 $(|\phi\rangle + \lambda|\chi\rangle) \in \mathcal{H}$

Hilbert space  $\Rightarrow$  positive-definite scalar product:

$$\langle \chi | \phi \rangle$$

$\rightarrow$  linearity:  $\langle \chi | (\phi_1 + \lambda\phi_2) \rangle = \langle \chi | \phi_1 \rangle + \lambda \langle \chi | \phi_2 \rangle$

$\rightarrow$  complex conjugation:  $\langle \chi | \phi \rangle = \langle \phi | \chi \rangle^* \rightarrow \langle \phi | \phi \rangle$  real!

$\langle \chi | \phi \rangle$  linear in  $|\phi\rangle$ , and antilinear in  $|\chi\rangle$ :

$$\langle (\chi_1 + \lambda\chi_2) | \phi \rangle = \langle \chi_1 | \phi \rangle + \lambda^* \langle \chi_2 | \phi \rangle$$

The scalar product is positive-definite  $\Rightarrow \langle \phi | \phi \rangle = 0 \iff |\phi\rangle = 0$

→ orthonormal basis  $\{ |n\rangle \}$  of an N-dim. Hilbert space:

$$\{ |n\rangle \} \equiv \{ |1\rangle, |2\rangle, \dots, |n\rangle, \dots, |N\rangle \} \quad \longrightarrow \quad \langle n|m\rangle = \delta_{nm}$$

Any vector  $|\phi\rangle \in \mathcal{H}$  can be decomposed on this basis with coefficients  $c_n$  which are the components of  $|\phi\rangle$  in this basis:

$$|\phi\rangle = \sum_{n=1}^N c_n |n\rangle \quad c_m = \langle m|\phi\rangle$$

→ scalar product: 
$$\langle \chi|\phi\rangle = \sum_{n,m=1}^N d_m^* c_n \langle m|n\rangle = \sum_{n=1}^N d_n^* c_n$$

DEF. the *norm* of  $|\phi\rangle$ : 
$$\|\phi\|^2 = \langle \phi|\phi\rangle = \sum_{n=1}^N |c_n|^2 \geq 0$$

The Schwarz inequality:

$$|\langle \chi|\phi\rangle|^2 \leq \langle \chi|\chi\rangle \langle \phi|\phi\rangle = \|\chi\|^2 \|\phi\|^2$$

Hilbert space: linear vector space, complete and separable, on which the scalar product is defined.

# Linear operators on $\mathcal{H}$

## Linear, Hermitian, unitary operators


A linear operator A:  $|A(\varphi + \lambda\chi)\rangle = |A\varphi\rangle + \lambda|A\chi\rangle$

This operator is represented in a given basis  $\{|n\rangle\}$  by a matrix with elements  $A_{nm}$ :

$$|A\varphi\rangle = \sum_{n=1}^N c_n |An\rangle$$

The components  $d_m$  of  $|A\varphi\rangle = \sum_m d_m |m\rangle$ :

$$d_m = \langle m|A\varphi\rangle = \sum_{n=1}^N c_n \langle m|An\rangle = \sum_{n=1}^N A_{mn} c_n$$

  $A_{mn} = \langle m|An\rangle$

The *Hermitian conjugate* (or adjoint) of A,  $A^\dagger$ , is defined:  $\langle\chi|A^\dagger\varphi\rangle = \langle A\chi|\varphi\rangle = \langle\varphi|A\chi\rangle^*$

$$(A^\dagger)_{mn} = A_{nm}^*$$

The Hermitian conjugate of the product AB of two operators is B<sup>†</sup>A<sup>†</sup>:

$$\langle \chi | (AB)^\dagger \varphi \rangle = \langle AB \chi | \varphi \rangle = \langle B \chi | A^\dagger \varphi \rangle = \langle \chi | B^\dagger A^\dagger \varphi \rangle$$

An operator satisfying  $A = A^\dagger$  is termed *Hermitian* or *self-adjoint*.

A unitary operator:  $UU^\dagger = U^\dagger U = I$    $U^{-1} = U^\dagger$

In a finite-dimensional space the necessary and sufficient condition for an operator U to be unitary is that it leaves unchanged the norm:

$$\|U\varphi\|^2 = \|\varphi\|^2 \quad \text{or} \quad \langle U\varphi | U\varphi \rangle = \langle \varphi | \varphi \rangle \quad \forall \varphi \in \mathcal{H}$$

*Proof:*


$$\langle \varphi + \lambda\chi | \varphi + \lambda\chi \rangle = \langle \varphi | \varphi \rangle + |\lambda|^2 \langle \chi | \chi \rangle + 2\text{Re}(\lambda \langle \varphi | \chi \rangle)$$

$$\langle U(\varphi + \lambda\chi) | U(\varphi + \lambda\chi) \rangle = \langle U\varphi | U\varphi \rangle + |\lambda|^2 \langle U\chi | U\chi \rangle + 2\text{Re}(\lambda \langle U\varphi | U\chi \rangle)$$

