

3. QUANTUM COMPUTING

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Chapter 3: HILBERT SPACE BASICS

ABSTRACT

Hilbert space is a mathematical framework suitable for describing concepts, principles, processes and laws of the theory of quantum world called (for historical reasons) **quantum mechanics**, in general; and quantum information processing and communication (QIPC) in particular.

In this chapter those basics of Hilbert space theory are introduced and illustrated that play an important role in QIPC.

QUANTUM SYSTEM = HILBERT SPACE

Hilbert space H_n is n -dimensional complex vector space with

scalar product (dot product)

$$\langle \psi | \phi \rangle = \sum_{i=1}^n \phi_i \psi_i^* \quad \text{of vectors } |\phi\rangle = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_n \end{pmatrix}, |\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{pmatrix},$$

norm of vectors

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

and the **metric**

$$\text{dist}(\phi, \psi) = \|\phi - \psi\|.$$

This allows us to introduce on H a metric topology and such concepts as continuity.

All n -dimensional Hilbert spaces are isomorphic. Their vectors of norm 1 are called **pure quantum states**. Their physical counterparts are **n -level quantum systems**.

MORE ABOUT RELATIONS BETWEEN QUANTUM SYSTEMS AND HILBERT SPACES

Basic assumption With every quantum systems \mathcal{S} there is associated a Hilbert space $\mathcal{H}_{\mathcal{S}}$, whose dimension depends on the nature of the degree of freedom being considered for the system.

Example: If only spin orientation of electron (a spin-1/2 particle) is considered, then the corresponding Hilbert space is two dimensional Hilbert space \mathcal{H}_2 .

However, if the position of an electron is of concern, which can be in any point of some space, then the corresponding Hilbert space is usually taken to be continuous and therefore infinite dimensional.

BRA-KET NOTATION

Dirac introduced a very handy notation, so called bra-ket notation, to deal with amplitudes, quantum states and linear functionals $f : H \rightarrow \mathbb{C}$.

If $\psi, \phi \in H$, then

$\langle \psi | \phi \rangle$ — **scalar product** of ψ and ϕ
(an amplitude of going from ϕ to ψ).

$|\phi\rangle$ — **ket-vector** — an equivalent to ϕ

$\langle \psi |$ — **bra-vector** a linear functional on H (and a dual vector to $|\phi\rangle$)
such that $\langle \psi | (|\phi\rangle) = \langle \psi | \phi \rangle$

Example For states $\phi = (\phi_1, \dots, \phi_n)$ and $\psi = (\psi_1, \dots, \psi_n)$ we have

$$|\phi\rangle = \begin{pmatrix} \phi_1 \\ \dots \\ \phi_n \end{pmatrix}, \langle \phi | = (\phi_1^*, \dots, \phi_n^*); \langle \phi | \psi \rangle = \sum_{i=1}^n \phi_i^* \psi_i; |\phi\rangle \langle \psi | = \begin{pmatrix} \phi_1 \psi_1^* & \dots & \phi_1 \psi_n^* \\ \vdots & \ddots & \vdots \\ \phi_n \psi_1^* & \dots & \phi_n \psi_n^* \end{pmatrix}$$

GENERAL DEFINITION

Definition 0.1 *An inner-product space H is a complex vector space, equipped with an inner product $\langle \cdot | \cdot \rangle : H \times H \rightarrow \mathbb{C}$ satisfying the following axioms for any vectors $\phi, \psi, \phi_1, \phi_2 \in H$, and any $c_1, c_2 \in \mathbb{C}$.*

$$\begin{aligned}\langle \phi | \psi \rangle &= \langle \psi | \phi \rangle^*, \\ \langle \psi | \psi \rangle &\geq 0 \text{ and } \langle \psi | \psi \rangle = 0 \text{ if and only if } \psi = \mathbf{0}, \\ \langle \psi | c_1 \phi_1 + c_2 \phi_2 \rangle &= c_1 \langle \psi | \phi_1 \rangle + c_2 \langle \psi | \phi_2 \rangle.^1\end{aligned}$$

The inner product introduces on H the norm (length)

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

and the metric (Euclidean distance)

$$\text{dist}(\phi, \psi) = \|\phi - \psi\|.$$

This allows us to introduce on H a metric topology and such concepts as continuity.

Some basic properties of the norm:

- $\|\phi\| \geq 0$ for all $\phi \in H$ and $\|\phi\| = 0$ if and only if $\phi = \mathbf{0}$
- $\|\phi + \psi\| \leq \|\phi\| + \|\psi\|$ (**triangle inequality**);
- $\|a\phi\| = |a| \|\phi\|$; (e) $|\langle \phi, \psi \rangle| \leq \|\phi\| \|\psi\|$ (**Schwarz inequality**).

COMPLETENESS, ISOMORPHISM and DUAL SPACE

Definition 0.2 An inner-product space H is called **complete**, if for any sequence

$$\{\phi_i\}_{i=1}^{\infty},$$

with $\phi_i \in H$, and with the property that

$$\lim_{i,j \rightarrow \infty} \|\phi_i - \phi_j\| = 0,$$

there is a unique element $\phi \in H$ such that

$$\lim_{i \rightarrow \infty} \|\phi - \phi_i\| = 0.$$

A complete inner-product space is called a **Hilbert space**.

Two Hilbert spaces H_1 and H_2 are said to be **isomorphic**, notation $H_1 \simeq H_2$, if the underlying vector spaces are isomorphic and their isomorphism preserves the inner product.

BASIC EXAMPLES of HILBERT SPACES

Let us start with the two most important examples of Hilbert spaces.

Example 0.3 *Hilbert spaces $l_2(D)$* For any countable set D , let $l_2(D)$ be the space of all complex valued functions on D bounded by the so-called l_2 -norm, i.e.

$$l_2(D) = \{x \mid x : D \rightarrow \mathbf{C}, \left(\sum_{i \in D} x(i)x^*(i) \right)^{1/2} < \infty\}^2.$$

We say that $l_2(D)$ is a Hilbert space with respect to the inner product $\langle \cdot | \cdot \rangle : l_2(D) \times l_2(D) \rightarrow \mathbf{C}$, defined by

$$\langle x_1 | x_2 \rangle = \sum_{i \in D} x_1^*(i)x_2(i).$$

Elements of $l_2(D)$ are usually called vectors (to be indexed by elements of D). The notation $l_2 = l_2(\mathbf{N})$ is usually used in the case $D = \mathbf{N}$.

² x^* denotes the conjugate of the com x ; i.e., $x^* = a - bi$ if $x = a + bi$, where a, b are real.

