The Mathematics of Quantum Mechanics

Hilbert spaces of finite dimension

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

$\lambda, \mu \in \mathbb{C} \Rightarrow$ linear vector space: if $|\phi>, |\chi>, \ldots \in \mathcal{H} \Rightarrow$

$$\lambda|\varphi\rangle \equiv |\lambda\varphi\rangle \in \mathcal{H}$$

$$(|\varphi\rangle + \lambda|\chi\rangle) \in \mathcal{H}$$

Hilbert space $\Rightarrow$ positive-definite scalar product: $\langle\chi|\varphi\rangle$

$\rightarrow$ linearity: $\langle\chi|(\varphi_1 + \lambda\varphi_2)\rangle = \langle\chi|\varphi_1\rangle + \lambda\langle\chi|\varphi_2\rangle$

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

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

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

The scalar product is positive-definite$\Rightarrow$ $\langle\varphi|\varphi\rangle = 0 \Longleftrightarrow |\varphi\rangle = 0$

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

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

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

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

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

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

The Schwarz inequality: $$\boxed{|\langle\chi|\varphi\rangle|^2 \leq \langle\chi|\chi\rangle\langle\varphi|\varphi\rangle = ||\chi||^2\, ||\varphi||^2}$$

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 >} by a matrix with elements A_{nm}:

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

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

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

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

The *Hermitian conjugate* (or adjoint) of A, A†, 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 $B^\dagger A^\dagger$:

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

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:

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

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

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

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

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

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

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

The transformation of matrix elements:

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

Projection operators and Dirac notation

$\mathscr{H}_1$ → subspace of $\mathscr{H}$, and $\mathscr{H}_2$ is the orthogonal subspace. Any vector |ϕ> can be decomposed uniquely:

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

The projector P_1 onto $\mathscr{H}_1$ is defined by its action on an arbitrary vector |ϕ> ∈ $\mathscr{H}$:

$$\boxed{|\mathcal{P}_1\varphi\rangle = |\varphi_1\rangle}$$

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

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

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

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

Proof: $\mathcal{P}_1^\dagger = \mathcal{P}_1$ ⇒ the vectors $P_1|\phi>$ 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 notaion 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: $\{|1\rangle, \ldots, |M\rangle\},\ M \leq N$ 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 |ϕ> and a complex number *a* such that:

$$\boxed{A|\varphi\rangle = a|\varphi\rangle}$$

⇒ |ϕ> is an eigenvector, and *a* an eigenvalue of the operator A. The eigenvalues are solutions of the equation:

$$\boxed{\det(A - aI) = 0}$$

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

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

$$= \langle A\varphi|\varphi\rangle = \langle a\varphi|\varphi\rangle = a^*||\varphi||^2 \Rightarrow \boxed{a = a^*}$$

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

$$\Rightarrow \langle\chi|\varphi\rangle = 0 \text{ if } a \neq b$$

The eigenvectors of a Hermitian operator normalized to unity form an orthonormal basis of $\mathscr{H}$ 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

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

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

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

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

Let the vector $|\phi\rangle \in \mathcal{H} \Rightarrow$

$$A|\varphi\rangle = \sum_n A\mathcal{P}_n|\varphi\rangle = \sum_n a_n\mathcal{P}_n|\varphi\rangle$$

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

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 $A_1,\ldots A_M$ 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* an *of a unitary operator have modulus unity*: $a_n = \exp(i\alpha_n)$, *α_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 P_n as*

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

Let $A = \sum_n a_n \mathcal{P}_n$ be a Hermitian operator ⇒ $U = \sum_n e^{i\alpha a_n} \mathcal{P}_n = e^{i\alpha A}$ 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 $|z|<R$:

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

$\Rightarrow$ operator-valued function: $f(A) = \sum_{p=0}^{\infty} c_p A^p = \sum_{p=0}^{\infty} c_p X D^p X^{-1} = X \left[\sum_{p=0}^{\infty} c_p D^p \right] X^{-1}$

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: $A = \sum_n a_n \mathcal{P}_n$

$\Rightarrow$ 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* $|\phi\rangle$ → an element of a complex Hilbert space $\mathscr{H}$ (*space of states*).

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

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

$$|\psi\rangle = \frac{\lambda|\varphi\rangle + \mu|\chi\rangle}{||\lambda|\varphi\rangle + \mu|\chi\rangle||}$$

$\in \mathscr{H}$ is a state vector (λ, μ are complex numbers).

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

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

⇒ the probability:

$$\mathrm{p}(\varphi \to \chi) = |a(\varphi \to \chi)|^2 = |\langle \chi | \varphi \rangle|^2$$

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 $\mathcal{A} \to$ 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 $|\phi\rangle$

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

result of the p-th measurement

number of measurements

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

$$\langle A\rangle_\varphi = \sum_n \mathsf{p}_n a_n = \sum_n \langle\varphi|n\rangle a_n \langle n|\varphi\rangle = \langle\varphi|A|\varphi\rangle$$

→ general case with degenerate eigenvalues:

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

→ the probability of observing the eigenvalue a_n:

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

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

→ 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 $|\phi\rangle$:

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

$$\boxed{\langle A\rangle_\varphi = \langle\varphi|A|\varphi\rangle}$$

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.