Subtracting the second of these equations from the first  $\Rightarrow \langle U\varphi | U\varphi \rangle = \langle \varphi | \varphi \rangle \quad \forall \varphi \in \mathcal{H}$

  $\text{Re}(\lambda \langle \varphi | \chi \rangle) = \text{Re}(\lambda \langle U\varphi | U\chi \rangle)$    $\langle U\varphi | U\chi \rangle = \langle \varphi | \chi \rangle \Rightarrow U^\dagger U = I$

Unitary operators change the orthonormal basis in  $\mathcal{H}$ :  $|n'\rangle = |Un\rangle$

  $\langle m'|n'\rangle = \langle Um|Un\rangle = \langle m|n\rangle = \delta_{mn} = \delta_{m'n'}$

The components of a vector:  $c'_n = \langle n'|\varphi\rangle = \langle Un|\varphi\rangle = \langle n|U^\dagger\varphi\rangle = \sum_{m=1}^N U_{nm}^\dagger c_m$

The transformation of matrix elements:

$$A'_{mn} = \langle m'|An'\rangle = \langle Um|AUn\rangle = \langle m|U^\dagger AUn\rangle = \sum_{k,l=1}^N U_{mk}^\dagger A_{kl} U_{ln}$$

## Projection operators and Dirac notation

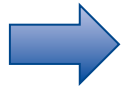
$\mathcal{H}_1 \rightarrow$  subspace of  $\mathcal{H}$ , and  $\mathcal{H}_2$  is the orthogonal subspace. Any vector  $|\phi\rangle$  can be decomposed uniquely:

$$|\phi\rangle = |\varphi_1\rangle + |\varphi_2\rangle, \quad |\varphi_1\rangle \in \mathcal{H}_1, \quad |\varphi_2\rangle \in \mathcal{H}_2, \quad \langle \varphi_1|\varphi_2\rangle = 0.$$

The projector  $P_1$  onto  $\mathcal{H}_1$  is defined by its action on an arbitrary vector  $|\phi\rangle \in \mathcal{H}$ :

$$|\mathcal{P}_1\phi\rangle = |\varphi_1\rangle$$

Projectors  $\rightarrow$  linear and hermitian operators: if  $|\chi\rangle = |\chi_1\rangle + |\chi_2\rangle$

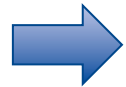

$$\begin{aligned}\langle\chi|\mathcal{P}_1\varphi\rangle &= \langle\chi|\varphi_1\rangle = \langle\chi_1|\varphi_1\rangle, \\ \langle\chi|\mathcal{P}_1^\dagger\varphi\rangle &= \langle\mathcal{P}_1\chi|\varphi\rangle = \langle\chi_1|\varphi\rangle = \langle\chi_1|\varphi_1\rangle.\end{aligned}$$

$$\boxed{|\mathcal{P}_1^2\varphi\rangle = |\mathcal{P}_1\varphi_1\rangle = |\varphi_1\rangle \Rightarrow \mathcal{P}_1^2 = \mathcal{P}_1} \Rightarrow \text{eigenvalues 0 or 1.}$$

Every linear operator satisfying:  $\mathcal{P}_1^\dagger\mathcal{P}_1 = \mathcal{P}_1 \Rightarrow$  PROJECTOR.

*Proof:*  $\mathcal{P}_1^\dagger = \mathcal{P}_1 \Rightarrow$  the vectors  $\mathcal{P}_1|\phi\rangle$  form a vector subspace  $\mathcal{H}_1$ .

$$|\varphi\rangle = |\mathcal{P}_1\varphi\rangle + (|\varphi\rangle - |\mathcal{P}_1\varphi\rangle) = |\mathcal{P}_1\varphi\rangle + |\varphi_2\rangle$$



$|\varphi_2\rangle$  is orthogonal to every vector  $|\mathcal{P}_1\chi\rangle$

$$\langle\varphi - \mathcal{P}_1\varphi|\mathcal{P}_1\chi\rangle = \langle\mathcal{P}_1\varphi - \mathcal{P}_1^2\varphi|\chi\rangle = 0.$$