Example 0.4 Hilbert space L_2 ³ Let (a, b) be an interval, with finite or infinite bounds, on the real axis. By $L_2((a, b))$, or simply L_2 , we denote the set of all complex valued functions such that $\int_a^b |f(x)|^2 dx$ exists, equipped with the inner product

$$\langle f|g \rangle = \int_a^b f^*(t)g(t) dt < \infty.$$

If f and g are such that $|f|^2$ and $|g|^2$ are integrable functions (with respect to Lebesgue measure) on (a, b) , then so are functions cf and $f + g$, for any complex number c , and therefore L_2 is a linear space.⁴

Surprisingly, for two Hilbert spaces introduced in the last examples it holds

$$l_2 \simeq L_2$$

that is they are isomorphic (so-called Riesz-Fischer Theorem.)

The Hilbert space corresponding to a simple harmonic oscillator is L_2 of all complex valued functions, each of which is square integrable over the entire real line.

³Hilbert studied spaces l_2 and L_2 , in his work on linear integral systems, and that is why von Neumann all spaces of such types named as Hilbert spaces.

⁴To be more precise L_2 is to be the set of Lebesgue integrable functions on (a, b) and we do not consider as different a pair of functions that differ only on a set of measure zero. In such a linear space the zero element is a function that is equal to zero almost everywhere on (a, b) .

DUAL HILBERT SPACE

The set of dual vectors of a Hilbert space \mathcal{H} forms so called **Dual Hilbert space** \mathcal{H}^* . A dual vector $\langle \phi |$ to a vector $|\phi\rangle$ is often denoted as $|\phi\rangle^\dagger$.

If $\{|\beta_i\rangle\}_{i=1}^n$ forms an orthogonal basis of a Hilbert space \mathcal{H} , then $\{\langle\beta_i|\}_{i=1}^n$ forms an orthogonal basis of \mathcal{H}^* .

If \mathcal{H} is a Hilbert space, then the set of linear operators on \mathcal{H} forms again a Hilbert space, denoted usually $\mathcal{L}(\mathcal{H})$ and all inner products of an orthogonal basis of \mathcal{H} forms an orthogonal basis of $\mathcal{L}(\mathcal{H})$. As a consequence if $\{|\beta_i\rangle\}_{i=1}^n$ form an orthogonal basis on \mathcal{H} , then every linear operator O on \mathcal{H} can be expressed in the form

$$O = \sum_n \sum_m t_{n,m} |\beta_n\rangle \langle \beta_m|$$

for some constants $t_{n,m} = \langle \beta_n | O | \beta_m \rangle$

ORTHOGONALITY of STATES

Two vectors $|\phi\rangle$ and $|\psi\rangle$ are called **orthogonal vectors** if $\langle\phi|\psi\rangle = 0$.

Physically are fully distinguishable only orthogonal vectors (states).

By a basis \mathcal{B} of H_n we will understand any set of n vectors $|b_1\rangle, |b_2\rangle, \dots, |b_n\rangle$ in \mathcal{H}_n of the norm 1 which are mutually orthogonal.

Given a basis \mathcal{B} , any vector $|\psi\rangle$ from H_n can be uniquely expressed in the form

$$|\psi\rangle = \sum_{i=1}^n \alpha_i |b_i\rangle.$$

A set S of vectors is called orthonormal if all vectors of S have norm 1 and are mutually orthogonal.

Definition A subspace G of a Hilbert space H is a subset of H closed under addition and scalar multiplication.

An important property of Hilbert spaces is their decomposability into mutually orthogonal subspaces. It holds:

Theorem For each closed subspace W of a Hilbert space H there exists a unique subspace W^\perp such that $\langle \phi | \psi \rangle = 0$, whenever $\phi \in W$ and $\psi \in W^\perp$

and

each $\psi \in H$ can be uniquely expressed in the form $\psi = \phi_1 + \phi_2$, with $\phi_1 \in W$ and $\phi_2 \in W^\perp$. In such a case we write $H = W \oplus W^\perp$ and we say that W and W^\perp form an orthogonal decomposition of H .

In a natural way we can make a generalization of an orthogonal decomposition

$$H = W_1 \oplus W_2 \oplus \dots \oplus W_n,$$

of H into mutually orthogonal subspaces W_1, \dots, W_n such that each $\psi \in H$ has a unique representation as $\psi = \phi_1 + \phi_2 + \dots + \phi_n$, with $\phi_i \in W_i, 1 \leq i \leq n$.

OPERATORS of HILBERT SPACES

A linear operator on a Hilbert space H is a linear mapping

$$A : H \rightarrow H.$$

An application of a linear operator A to a vector $|\psi\rangle$ is denoted $A|\psi\rangle$.

A is also a linear operator of the dual Hilbert space H^* , mapping each linear functional $\langle\phi|$ of the dual space to the linear functional, denoted by $\langle\phi|A$.

A linear operator A is called **positive** or **semi-definite**, notation $A \geq 0$, if $\langle\psi|A\psi\rangle \geq 0$ for every $|\psi\rangle \in H$.

The **norm** $\|A\|$ of a linear operator A is defined as

$$\|A\| = \sup_{\|\phi\|=1} \|A|\phi\rangle\|.$$

A linear operator is called bounded if its norm is finite.

Projections have a special role among linear operators.

If $H = W_1 \oplus W_2$ is an orthogonal decomposition of a Hilbert space H into subspaces W_1 and W_2 , then, as mentioned above, each $\psi \in H$ has a unique representation $\psi = \psi_1 + \psi_2$, where $\psi_1 \in W_1$ and $\psi_2 \in W_2$.

$$P_{W_1}(\psi) = \psi_1 \quad \text{and} \quad P_{W_2}(\psi) = \psi_2$$

are called **projections** onto the subspaces W_1 and W_2 , respectively.

Example If $\phi \in H$ for $\|\phi\| = 1$ and a Hilbert space H , then the operator defined by $|\phi\rangle\langle\phi|$ and defined by

$$|\phi\rangle\langle\phi|(|\psi\rangle) = \langle\phi|\psi\rangle|\phi\rangle$$

is a projection into the one-dimensional subspace spanned by the vector $|\phi\rangle$.