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

$\{|\varphi\rangle, |\chi\rangle\}$ → 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:

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

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

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

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

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

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⊗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 $|\phi\otimes\chi\rangle$:

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

⇒ its matrix elemnts 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⊗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 $\mathcal{H}_1^N$ i $\mathcal{H}_2^M$)

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

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

$|\Psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ → 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 ⇒ a *pure state* (complete information about the system is available)

ii) when the information on the system is incomplete ⇒ a *mixture* (the system is described by a *density operator*)

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

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

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

$\{|n\rangle\}$ → an orthonormal basis of $\mathscr{H}$ ⇒ the expectation value of an observable:

$$\langle A\rangle = \langle\varphi|A|\varphi\rangle = \sum_{n,m}\langle\varphi|n\rangle\langle n|A|m\rangle\langle m|\varphi\rangle$$
$$= \sum_{n,m}\langle m|\varphi\rangle\langle\varphi|n\rangle\langle n|A|m\rangle$$
$$= \sum_{m}\langle m|\mathcal{P}_{\varphi}A|m\rangle = \mathrm{Tr}(\mathcal{P}_{\varphi}A).$$

<u>Mixture of quantum states:</u>

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

DEF. Density operator (state operator)

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

⇒

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

Properties: → ρ is Hermitian $\rho=\rho^\dagger$
→ Tr ρ = 1
→ ρ is a positive operator (Hermitian and has positive eigenvalues)

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

→ a necessary and sufficient condition for ρ to describe a pure state is $\rho^2 = \rho$.
→ spectral decomposition:

$$\rho = \sum_n \mathrm{p}_n |n\rangle\langle n|$$

The reduced density operator

A density operator ρ 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 ⇒ define a density operator $\rho^{(1)}$ acting in $\mathcal{H}_1$ such that:

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

$$\langle A\otimes I_2\rangle = \mathrm{Tr}([A\otimes I_2]\rho) = \sum_{n_1 m_1; n_2 m_2} A_{n_1 m_1}\delta_{n_2 m_2}\rho_{m_1 m_2; n_1 n_2} = \sum_{n_1 m_1} A_{n_1 m_1}\sum_{n_2}\rho_{m_1 n_2; n_1 n_2}$$

$$= \sum_{n_1 m_1} A_{n_1 m_1}\rho^{(1)}_{m_1 n_1} = \mathrm{Tr}(A\rho^{(1)}).$$

The *reduced* density operator:

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

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

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

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

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

→ 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 $<\mathbf{r}|\phi>$ for finding the particle in the state $|\phi>$ localized at position **r**. Normalization:

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

Diagonalization of *X* and *P* and wave functions

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

$$X\Big[\exp\Big(-\mathrm{i}\frac{Pa}{\hbar}\Big)|x\rangle\Big] = \exp\Big(-\mathrm{i}\frac{Pa}{\hbar}\Big)(X + aI)|x\rangle$$
$$= (x+a)\Big[\exp\Big(-\mathrm{i}\frac{Pa}{\hbar}\Big)|x\rangle\Big]$$

The vector $\exp(-\mathrm{i}Pa/\hbar)|x>$, with *a* real, is an eigenvector of *X* with eigenvalue $(x+a)$, and since *a* is arbitrary ⇒ all real values of *x* between $-\infty$ and $+\infty$ are eigenvalues of X.

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

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

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

→ 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: $\int_{-\infty}^{\infty} |x\rangle\, \mathrm{d}x\, \langle x| = I$

The projector *P*[a,b] onto the subspace of eigenvalues of *X* in the interval [a,b]:

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

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

|ϕ> → a normalized vector of $\mathscr{H}$ representing a physical state:

$$|\varphi\rangle = \int_{-\infty}^{\infty} |x\rangle \, \mathrm{d}x \, \langle x|\varphi\rangle$$

probability amplitude of finding the particle localized at point x

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

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

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

→ the scalar product: $\langle \chi|\varphi\rangle = \int_{-\infty}^{\infty} \mathrm{d}x \, \langle \chi|x\rangle \langle x|\varphi\rangle = \int_{-\infty}^{\infty} \mathrm{d}x \, \chi^*(x)\varphi(x)$

$$\int_{-\infty}^{\infty} \mathrm{d}x \, |\varphi(x)|^2 = 1$$

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

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

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

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

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

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

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

If |ϕ> is the state vector of a particle, the "wave function in the *p*-representation"will be:

$$\tilde{\varphi}(p) = \langle p|\varphi\rangle = \int_{-\infty}^{\infty} \langle p|x\rangle\, \mathrm{d}x\, \langle x|\varphi\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}px/\hbar}\, \varphi(x)$$

…just the Fourier transform of the wave function ϕ(x) = <x|ϕ> in the *x*-representation.

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

$$\varphi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \mathrm{d}p \, \mathrm{e}^{\mathrm{i}px/\hbar} \, \tilde{\varphi}(p)$$

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

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

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

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

⇒ the time-dependent Schrödinger equation:

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

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:

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