## Dirac notation:

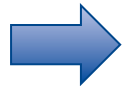
$|\phi\rangle \in \mathcal{H} \rightarrow$  "ket" and  $\langle\phi| \rightarrow$  "bra". Instead of  $|A\phi\rangle$ , in this notation we use  $A|\phi\rangle$ . The scalar product:

$$\langle\chi|A\varphi\rangle \rightarrow \langle\chi|A|\varphi\rangle$$

$$\langle\lambda\varphi|\chi\rangle = \lambda^* \langle\varphi|\chi\rangle$$

Projectors:

$$\mathcal{P}_\varphi = |\varphi\rangle\langle\varphi|$$



decomposition:

$$|\chi\rangle = |\varphi\rangle\langle\varphi|\chi\rangle + (|\chi\rangle - |\varphi\rangle\langle\varphi|\chi\rangle) = |\varphi\rangle\langle\varphi|\chi\rangle + |\chi_\perp\rangle = \mathcal{P}_\varphi|\chi\rangle + |\chi_\perp\rangle$$

If the vectors:  $\{|1\rangle, \dots, |M\rangle\}$ ,  $M \leq N$  form an orthonormal basis of the subspace  $\mathcal{H}_1 \Rightarrow$

$$\mathcal{P}_1 = \sum_{n=1}^M |n\rangle\langle n|$$

If  $M = N$  we obtain the decomposition of the identity operator:

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



# Spectral decomposition of Hermitian operators

## Diagonalization of a Hermitian operator

Let  $A$  be a linear operator. If there exists a vector  $|\varphi\rangle$  and a complex number  $a$  such that:

$$A|\varphi\rangle = a|\varphi\rangle$$

$\Rightarrow |\varphi\rangle$  is an eigenvector, and  $a$  an eigenvalue of the operator  $A$ . The eigenvalues are solutions of the equation:

$$\det(A - aI) = 0$$

*Theorem. The eigenvalues of a Hermitian operator are real and the eigenvectors corresponding to two different eigenvalues are orthogonal.*

*Proof:*  $\langle\varphi|A|\varphi\rangle = \langle\varphi|a\varphi\rangle = a\|\varphi\|^2$   
 $= \langle A\varphi|\varphi\rangle = \langle a\varphi|\varphi\rangle = a^*\|\varphi\|^2 \quad \Rightarrow \quad a = a^*$

$$\begin{array}{l} A|\varphi\rangle = a|\varphi\rangle \\ A|\chi\rangle = b|\chi\rangle \end{array} \Rightarrow \langle\chi|A\varphi\rangle = a\langle\chi|\varphi\rangle = \langle A\chi|\varphi\rangle = b\langle\chi|\varphi\rangle \Rightarrow \langle\chi|\varphi\rangle = 0 \text{ if } a \neq b$$

The eigenvectors of a Hermitian operator normalized to unity form an orthonormal basis of  $\mathcal{H}$  if the eigenvalues are all distinct.

If  $a_n$  is a multiple root of  $\det(A-aI)=0$ , the eigenvalue  $a_n$  is then said to be *degenerate*.

*Theorem.* If an operator  $A$  is Hermitian, it is always possible to find a (nonunique) unitary matrix  $U$  such that  $U^{-1}AU$  is a diagonal matrix, where the diagonal elements are the eigenvalues of  $A$ , each of which appears a number of times equal to its multiplicity.

Let  $a_n$  be a degenerate eigenvalue and let  $G(n)$  be its multiplicity. Then there exist  $G(n)$  independent eigenvectors corresponding to this eigenvalue. These eigenvectors span a vector subspace of dimension  $G(n)$  called the *subspace of the eigenvalue*  $a_n$ , in which we can find a (nonunique) orthonormal basis

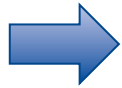
$$|n, r\rangle, \quad r = 1, \dots, G(n)$$

$$A|n, r\rangle = a_n|n, r\rangle$$

The projector onto this vector subspace:  $\mathcal{P}_n = \sum_{r=1}^{G(n)} |n, r\rangle\langle n, r|$

$$\sum_n \mathcal{P}_n = \sum_n \sum_{r=1}^{G(n)} |n, r\rangle\langle n, r| = I$$

Let the vector  $|\phi\rangle \in \mathcal{H} \Rightarrow A|\phi\rangle = \sum_n A\mathcal{P}_n|\phi\rangle = \sum_n a_n\mathcal{P}_n|\phi\rangle$



$$A = \sum_n a_n \mathcal{P}_n = \sum_n \sum_{r=1}^{G(n)} |n, r\rangle a_n \langle n, r|$$

*Spectral decomposition of the operator A.*

### Complete sets of compatible operators

Two operators A and B commute if  $AB = BA$ , and in this case their *commutator*  $[A, B]$  vanishes.

$$[A, B] = AB - BA$$

*Theorem.* Let A and B be two Hermitian operators such that  $[A, B] = 0$ . We can then find a basis of  $\mathcal{H}$  constructed from eigenvectors common to A and B.