REPRESENTATIONS

If $\beta = \{\theta_i\}_{i=1}^n$ is an orthonormal basis of a Hilbert space \mathcal{H} , then any state $|\phi\rangle$ has a unique representation

$$|\phi\rangle = \sum_{i=1}^n \langle\theta_i|\phi\rangle|\theta_i\rangle.$$

Each linear operator A of a countable Hilbert space H with a basis $\mathcal{B} = \{|\theta_i\rangle | i \in I\}$ can be represented by a matrix, in general infinitely dimensional, whose rows and columns are labeled by elements of I and with $\langle\theta_i|A|\theta_j\rangle = \langle\theta_i|A\theta_j\rangle$ in the i -th row and j -th column. Such a matrix is said to be **matrix representation of A relative to the basis β** .

Each operator A has also so-called **outer-product representation**:

$$A = \sum_{ij} \langle\theta_i|A|\theta_j\rangle |\theta_i\rangle\langle\theta_j|.$$

(here we use for $\langle\theta_i|A\theta_j\rangle$ Dirac's notation $\langle\theta_i|A|\theta_j\rangle$).

TRACE of OPERATORS

Definition 0.5 Let \mathcal{H} be an n -dimensional Hilbert space and \mathcal{B} be an orthogonal basis on \mathcal{H} . The trace (operator) of a linear mapping $M : \mathcal{H} \rightarrow \mathcal{H}$ is defined by

$$\text{Tr}(M) = \sum_{\phi \in \mathcal{B}} \langle \phi | M | \phi \rangle.$$

In addition, if A is the matrix representation of M in the basis \mathcal{B} . Then

$$\text{Tr}(M) = \text{Tr}(A) = \sum_{i=1}^n a_{ii},$$

where a_{ii} is the element of the matrix A at the position (i, i) .

Properties of the trace operator:

- Trace of a linear mapping does not depend on the basis chosen.
- $\text{Tr}(A + B) = \text{Tr}(A) + \text{Tr}(B)$.
- $\text{Tr}(AB) = \text{Tr}(BA)$; $\text{Tr}(A \otimes B) = \text{Tr}(A) \text{Tr}(B)$.
- $\text{Tr}(\alpha A) = \alpha \text{Tr}(A)$.
- $\text{Tr}(|\psi\rangle\langle\phi|) = \langle\phi|\psi\rangle$.

SELF-ADJOINT OPERATORS

Of special importance are **adjoint** and **self-adjoint** operators.

The adjoint operator T^* to a bounded linear operator T is an operator such that for any ϕ and $\psi \in H$,

$$\langle \psi | T \phi \rangle = \langle T^* \psi | \phi \rangle.$$

An operator T is self-adjoint if $T = T^*$.

Instead of $\langle \psi | T \phi \rangle$ notation $\langle \psi | T | \phi \rangle$ is used. Hence

$$\langle T^* \psi | \phi \rangle = \langle \psi | T | \phi \rangle = \langle \psi | T \phi \rangle.$$

SELF-ADJOINT OPERATORS — HERMITIAN MATRICES

To self-adjoint operators correspond Hermitian matrices, i.e., matrices A such that $A = A^*$.

Theorem 0.6 *Hermitian matrices have the following properties.*

1. *All eigenvalues of a Hermitian matrix are real.*
2. *The eigenvectors of an Hermitian matrix corresponding to distinct eigenvalues are orthogonal.*

Proof of property 1: If $A\phi = \lambda\phi$, then

$$\lambda^* \langle \phi | \phi \rangle = \langle \lambda \phi | \phi \rangle = \langle A\phi | \phi \rangle = \langle \phi | A\phi \rangle = \lambda \langle \phi | \phi \rangle.$$

hence $\lambda^* = \lambda$.

Proof of property 2 Assume that $\lambda \neq \lambda'$, $A\phi = \lambda\phi$, $A\phi' = \lambda'\phi'$. Since λ, λ' are real, it holds

$$\lambda' \langle \phi' | \phi \rangle = \langle A\phi' | \phi \rangle = \langle \phi' | A\phi \rangle = \lambda \langle \phi' | \phi \rangle$$

and therefore $\langle \phi' | \phi \rangle = 0$.

SPECTRAL REPRESENTATION of SELF-ADJOINT OPERATORS

A self-adjoint operator A of a finite dimensional Hilbert space H has the so-called **spectral representation**. If $\lambda_1, \dots, \lambda_k$ are its distinct eigenvalues, then A can be expressed in the form

$$A = \sum_{j=1}^k \lambda_j P_j,$$

where P_j is the projection operator into the subspace of H spanned by the eigenvectors corresponding to λ_j .

In a special case when all eigenvalues are distinct and $|\phi_i\rangle$ is the eigenstate/eigenvector corresponding to the eigenvalue λ_i , then

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

Since $P_i P_j = 0$ for two different projections, it holds for any polynomial p

$$p(A) = \sum_{i=1}^k p(\lambda_i) P_i.$$

This is generalized to define for any function $f : \mathbf{R} \rightarrow \mathbf{C}$ by

$$f(A) = \sum_{i=1}^k f(\lambda_i) P_i.$$

Example Pauli matrix σ_x has eigenvalues 1 and -1 and corresponding eigenvectors are $|0'\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ and $|1'\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$. Since

$$|0'\rangle\langle 0'| = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \quad |1'\rangle\langle 1'| = \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

and therefore

$$\begin{aligned} \sigma_x &= 1 \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} - 1 \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix} \\ \sqrt{\sigma_x} &= \sqrt{1} \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} + \sqrt{-1} \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix} \end{aligned}$$

that is

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

SPECTRAL REPRESENTATION of UNITARY OPERATORS

Each self-adjoint operator A has spectral decomposition $A = \sum_{j=1}^n \lambda_j |\phi_j\rangle\langle\phi_j|$ and therefore

$$e^{iA} = \sum_{j=1}^n e^{i\lambda_j} |\phi_j\rangle\langle\phi_j|$$

and therefore

$$(e^{iA})^* = \sum_{j=1}^n e^{-i\lambda_j} |\phi_j\rangle\langle\phi_j| = (e^{iA})^{-1}$$

what implies that the matrix e^{iA} is unitary.

We show now that each unitary matrix $U = e^{iH}$ for some self-adjoint operator H . Indeed, if U is decomposed into a “real and imaginary” part $U = A + iB$, then A and B are both self-adjoint and have spectral decompositions

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

$$B = \sum_{i=1}^n \mu_i |\phi_i\rangle\langle\phi_i|$$

All eigenvalues of a unitary matrix have absolute value 1 and self-adjoint matrices have eigenvalues real. Therefore, for each j an $\theta_j \in [0, 2\pi]$ has to exist such that $\lambda_j + i\mu_j = e^{i\theta_j}$. Hence for

$$H = \sum_{j=1}^n \theta_j |\phi_j\rangle\langle\phi_j|$$

we have

$$U = e^{iH}.$$

Example 1 Hadamard transform $H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ has as eigenvalues 1 and -1 and the corresponding eigenvectors are

$$\phi_1 = \frac{1}{\sqrt{4 + 2\sqrt{2}}} \begin{pmatrix} 1 + \sqrt{2} \\ 1 \end{pmatrix} \quad \phi_{-1} = \frac{1}{\sqrt{4 - 2\sqrt{2}}} \begin{pmatrix} 1 - \sqrt{2} \\ 1 \end{pmatrix}$$

The spectral decomposition of H is then

$$H = 1 \cdot |\phi_1\rangle\langle\phi_1| + (-1)|\phi_{-1}\rangle\langle\phi_{-1}|$$

and therefore $H = e^{iA}$, where

$$A = 0 \cdot |\phi_1\rangle\langle\phi_1| + \pi|\phi_{-1}\rangle\langle\phi_{-1}|$$

Example 2 It holds

$$R_\theta = \begin{pmatrix} \cos \theta & \sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} = e^{iA_\theta} \quad \text{where } A_\theta = \begin{pmatrix} 0 & i\theta \\ -i\theta & 0 \end{pmatrix}.$$

QUANTUM TIME EVOLUTION

It is natural to assume that for a Hilbert space \mathcal{H}_n there is a mapping $U_t : \mathcal{H}_n \rightarrow \mathcal{H}_n$ that depends on time t that maps the initial state $|\phi_0\rangle$ into the state $|\phi_t\rangle$ in time t , that is that

$$|\phi_t\rangle = U_t|\phi_0\rangle.$$

It is also natural to put the following four requirements on U_t :

1. U_t should map states into states, that is it should preserve norm:

$$\text{For each real } t > 0 \text{ and each state } |\phi\rangle, \|U_t|\phi\rangle\| = \|\phi\|.$$

2. U_t should be linear - what means that each basis state should develop independently. Namely: for each basis $\{\beta_i\}_{i=1}^n$,

$$U_t\left(\sum_{i=1}^n a_i|\beta_i\rangle\right) = \sum_{i=1}^n a_i U_t(|\beta_i\rangle)$$

.

3. U_t should be decomposable. Namely, for all $t_1 > 0, t_2 > 0$

$$U_{t_1+t_2} = U_{t_1}U_{t_2}.$$

4. Evolution should be smooth. Namely, for each real t_0

$$\lim_{t \rightarrow t_0} U_t |\phi_0\rangle = \lim_{t \rightarrow t_0} |\phi_t\rangle = |\phi_{t_0}\rangle.$$

Theorem If time evolution U_t satisfies the above four conditions, then U_t has to be unitary and $U_t = e^{-iHt}$ for some self-adjoint operator H . Hence

$$\frac{\partial \phi_t}{\partial t} = -iH e^{-itH} \phi_0 = -iH \phi_t$$

what is known as the abstract Schrödinger equation.

ANOTHER VIEW OF QUANTUM DYNAMICS

The time evolution of any state of a closed quantum system is unitary; i.e. the state $|\phi(t_1)\rangle$ of the system at time t_1 is related to the state $|\phi(t_2)\rangle$ of the system at a later time t_2 by a unitary operator U_{t_1,t_2} which depends on t_1 and t_2 :

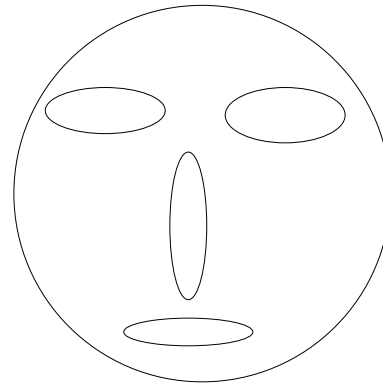
$$|\phi(t_2)\rangle = U_{t_1,t_2}|\phi(t_1)\rangle.$$

moreover such an evolution is linear, i.e.

$$U_{t_1,t_2} \sum_i \alpha_i |\phi_i\rangle = \sum_i \alpha_i U_{t_1,t_2} |\phi_i\rangle.$$

QUANTUM (PROJECTION) MEASUREMENT - OBSERVABLES

Informally, a quantum state $|\psi\rangle$ is observed (measured) with respect to an **observable** — a Hermitian matrix A which specifies a decomposition of the Hilbert space into orthogonal subspaces (such that each vector can be uniquely represented as a sum of vectors of these subspaces) that are subspaces generated by eigenvectors corresponding to different eigenvalues of the operator A .



There are two outcomes of a projection measurement of a state $|\phi\rangle$:

1. Information into which subspace projection of $|\phi\rangle$ took place.
2. Resulting projection (a new quantum state) $|\phi'\rangle$.

The subspace into which projection is made is chosen **randomly** and the corresponding probability is uniquely determined by the amplitudes at the representation of $|\phi\rangle$ at the basis states of the subspace.

Namely, if

$$A = \sum_{i=1}^k \lambda_i P_i$$

for a self-adjoint operator A , where P_i are projections into mutually orthogonal subspaces, then by measuring (observing) a state $|\phi\rangle$ with respect to A , this state collapses into the state

$$\frac{P_i|\phi\rangle}{\sqrt{\langle\phi|P_i|\phi\rangle}}$$

with probability

$$\langle\phi|P_i|\phi\rangle$$

and we also say that with the same probability the value λ_i is observed in the classical world.

PROJECTION MEASUREMENT - OTHER VIEW

For any decomposition of a unitary operator

$$I = \sum_i P_i$$

into orthogonal projectors P_i there exists a projective measurement that outputs, if a state $|\phi\rangle$ is measured, as the outcome an i with probability

$$\mathbf{Pr}(i) = \langle \phi | P_i | \phi \rangle$$

and leaves the system in the state

$$\frac{P_i |\phi\rangle}{\sqrt{\mathbf{Pr}(i)}}$$

EXAMPLE

Observable $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ has eigenvalues $\{1, -1\}$ and eigenvectors $\{|0'\rangle, |1'\rangle\}$.

A measurement with respect to the observable σ_x is therefore measurement with respect to the dual basis.

Observable $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ has eigenvalues $\{1, -1\}$ and eigenvectors $\{|0\rangle, |1\rangle\}$.

A measurement with respect to the observable σ_x is therefore measurement with respect to the standard (computational) basis.

PROBABILITIES

To the key outcomes of quantum mechanics belong rules for determining probabilities of the outcomes of quantum measurements.