$\Rightarrow$  an ensemble of Hermitian operators  $A_1, \dots, A_M$  that commute pairwise and whose eigenvalues unambiguously define the vectors of a basis of  $\mathcal{H}$  is called a *complete set of compatible operators* (or a complete set of commuting operators).

## Unitary operators and Hermitian operators

*Theorem.* (a) The eigenvalues of a unitary operator have modulus unity:  $a_n = \exp(i\alpha_n)$ ,  $\alpha_n$  real. (b) The eigenvectors corresponding to two different eigenvalues are orthogonal. (c) The spectral decomposition of a unitary operator is written as a function of pairwise orthogonal projectors  $\mathcal{P}_n$  as

$$U = \sum_n a_n \mathcal{P}_n = \sum_n e^{i\alpha_n} \mathcal{P}_n \quad \sum_n \mathcal{P}_n = I$$

Let  $A = \sum_n a_n \mathcal{P}_n$  be a Hermitian operator  $\Rightarrow U = \sum_n e^{i\alpha_n} \mathcal{P}_n = e^{iA}$  unitary operator.

## Operator-valued functions

A function  $f(A)$  of an operator?

1) If the operator  $A$  can be diagonalized:  $A = XDX^{-1}$ , where  $D$  is a diagonal matrix whose elements are  $d_n$ . Let us assume that a function  $f$  is defined by a Taylor series which converges in a certain region of the complex plane  $|z| < R$ :

$$f(z) = \sum_{p=0}^{\infty} c_p z^p$$

$$\Rightarrow \text{operator-valued function: } f(A) = \sum_{p=0}^{\infty} c_p A^p = \sum_{p=0}^{\infty} c_p X D^p X^{-1} = X \underbrace{\left[ \sum_{p=0}^{\infty} c_p D^p \right]}_{\text{diagonal matrix with elements } f(d_n), \text{ well defined if } |d_n| < R \forall n.} X^{-1}$$

diagonal matrix with elements  $f(d_n)$ , well defined if  $|d_n| < R \forall n$ .

The exponential of an operator: 
$$\exp A = \sum_{p=0}^{\infty} \frac{A^p}{p!}$$

Generally: 
$$\exp A \exp B \neq \exp B \exp A$$

A sufficient (but not necessary!) condition for the equality to hold is that A and B commute.

For a Hermitian operator A whose spectral decomposition is given by: 
$$A = \sum_n a_n \mathcal{P}_n$$



any function of A can be defined:

$$f(A) = \sum_n f(a_n) \mathcal{P}_n$$

# State vectors and physical properties

## The superposition principle

The space of states: the properties of a quantum system are completely defined by its *state vector*  $|\phi\rangle \rightarrow$  an element of a complex Hilbert space  $\mathcal{H}$  (*space of states*).

$\rightarrow$  normalized state vector:  $\|\varphi\|^2 = \langle\varphi|\varphi\rangle = 1$

$\rightarrow$  linearity of the space of states  $\Rightarrow$  *superposition principle*: if  $|\phi\rangle$  i  $|\chi\rangle \in \mathcal{H}$  are state vectors  $\Rightarrow$

$$|\psi\rangle = \frac{\lambda|\varphi\rangle + \mu|\chi\rangle}{\|\lambda|\varphi\rangle + \mu|\chi\rangle\|} \in \mathcal{H} \text{ is a state vector } (\lambda, \mu \text{ are complex numbers}).$$

Probability amplitudes and probabilities: if  $|\phi\rangle$  i  $|\chi\rangle \in \mathcal{H}$  are state vectors of a quantum system, there exists a probability amplitude of finding  $|\phi\rangle$  in the state  $|\chi\rangle$  given by the scalar product on  $\mathcal{H}$ :

$$\mathcal{H}: a(\varphi \rightarrow \chi) = \langle \chi | \varphi \rangle$$

⇒ the probability:

$$p(\varphi \rightarrow \chi) = |a(\varphi \rightarrow \chi)|^2 = |\langle \chi | \varphi \rangle|^2$$

## Physical properties and measurement

Physical properties and operator: with every physical property (observable)  $\mathcal{A}$  there exists an associated Hermitian operator  $A$  that acts on the Hilbert space of states.

Example: an observable  $\mathcal{A} \rightarrow$  Hermitian operator  $A$  with nondegenerate eigenvalues:

$$A = \sum_n |n\rangle a_n \langle n|$$

If the quantum system is in a state  $|\phi\rangle \equiv |n\rangle$ , the value of the operator  $A$  in this states is  $a_n$ , that is, the physical property  $\mathcal{A}$  takes the exact numerical value  $a_n$ .