The classical outcome of a measurement of a state $|\psi\rangle$ with respect to an observable A is one of the eigenvalues of A and quantum impact of such a measurement is a “collapse” of $|\psi\rangle$ into a state $|\psi'\rangle$. In the measurement the eigenvalue λ_i is obtained with probability

$$Pr(\lambda_i) = \|P_i|\psi\rangle\|^2 = \langle\psi|P_i|\psi\rangle,$$

and the new state $|\psi'\rangle$, into which $|\psi\rangle$ collapses, has the form

$$|\psi'\rangle = \frac{P_i|\psi\rangle}{\sqrt{\langle\psi|P_i|\psi\rangle}}.$$

ANOTHER VIEW of MEASUREMENT

Quantum measurement is described by a finite set $\{P_m\}$ of projectors acting on the state space of the system being measured and such that $\sum_m P_m = I$ - the index m refers to the potential classical outcomes of a measurement.

If a state $|\phi\rangle$ is measured with respect to $\{P_m\}$, then the result m occurs with probability

$$\Pr(m) = \langle \phi | P_m | \phi \rangle$$

and if such a result occurs the state of the system immediately after measurement is

$$\frac{P_m |\phi\rangle}{\sqrt{\langle \phi | P_m | \phi \rangle}} = \frac{P_m |\phi\rangle}{\sqrt{\Pr(m)}}.$$

If α is a real number, we say that states $|\phi\rangle$ and $e^{i\alpha}|\phi\rangle$ are equivalent, or equal up to a phase factor. Two such states give the same measurement statistics, what follows from the relations

$$\langle e^{i\alpha} \phi | P_m | e^{i\alpha} \phi \rangle = e^{-i\alpha} e^{i\alpha} \langle \phi | P_m | \phi \rangle = \langle \phi | P_m | \phi \rangle.$$

IMPORTANT OBSERVATION

Quantum mechanics is a probabilistic mathematical theory for describing the physical world.

However, probability involved is not probability of some dynamic variables having a particular value in some state.

Rather, it represents the probability of finding a particular value of a dynamical variable if that dynamical variable is measured.

Quantum mechanics says nothing about values of dynamical variables when the system is not subjected to any measurement.

EXPECTATION VALUE

Let A be self-adjoint operator of a Hilbert space H , with spectral decomposition

$$A = \sum_{i=1}^k \lambda_i P_{\lambda_i}.$$

The expectation value of A in the state ψ is defined by

$$\begin{aligned} \exp_{\psi}(A) &= \sum_{i=1}^k \lambda_i \text{prob}_{\psi}(\lambda_i) \\ &= \sum_{i=1}^k \lambda_i \langle P_{\lambda_i} \psi | P_{\lambda_i} \psi \rangle \\ &= \sum_{i=1}^k \lambda_i \langle \psi | P_{\lambda_i} \psi \rangle \\ &= \langle \psi | \sum_{i=1}^k \lambda_i P_{\lambda_i} | \psi \rangle \\ &= \langle \psi | A \psi \rangle \\ &= \langle \psi | A P_{\psi} \psi \rangle = \text{Tr}(A P_{\psi}) = \text{Tr}(P_{\psi} A). \end{aligned}$$

MIXED STATES — DENSITY MATRICES

Pure states are fundamental objects for quantum mechanics in the sense that the evolution of any closed quantum system can be seen as a unitary evolution of pure states.

However, to deal with unisolated and composed quantum systems the concept of mixed states is of importance.

A probability distribution $\{(p_i, \phi_i) \mid 1 \leq i \leq k\}$ on pure states $\{\phi_i\}_{i=1}^k$, with probabilities $0 < p_i \leq 1$, $\sum_{i=1}^k p_i = 1$ is called a **mixed state** or **mixture**, and denoted by $[\psi] = \{(p_i, \phi_i) \mid 1 \leq i \leq k\}$. For example, a mixed state is created if a source produces pure state $|\phi_i\rangle$ with probability p_i and $\sum_{i=1}^k p_i = 1$.

To each mixed state $[\psi] = \{(p_i, \phi_i) \mid 1 \leq i \leq k\}$ corresponds a **density operator**

$$\rho_{[\psi]} = \sum_{i=1}^k p_i |\phi_i\rangle\langle\phi_i|.$$

Key observation Two mixed states with the same density matrix are physically undistinguishable.

EXAMPLES

The density matrix corresponding to the mixed state

$$\left(\frac{1}{2}, |0\rangle\right) \oplus \left(\frac{1}{2}, |1\rangle\right)$$

has the form

$$\frac{1}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} (0, 1) + \frac{1}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix} (0, 1) = \frac{1}{2} I.$$

For any pure one qubit state $\alpha|0\rangle + \beta|1\rangle$, to the mixed state

$$\left(\frac{1}{4}, \alpha|0\rangle + \beta|1\rangle\right) \oplus \left(\frac{1}{4}, \alpha|0\rangle - \beta|1\rangle\right) \oplus \left(\frac{1}{4}, \beta|0\rangle + \alpha|1\rangle\right) \oplus \left(\frac{1}{4}, \beta|0\rangle - \alpha|1\rangle\right)$$

corresponds the density matrix

$$\begin{aligned} & \frac{1}{4} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} (\alpha^*, \beta^*) + \frac{1}{4} \begin{pmatrix} \alpha \\ -\beta \end{pmatrix} (\alpha^*, -\beta^*) \\ & + \frac{1}{4} \begin{pmatrix} \beta \\ \alpha \end{pmatrix} (\beta^*, \alpha^*) + \frac{1}{4} \begin{pmatrix} \beta \\ -\alpha \end{pmatrix} (\beta^*, -\alpha^*) = \frac{1}{2} I \end{aligned}$$

REPRESENTATION of MIXED STATES

If ρ is a density matrix and in a basis $\{\beta_i\}_{i=1}^n$

$$\rho = \{\rho_{i,j}\}_{i,j=1}^n,$$

then

$$\rho = \sum_{i,j=1}^n \rho_{i,j} |\beta_i\rangle \langle \beta_j|.$$

As a consequence, for any k, l ,

$$\langle \beta_k | \rho | \beta_l \rangle = \rho_{k,l}.$$

PROPERTIES of DENSITY MATRICES

1. Any density matrix ρ is Hermitian, nonnegative, has only nonnegative eigenvalues and $\text{Tr}(\rho) = 1$.
2. If ρ_1, ρ_2 are density matrices on a Hilbert space \mathcal{H} , then $p\rho_1 + (1 - p)\rho_2$, $0 \leq p \leq 1$ is a density matrix on \mathcal{H} .
3. If ρ is a density matrix, then so is the matrix ρ^T .
4. If ρ_1 is a density matrix on a Hilbert space \mathcal{H}_1 and ρ_2 is a density matrix on a Hilbert space \mathcal{H}_2 , then $\rho_1 \otimes \rho_2$ is density matrix on the Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$.
5. A matrix ρ is a density matrix if it is Hermitian, nonnegative and $\text{Tr}\rho = 1$.
6. If $\rho^2 = \rho$ for a density matrix ρ , then ρ is a pure state, i.e. $\rho = |\phi\rangle\langle\phi|$ for a pure state $|\phi\rangle$.

DENSITY OPERATORS as STATES

We had a description of quantum (pure) states in terms of vectors of the norm one of a Hilbert space.

An alternative description is in terms of density operators which is very useful in describing states of subsystems of a composite quantum systems.

Quantum states are therefore often (mostly) associated with density operators (positive trace 1 operators).

BLOCH VECTORS REPRESENTATION of MIXED QUBIT STATES

For qubits, any density operator ρ (matrix) can be written uniquely in the form

$$\rho = \frac{1}{2}[I + a_x\sigma_x + a_y\sigma_y + a_z\sigma_z]$$

where a_i are real numbers such that for $i \in \{x, y, z\}$, $\sum_i |a_i|^2 \leq 1$ (because the set of matrices $\{I, \sigma_x, \sigma_y, \sigma_z\}$ form a basis) .

In short, ρ can be written as

$$\rho = \frac{1}{2}[I + a \cdot \sigma]$$

where a is a vector with components a_i and the notation $r \cdot \sigma$ means $\sum_i a_i \sigma_i$.

Therefore there is one-to-one correspondence between density operators for qubits and points of the Bloch/Poincare sphere.

Example Totally mixed state $\{(\frac{1}{2}, |0\rangle), (\frac{1}{2}, |1\rangle)\}$ that is identical with $\{(\frac{1}{2}, |0\rangle\langle 0|), (\frac{1}{2}, |1\rangle\langle 1|)\}$ corresponds to the centre of the Bloch sphere.

EVOLUTION of MIXED STATES and DENSITY MATRICES

If a unitary matrix U is applied to a mixed state

$$\{(p_1, |\phi_i\rangle), \dots, (p_k, \phi_k)\}$$

with the density matrix

$$\rho = \sum_{i=1}^k p_i |\phi_i\rangle \langle \phi_i|$$

then the resulting mixed state is

$$\{(p_1, |U\phi_i\rangle), \dots, (p_k, U\phi_k)\}$$

and the corresponding density matrix is

$$\sum_{i=1}^k p_i U |\phi_i\rangle \langle \phi_i| U^\dagger = U \left(\sum_{i=1}^k p_i |\phi_i\rangle \langle \phi_i| \right) U^\dagger = U \rho U^\dagger$$

TRACING OUT OPERATION

One of the profound differences between the quantum and classical systems lies in the relation between a system and its subsystems.

As discussed below a state of a Hilbert space $H = H_A \otimes H_B$ cannot be always decomposed into states of its subspaces H_A and H_B . We also cannot define any natural mapping from the space of linear operators on H into the space of linear operators on H_A (or H_B).

However, density operators are much more robust and that is also one reason for their importance. A density operator ρ on H can be “projected” into H_A by the operation of **tracing out** H_B , to give the density operator (for finite dimensional Hilbert spaces):

$$\rho_{H_A} = \text{Tr}_{H_B}(\rho) = \sum_{|\phi\rangle, |\phi'\rangle \in \mathcal{B}_{H_A}} |\phi\rangle \left(\sum_{|\psi\rangle \in \mathcal{B}_{H_B}} \langle \phi, \psi | \rho | \phi', \psi \rangle \right) \langle \phi'|,$$

where \mathcal{B}_{H_A} (\mathcal{B}_{H_B}) is an orthonormal basis of the Hilbert space H_A (H_B).

MEANING of TRACING OUT OPERATIONS

If $\dim(H_A) = n$, $\dim(H_B) = m$, then ρ is an $nm \times nm$ matrix which can be seen as an $n \times n$ matrix consisting of $m \times m$ blocks ρ_{ij} as follows:

$$\rho = \begin{pmatrix} \rho_{11} & \cdots & \rho_{1n} \\ \vdots & \ddots & \\ \rho_{n1} & \cdots & \rho_{nn} \end{pmatrix}$$

and in such a case

$$\rho_{H_A} = \begin{pmatrix} \mathbf{Tr}(\rho_{11}) & \cdots & \mathbf{Tr}(\rho_{1n}) \\ \vdots & \ddots & \vdots \\ \mathbf{Tr}(\rho_{n1}) & \cdots & \mathbf{tr}(\rho_{nn}) \end{pmatrix}$$

WHY SUCH a TRACING OUT OPERATION?

The following fact is the main mathematical justification that strangely looking tracing out operation has the proper physical meaning:

If $H = \mathcal{H}_A \otimes \mathcal{H}_B$ and ρ is a density matrix of H , then $\rho_A = \text{Tr}_B(\rho)$ is the unique density matrix of \mathcal{H}_A such that

$$\text{Tr}(\rho_A \cdot O) = \text{Tr}(\rho \cdot (O \otimes I))$$

for each observable (Hermitian matrix) O of \mathcal{H}_A .

In other words the average value of the measurement of ρ_A on \mathcal{H}_A with respect to the observable O , on \mathcal{H}_A , equals the average value of the measurement of ρ on \mathcal{H} with respect to the observable $O \otimes I$ on \mathcal{H} .

Informally, one often says that in order to get the density matrix of a subsystem, given the density matrix of the whole system, one should trace over the degrees of freedom of the rest of the system.