→ in the general case we define the expectation value of the observable  $\mathcal{A}$  in the state  $|\phi\rangle$

$$\langle A \rangle_\phi = \lim_{\mathcal{N} \rightarrow \infty} \frac{1}{\mathcal{N}} \sum_{p=1}^{\mathcal{N}} \mathcal{A}_p$$

↙
↘

number of measurements result of the p-th measurement

The expectation value is a function of A and  $|\phi\rangle$ :

➔ 
$$\langle A \rangle_\phi = \sum_n p_n a_n = \sum_n \langle \phi | n \rangle a_n \langle n | \phi \rangle = \langle \phi | A | \phi \rangle$$

→ general case with degenerate eigenvalues:

$$|\phi\rangle = \sum_{n,r} |n, r\rangle \langle n, r | \phi \rangle = \sum_{n,r} c_{nr} |n, r\rangle$$

→ the probability of observing the eigenvalue  $a_n$ :

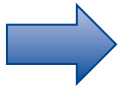
$$p(a_n) = \sum_r |c_{nr}|^2 = \sum_r \langle \phi | n, r \rangle \langle n, r | \phi \rangle$$

$$= \langle \phi | \mathcal{P}_n | \phi \rangle,$$

$$\mathcal{P}_n = \sum_r |n, r\rangle \langle n, r|$$

→ projector on the subspace  $a_n$





the expectation value  $\langle A \rangle_\phi$  of the physical property  $\mathcal{A}$  of the system in the state  $|\phi\rangle$ :

$$\langle A \rangle_\phi = \sum_n a_n \mathbf{p}(a_n) = \sum_{n,r} \langle \phi | n, r \rangle a_n \langle n, r | \phi \rangle$$

$$\langle A \rangle_\phi = \langle \phi | A | \phi \rangle$$

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# The tensor product of two vector spaces

Two QM systems: the corresponding spaces of states  $\mathcal{H}_1^N$  and  $\mathcal{H}_2^M$ , of dimensions  $N$  and  $M$ .

$$|\varphi\rangle \in \mathcal{H}_1^N \quad |\chi\rangle \in \mathcal{H}_2^M$$

$\{|\varphi\rangle, |\chi\rangle\}$  → a vector that belongs to a space of dimension  $NM$  ⇒ *tensor product* of spaces:

$$\boxed{\mathcal{H}_1^N \otimes \mathcal{H}_2^M}$$

Orthonormal bases  $|n\rangle \in \mathcal{H}_1^N$  and  $|m\rangle \in \mathcal{H}_2^M$ :

$$|\varphi\rangle = \sum_{n=1}^N c_n |n\rangle, \quad |\chi\rangle = \sum_{m=1}^M d_m |m\rangle$$

$\mathcal{H}_1^N \otimes \mathcal{H}_2^M$  → vector space of dimension  $NM$  on which an orthonormal basis is defined:  $\{|n\rangle, |m\rangle\} \equiv |n\rangle \otimes |m\rangle$

$$\boxed{\langle n' \otimes m' | n \otimes m \rangle = \delta_{n'n} \delta_{m'm}}$$

The tensor product of the vectors  $|\phi\rangle$  i  $|\chi\rangle$ :

$$|\varphi \otimes \chi\rangle = \sum_{n,m} c_n d_m |n \otimes m\rangle$$

→ linearity:

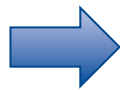
$$|\varphi \otimes (\chi_1 + \lambda \chi_2)\rangle = |\varphi \otimes \chi_1\rangle + \lambda |\varphi \otimes \chi_2\rangle$$

$$|(\varphi_1 + \lambda \varphi_2) \otimes \chi\rangle = |\varphi_1 \otimes \chi\rangle + \lambda |\varphi_2 \otimes \chi\rangle$$

The tensor product is independent of the choice of basis. Let the new bases of  $\mathcal{H}_1^N$  i  $\mathcal{H}_2^M$  be defined by the unitary transformations:

$$|i\rangle = \sum_n R_{in} |n\rangle, \quad |j\rangle = \sum_m S_{jm} |m\rangle$$

$$R^{-1} = R^\dagger \quad S^{-1} = S^\dagger$$



$$|i \otimes j\rangle = \sum_{n,m} R_{in} S_{jm} |n \otimes m\rangle$$

$$|\varphi\rangle = \sum_{i=1}^N \bar{c}_i |i\rangle, \quad |\chi\rangle = \sum_{j=1}^M \bar{d}_j |j\rangle$$



$$\sum_{i,j} \bar{c}_i \bar{d}_j |i \otimes j\rangle = |\varphi \otimes \chi\rangle$$

Postulate: The space of states of two interacting quantum systems is:  $\mathcal{H}_1^N \otimes \mathcal{H}_2^M$

The most general state vector: 
$$|\Phi\rangle = \sum_{n,m} b_{nm} |n \otimes m\rangle$$

→ in general, it cannot be written as a tensor product  $|\phi \otimes \chi\rangle$ , except for independent systems. In that case  $b_{nm} = c_n d_m$ . State vectors which can be written as a tensor product form a subset (but not a subspace) of  $\mathcal{H}_1^N \otimes \mathcal{H}_2^M$ . A state vector which cannot be written in the form of a tensor product is termed *entangled state*.