TRACING OUT OPERATION

Perhaps the simplest way to introduce tracing out operation is to say that it is a linear operation such that for any bipartite system $A \otimes B$ and any states $|\phi_1\rangle$ and $|\phi_2\rangle$ of A and any states $|\psi_1\rangle$ and $|\psi_2\rangle$ of B

$$\mathbf{Tr}_B(|\phi_1\rangle\langle\phi_2| \otimes |\psi_1\rangle\langle\psi_2|) = |\phi_1\rangle\langle\phi_2| \mathbf{Tr}(|\psi_1\rangle\langle\psi_2|) = \langle\psi_2|\psi_1\rangle |\phi_1\rangle\langle\phi_2|.$$

EXAMPLES

Example 1. For

$$\rho = \frac{1}{2}(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|)$$

it holds

$$\mathbf{Tr}(\rho) = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$$

MEASUREMENT of PURE STATES

Let us assume that we are measuring (with respect to) the observable X with spectral decomposition

$$X = \sum_j \lambda_j |j\rangle\langle j|.$$

From the hermiticity of X it follows that the eigenvalues λ_j are real. For simplicity we assume that eigenvalues are nondegenerate (all different) and the corresponding eigenvectors, $\{|j\rangle\}_j$, form an orthonormal basis. Then:

1. The projectors $P_j = |j\rangle\langle j|$ span the entire Hilbert space, $\sum_j P_j = 1$.
2. From the orthogonality of the basis states we have $P_i P_j = \delta_{ij} P_i$. in particular, $P_i^2 = P_i$, what implies that eigenvalues of any projector are -1 and 1 .
3. Each measurement of a state $|\phi\rangle$ with respect to X yields, on a classical level, one of the eigenvalues λ_j .

4. (Collapse postulate) The quantum state of the system immediately, after the measurement of $|\phi\rangle$ with respect to X , is

$$|\phi_j\rangle = \frac{P_j|\phi\rangle}{\sqrt{\langle\phi|P_j|\phi\rangle}}$$

if the classical outcome is λ_j .

5. (Born's rule) The probability that this particular outcome is found as the measurement result is

$$p_j = \|P_j|\phi\rangle\|^2 = \langle\phi|P_j^2|\phi\rangle = \langle\phi|P_j|\phi\rangle,$$

where we used the property 2.

6. If we perform the measurement as above, but we do not record the result, then the postmeasurement state can be described by the density operator

$$\rho = \sum_j p_j |\phi_j\rangle\langle\phi_j| = \sum_j P_j|\phi\rangle\langle\phi|P_j.$$

The above six rules (postulates) describe what happens to the system during the measurement if it was initially in a pure state.

MEASUREMENT of MIXED STATES

If the quantum system is initially in a mixed state ρ , then the last three postulates are to be replaced by their immediate generalisations:

1. The projectors $P_j = |j\rangle\langle j|$ span the entire Hilbert space, that is $\sum_j P_j = 1$.
2. From the orthogonality of the basis states we have $P_i P_j = \delta_{ij} P_i$. in particular, $P_i^2 = P_i$, what implies that eigenvalues of any projector are -1 and 1 .
3. Each measurement of a state $|\phi\rangle$ with respect to X yields, on the classical level, one of the eigenvalues λ_j .

4. The quantum state of the system after the measurement is

$$\rho_j = \frac{P_j \rho P_j}{\text{Tr}(P_j \rho P_j)} = \frac{P_j \rho P_j}{\text{Tr}(P_j \rho)}$$

if the classical outcome is λ_j .

5. The probability that this particular outcome is found as the measurement result is

$$p_j = \text{Tr}(P_j \rho P_j) = \text{Tr}(P_j^2 \rho) = \text{Tr}(P_j \rho)$$

where, again, we used the property 2.

6. If measurement is performed, but result is not recorded, then the postmeasurement state can be described by the density operator

$$\rho_0 = \sum_j \lambda_j P_j \rho P_j.$$

SUPEROPERATORS

- A **superoperator (SO)** is a linear mapping/map on linear operators of a Hilbert space.
- A **positive superoperator (PSO)** is a superoperator that maps density matrices into density matrices.
- A **completely positive superoperator/map (CPO)** G is a PSO such that, for all positive integer m , $G \otimes I_m$ is also a PSO, where I_m is the identity matrix.

CPO are exactly (all) physically allowed transformations on density matrices.

Examples: encoders, decoders, **quantum channels**, quantum measurements.

CPO — INFORMAL VIEW

Informally, the best way is to see a CPO S applied to a state $|\phi\rangle$ of a Hilbert space H as follows:

Take at first an auxiliary state (called usually ancilla) of another Hilbert space H' , then apply a unitary operator U to the state $|\phi\rangle \otimes |\psi\rangle$ and, finally, discard (trace out) the H' -part of the resulting state.

WHAT ARE QUANTUM OPERATIONS?

The main question we deal with in this section is very fundamental. What are physically realizable operations one can perform (at least theoretically) on (mixed) states (to get again (mixed) states)?

In closed quantum systems unitary operations are actually the only quantum operations that are available. Measurements are actually outside of the closed quantum system framework, an interface from the quantum to classical world, but surely they are operations we should consider as physically realizable.

Of the main importance are quantum operations in open quantum systems. Actually, all actions that are performed in/on quantum systems are quantum operations: unitary operations , measurements, channel transmissions, flow of time, noise impacts,

The concept of quantum operations is therefore very general and very fundamental.

It is perhaps a bit surprising, but actually nice, useful and natural, that we can actually study and consider open quantum systems in the framework of closed quantum systems. We can consider as the basic setting that our (principal) quantum system and its environment form a closed quantum system in which we operate.

The requirement to consider only physically realizable (at least theoretically) operation is, of course, logical. As we shall see this question has, in a sense and at least theoretically, clear and simple answer. They are, as discussed later, *trace preserving completely positive linear maps*.

THREE APPROACHES

There are basically three main approaches to define what are “physically realizable quantum operations” (superoperators) \mathcal{E} .

A physically motivated **axiomatic approach** says that for a Hilbert space \mathcal{H} we should consider as physically realizable operations/maps $\mathcal{B}(\mathcal{H}) \rightarrow \mathcal{B}(\mathcal{H})$ which are *consistent with the (statistical) interpretation of quantum theory*.

That is physically realisable quantum operations are maps that are **linear** (to preserve superpositions), **positive** and **trace preserving** (to map density operators to density operators) and actually **completely positive** (to be sure that if a superoperator is applied to a subsystem, then the whole system is again in a quantum state).

A **pragmatic approach** says that superoperators are those operations that can be combined from unitary operations, adding ancillas, performing (non-selective) projective measurement and discarding subsystems (ancillas), by performing a tracing out operation.

A **mathematical approach** says that all basic quantum operations: adding and discarding quantum subsystems, unitary operations and non-selective projective measurements are those operations that have Kraus operator-sum representation

$$\rho \rightarrow \sum_{i=1}^k E_i \rho E_i^\dagger,$$

where so called *Kraus operators* $E_i : \mathcal{H} \rightarrow \mathcal{H}$ are not necessarily Hermitian operators, but they should be positive and should form a “decomposition of the identity operator”, that is it should hold:

$\sum_{i=1}^k E_i^\dagger E_i = I_{\mathcal{H}}$ – so called completeness condition.