The tensor product  $C = A \otimes B$  of two linear operators  $A$  and  $B$  acting respectively in the spaces  $\mathcal{H}_1^N$  i  $\mathcal{H}_2^M$  is defined by its action on the tensor product vector  $|\phi \otimes \chi\rangle$ :

$$(A \otimes B)|\phi \otimes \chi\rangle = |A\phi \otimes B\chi\rangle$$

⇒ its matrix elements in the basis  $|n \otimes m\rangle$

$$\langle n' \otimes m' | A \otimes B | n \otimes m \rangle = A_{n'n} B_{m'm}$$

In general, an operator  $C$  acting on  $\mathcal{H}_1^N \otimes \mathcal{H}_2^M$  will not be of the form  $A \otimes B$ :

$$\langle n' \otimes m' | C | n \otimes m \rangle = C_{n'm'; nm}$$

Special case:  $A=I_1$  or  $B=I_2$  (identity operators on  $\mathcal{H}_1^N$  ;  $\mathcal{H}_2^M$ )

$$(A \otimes I_2)|\varphi \otimes \chi\rangle = |A\varphi \otimes \chi\rangle, \quad (I_1 \otimes B)|\varphi \otimes \chi\rangle = |\varphi \otimes B\chi\rangle$$

Matrix elements:

$$\langle n' \otimes m' | A \otimes I_2 | n \otimes m \rangle = A_{n'n} \delta_{m'm}, \quad \langle n' \otimes m' | I_1 \otimes B | n \otimes m \rangle = \delta_{n'n} B_{m'm}$$

If  $|\phi\rangle$  is an eigenvector of the operator  $A$ :  $A|\phi\rangle = a|\phi\rangle \Rightarrow |\phi \otimes \chi\rangle$  is an eigenvector of the operator  $A \otimes I_2$ :  $A \otimes I_2 |\phi \otimes \chi\rangle = a |\phi \otimes \chi\rangle$

Notation:  $A|\varphi \otimes \chi\rangle = a|\varphi \otimes \chi\rangle$

$$A|\varphi \chi\rangle = a|\varphi \chi\rangle$$

# The density operator

## Definition and properties

$|\Psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2 \rightarrow$  if  $|\psi\rangle = |\phi_1 \otimes \phi_2\rangle$ , the state vector of system ① is  $|\phi_1\rangle$ . In the general case when  $|\psi\rangle$  is not a tensor product but rather an entangled state, it is not possible to associate a definite state vector in  $\mathcal{H}_1$  to the system ① or a vector in  $\mathcal{H}_2$  to ②.

- i) when a quantum system can be described by a vector in the Hilbert space of states  $\Rightarrow$  a *pure state* (complete information about the system is available)
- ii) when the information on the system is incomplete  $\Rightarrow$  a *mixture* (the system is described by a *density operator*)

Pure state:  $|\varphi\rangle \in \mathcal{H}$

$\rightarrow$  the projector onto  $|\varphi\rangle$ :  $\mathcal{P}_\varphi = |\varphi\rangle\langle\varphi|$

is invariant with respect to a phase transformation:  $|\varphi\rangle \rightarrow e^{i\alpha} |\varphi\rangle$

$\{|n\rangle\} \rightarrow$  an orthonormal basis of  $\mathcal{H} \Rightarrow$  the expectation value of an observable:

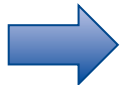
$$\begin{aligned}\langle A \rangle &= \langle \varphi | A | \varphi \rangle = \sum_{n,m} \langle \varphi | n \rangle \langle n | A | m \rangle \langle m | \varphi \rangle \\ &= \sum_{n,m} \langle m | \varphi \rangle \langle \varphi | n \rangle \langle n | A | m \rangle \\ &= \sum_m \langle m | \mathcal{P}_\varphi A | m \rangle = \text{Tr}(\mathcal{P}_\varphi A).\end{aligned}$$

Mixture of quantum states:

$p_\alpha$  ( $0 \leq p_\alpha \leq 1, \sum_\alpha p_\alpha = 1$ )  $\rightarrow$  probability that the system is in the state  $|\phi_\alpha\rangle$ . It is not possible to associate a definite state vector of  $\mathcal{H}$  to the system, but only a mixture of states with corresponding probabilities.

DEF. Density operator (state operator)

$$\rho = \sum_\alpha p_\alpha |\phi_\alpha\rangle \langle \phi_\alpha| = \sum_\alpha p_\alpha \mathcal{P}_{\phi_\alpha}$$



$$\langle A \rangle = \sum_\alpha p_\alpha \langle A \rangle_\alpha = \sum_\alpha p_\alpha \langle \phi_\alpha | A | \phi_\alpha \rangle = \text{Tr}(\rho A)$$

Properties:  $\rightarrow \rho$  is Hermitian  $\rho = \rho^\dagger$

$\rightarrow \text{Tr } \rho = 1$

$\rightarrow \rho$  is a positive operator (Hermitian and has positive eigenvalues)

$$\langle \varphi | \rho | \varphi \rangle \geq 0$$

$\rightarrow$  a necessary and sufficient condition for  $\rho$  to describe a pure state is  $\rho^2 = \rho$ .

$\rightarrow$  spectral decomposition:

$$\rho = \sum_n p_n |n\rangle \langle n|$$

### The reduced density operator

A density operator  $\rho$  acting in the space  $\mathcal{H}_1 \otimes \mathcal{H}_2$ . What is the density operator of the system ①? An observable  $C = A \otimes I_2$  which depends only on ①  $\Rightarrow$  define a density operator  $\rho^{(1)}$  acting in  $\mathcal{H}_1$  such that:

$$\langle A \rangle = \text{Tr}(\rho^{(1)} A)$$

$$\begin{aligned} \langle A \otimes I_2 \rangle &= \text{Tr}([A \otimes I_2] \rho) = \sum_{n_1 m_1; n_2 m_2} A_{n_1 m_1} \delta_{n_2 m_2} \rho_{m_1 m_2; n_1 n_2} = \sum_{n_1 m_1} A_{n_1 m_1} \sum_{n_2} \rho_{m_1 n_2; n_1 n_2} \\ &= \sum_{n_1 m_1} A_{n_1 m_1} \rho_{m_1 n_1}^{(1)} = \text{Tr}(A \rho^{(1)}). \end{aligned}$$



The *reduced* density operator:

$$\rho_{n_1 m_1}^{(1)} = \sum_{n_2} \rho_{n_1 n_2; m_1 n_2} \quad \text{or} \quad \rho^{(1)} = \text{Tr}_2 \rho$$

partial trace on  
the space  $\mathcal{H}_2$

Time dependence of the density operator:

→ density operator for a pure state:  $\mathcal{P}_\varphi(t) = |\varphi(t)\rangle\langle\varphi(t)|$

From the time evolution equation:  $i\hbar \frac{d|\varphi(t)\rangle}{dt} = H(t)|\varphi(t)\rangle$  →

$$i\hbar \frac{d}{dt} \mathcal{P}_{\varphi(t)} = i\hbar \frac{d}{dt} (|\varphi(t)\rangle\langle\varphi(t)|) = H(t)\mathcal{P}_{\varphi(t)} - \mathcal{P}_{\varphi(t)}H(t) = [H(t), \mathcal{P}_{\varphi(t)}]$$

For a mixture of states:  $\rho = \sum_{\alpha} p_{\alpha} |\varphi_{\alpha}\rangle\langle\varphi_{\alpha}| = \sum_{\alpha} p_{\alpha} \mathcal{P}_{\varphi_{\alpha}}$

$$i\hbar \frac{d\rho(t)}{dt} = [H(t), \rho(t)]$$

→ the evolution equation  
for the density operator.

# Wave mechanics

→ a state vector can be identified with an element  $\phi(\mathbf{r})$  of the Hilbert space  $L^2_r(\mathbb{R}^3)$  of functions which are square-integrable in the three-dimensional space  $\mathbb{R}^3$ . This state vector is called the *wave function* → probability amplitude  $\langle \mathbf{r} | \phi \rangle$  for finding the particle in the state  $|\phi\rangle$  localized at position  $\mathbf{r}$ . Normalization:

$$\int_{-\infty}^{\infty} d^3 r |\varphi(\vec{r})|^2 = 1$$


## Diagonalization of $X$ and $P$ and wave functions

→ eigenvector of the position operator:  $X|x\rangle = x|x\rangle$

$$\begin{aligned} X \left[ \exp\left(-i\frac{Pa}{\hbar}\right) |x\rangle \right] &= \exp\left(-i\frac{Pa}{\hbar}\right) (X + aI) |x\rangle \\ &= (x + a) \left[ \exp\left(-i\frac{Pa}{\hbar}\right) |x\rangle \right] \end{aligned} \quad \Rightarrow$$

The vector  $\exp(-iPa/\hbar)|x\rangle$ , with  $a$  real, is an eigenvector of  $X$  with eigenvalue  $(x+a)$ , and since  $a$  is arbitrary  $\Rightarrow$  all real values of  $x$  between  $-\infty$  and  $+\infty$  are eigenvalues of  $X$ .