It is a consequence of the completeness condition, and a property of trace operation, that for any superoperator \mathcal{E} holds

$$\mathbf{Tr}(\mathcal{E}(\rho)) = \mathbf{Tr}\left(\sum_i E_i \rho E_i^\dagger\right) = \mathbf{Tr}\left(\sum_i E_i^\dagger E_i \rho\right) = \mathbf{Tr}\left(\left(\sum_i E_i^\dagger E_i\right)\rho\right) = \mathbf{Tr}(\rho) = 1.$$

STINESPRING DILATION THEOREM

So called *Stinespring dilation theorem*, discussed below, says that each superoperator can be realized in “one big three-stage-step” : adding an ancilla, performing a unitary operation on a composed quantum system and, finally, discarding the ancilla, see Figure 1

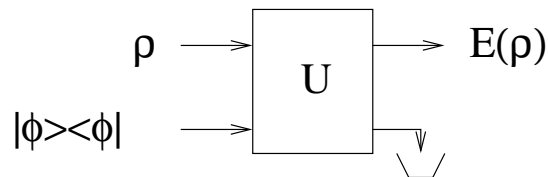


Figure 1: A Stinespring realization of a superoperator. In this view a superoperator \mathcal{E} performs the mapping $\mathcal{E}(\rho) = \text{Tr}_a(U(\rho \times \rho_a)U^\dagger)$, where ρ_a is the “initial state”, for example $|\phi\rangle\langle\phi|$ of an ancilla subsystem, U is a unitary operation on composed system and, finally, a tracing out operation is performed.

POVM (GENERALIZED QUANTUM MEASUREMENT)

Most general quantum observables (measurements) , so called POVM measurements, are given by a set $\{E_i\}_i$ of positive operators $0 \leq E_i \leq I$ such that $\sum_i E_i = I$.

A measurement of a state ρ with respect to such an observable provides i -th outcome with the probability

$$\text{Tr}[\rho E_i].$$

The idea of POVM occurs naturally when we consider projective measurements on composite systems. Indeed, the projective measurement on the tensor product Hilbert space of subsystems A and B may not remain projective on the Hilbert space associated with A and may result in a POVM on it.

By Neumark's theorem a POVM measurement on a Hilbert space can always be realized as projective measurement in a larger Hilbert space.

APPENDIX

SCHMIDT DECOMPOSITION THEOREM

If $|\psi\rangle$ is a state in a bipartite Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$, and $\{|\alpha_i\rangle\}_{i=1}^n$ is a basis of \mathcal{H}_A , $\{|\beta_j\rangle\}_{j=1}^m$ is a basis of \mathcal{H}_B , then

$$|\psi\rangle = \sum_{i=1}^n \sum_{j=1}^m p_{ij} |\alpha_i\rangle \otimes |\beta_j\rangle$$

for some amplitudes p_{ij} .

Schmidt decomposition theorem says that $|\psi\rangle$ can be expressed also through a one-sum superposition and not only through a two-sums superposition as above, what very often makes considerations and proofs much simpler.

Theorem If $|\psi\rangle$ is a vector of a bipartite Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$, then there exists an orthogonal basis $\{|\alpha_i\rangle\}$ of \mathcal{H}_A and an orthogonal basis $\{|\beta_j\rangle\}$ of \mathcal{H}_B and nonnegative integers $\{p_k\}$ such that

$$|\psi\rangle = \sum_k \sqrt{p_k} |\alpha_k\rangle \otimes |\beta_k\rangle.$$

The coefficients $\sqrt{p_k}$ are called **Schmidt coefficients** and $k = 1, \dots, \min\{n, m\}$.

PARTIAL TRACE and SCHMIDT DECOMPOSITION

If a state $|\psi\rangle$ of a bipartite Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ has the Schmidt decomposition

$$|\psi\rangle = \sum_k \sqrt{p_k} |\alpha_k\rangle \otimes |\beta_k\rangle.$$

where $\{|\alpha_i\rangle\}$ and $\{|\beta_j\rangle\}$ of \mathcal{H}_A and \mathcal{H}_B are orthogonal bases of \mathcal{H}_A and \mathcal{H}_B , then to trace out any of the subsystems is easy. Indeed

$$\text{Tr}_{\mathcal{H}_B}(|\psi\rangle\langle\psi|) = \sum_k p_k |\alpha_k\rangle\langle\alpha_k|$$

and

$$\text{Tr}_{\mathcal{H}_A}(|\psi\rangle\langle\psi|) = \sum_k p_k |\beta_k\rangle\langle\beta_k|$$

PARTIAL TRACE - A USEFUL FACT

The following fact concerning tracing out operation are often useful:

- If $\mathcal{H}_A \otimes \mathcal{H}_B$ is a bipartite system and ρ a state on it, then an application of a unitary operation U on A commute with operation of tracing out system B . Namely

$$\text{Tr}_B((U \otimes I)\rho(U^\dagger \otimes I)) = U(\text{Tr}_B\rho)U^\dagger.$$

MATHEMATICAL versus PHYSICAL NOTATION

If $|\phi\rangle$ is a vector of a Hilbert space \mathcal{H}_1 and $|\psi\rangle$ of a Hilbert space \mathcal{H}_2 , then

$$|\phi\rangle \otimes |\psi\rangle = |\phi\rangle|\psi\rangle$$

is a vector of $\mathcal{H}_1 \otimes \mathcal{H}_2$.

If we want to be more precise about to which Hilbert space vectors belong we specify them explicitly through indices as follows, for example,

$$|\phi_1\rangle|\psi_2\rangle.$$

In such a case for dual vectors mathematicians usually write

$$(|\phi_1\rangle|\psi_2\rangle)^\dagger = \langle\phi_1|\langle\psi_2|.$$

However, physicists usually write

$$(|\phi_1\rangle|\psi_2\rangle)^\dagger = \langle\psi_2|\langle\phi_1|.$$

If this convention is used, then we have

$$(|\phi\rangle|\psi\rangle)^\dagger|\alpha\rangle|\beta\rangle = \langle\psi|\langle\phi||\alpha\rangle|\beta\rangle = \langle\phi|\alpha\rangle\langle\psi|\beta\rangle$$

Moreover it holds

$$(|\phi_1\rangle \otimes |\psi_2\rangle)(\langle\alpha_1| \otimes \langle\beta_2|) = |\alpha_1\rangle\langle\alpha_1| \otimes |\psi_2\rangle\langle\beta_2|.$$