The spectrum of  $x$  is continuous  $\Rightarrow$  normalization:  $\langle x'|x\rangle = \delta(x - x')$

 translation operator:  $\exp\left(-i\frac{Pa}{\hbar}\right)|x\rangle = |x + a\rangle$

$\rightarrow$  matrix elements of  $X$ :  $\langle x'|X|x\rangle = x\langle x'|x\rangle = x\delta(x - x')$

$\rightarrow$  more generally, for a function of  $X$ :  $\langle x'|F(X)|x\rangle = F(x)\langle x'|x\rangle = F(x)\delta(x - x')$

The completeness relation:  $\int_{-\infty}^{\infty} |x\rangle dx \langle x| = I$

The projector  $\mathcal{P}[a,b]$  onto the subspace of eigenvalues of  $X$  in the interval  $[a,b]$ :

$$\mathcal{P}[a, b] = \int_a^b |x\rangle dx \langle x|$$

Realization in  $L^2_x(\mathbb{R}) \rightarrow$  space of square-integrable functions on  $\mathbb{R}$

$|\phi\rangle \rightarrow$  a normalized vector of  $\mathcal{H}$  representing a physical state:

$$|\phi\rangle = \int_{-\infty}^{\infty} |x\rangle dx \langle x|\phi\rangle$$

probability amplitude of finding the particle localized at point  $x$

$\langle x|\phi\rangle$  can be identified with a normalized function  $\phi(x)$  on  $L^2_x(\mathbb{R})$  such that:

$$[X\phi](x) = x\phi(x)$$

$$[P\phi](x) = -i\hbar \frac{\partial\phi}{\partial x}$$

$\rightarrow$  the scalar product:  $\langle\chi|\phi\rangle = \int_{-\infty}^{\infty} dx \langle\chi|x\rangle \langle x|\phi\rangle = \int_{-\infty}^{\infty} dx \chi^*(x)\phi(x)$

$$\int_{-\infty}^{\infty} dx |\phi(x)|^2 = 1$$

$|\phi(x)|^2 = |\langle x|\phi\rangle|^2 \Rightarrow$  probability density for the physical state of a particle moving on the  $x$  axis.

## Realization in $L^{(2)}_p(\mathbb{R})$

Let  $|p\rangle$  be an eigenvector of  $P$ :  $P|p\rangle = p|p\rangle$

$\Rightarrow$  the corresponding wave function  $\chi_p(x) = \langle x|p\rangle$  in the  $x$ -representation:

$$\chi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$$

$\Rightarrow$  normalization:  $\int_{-\infty}^{\infty} dx \chi_{p'}^*(x) \chi_p(x) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dx \exp\left[i \frac{(p-p')x}{\hbar}\right] = \delta(p-p')$

$\Rightarrow$  completeness:  $\int_{-\infty}^{\infty} dp \chi_p(x) \chi_p^*(x') = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dp \exp\left[i \frac{p(x-x')}{\hbar}\right] = \delta(x-x')$

If  $|\phi\rangle$  is the state vector of a particle, the “wave function in the  $p$ -representation” will be:

$$\tilde{\varphi}(p) = \langle p|\phi\rangle = \int_{-\infty}^{\infty} \langle p|x\rangle dx \langle x|\phi\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx e^{-ipx/\hbar} \varphi(x)$$

...just the Fourier transform of the wave function  $\phi(x) = \langle x|\phi\rangle$  in the  $x$ -representation.

⇒ conversely, the wave function in the  $x$ -representation:

$$\varphi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp e^{ipx/\hbar} \tilde{\varphi}(p)$$

The action of the operators  $X$  and  $P$  in the  $p$ -representation

$$[X\tilde{\varphi}](p) = i\hbar \frac{\partial}{\partial p} \tilde{\varphi}(p)$$

$$[P\tilde{\varphi}](p) = p \tilde{\varphi}(p).$$

## The Hamiltonian of the Schrödinger equation

The most general time-independent Hamiltonian compatible with Galilean invariance in dimension  $d = 1$ :

$$H = \frac{P^2}{2m} + V(X)$$

From the time evolution equation of a state vector:

$$i\hbar \frac{d|\varphi(t)\rangle}{dt} = H|\varphi(t)\rangle$$



⇒ the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial \varphi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \varphi(x, t)}{\partial x^2} + V(x)\varphi(x, t)$$

Since the potential  $V(x)$  is independent of time ⇒ stationary solutions:

$$|\varphi(t)\rangle = \exp\left(-i \frac{Et}{\hbar}\right) |\varphi(0)\rangle, \quad H|\varphi(0)\rangle = E|\varphi(0)\rangle$$

⇒ the time-independent Schrödinger equation:

$$\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \varphi(x) = E\varphi(x)$$

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