QUANTUM COMPUTING II

Jozef Gruska

Faculty of Informatics
Brno
Czech Republik

October 1, 2002

2. HILBERT SPACE BASICS

ABSTRACT

Hilbert space is a mathematical framework suitable for describing concepts, principles, processes and laws of quantum mechnics 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 important role in QIPC.

QUANTUM SYSTEM
=
HILBERT SPACE

Hilbert space H_n is n-dimensional complex vector space with

scalar product

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

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.
For each ϕ of a Hilbert space H the mapping $f_\phi : H \rightarrow \mathbf{C}$ defined by

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

is a linear mapping on H in the sense that $f_\phi(c\psi) = cf_\phi(\psi)$ and $f_\phi(\psi_1 + \psi_2) = f_\phi(\psi_1) + f_\phi(\psi_2)$. One can even show that we get all linear mappings from H to $\mathbf{C}$ by this construction. Namely, it holds:

Theorem To each continuous linear mapping $f : H \rightarrow \mathbf{C}$ there exists a unique $\phi_f \in H$ such that $f(\psi) = \langle\phi_f|\psi\rangle$ for any $\psi \in H$.

BRA-KET NOTATION

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

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

GENERAL DEFINITION

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

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

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 $\phi \in H$;
- $||\phi|| = 0$ 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, ISIMORPHISM 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 $\lim_{i,j\to\infty} ||\phi_i - \phi_j|| = 0$, there is a unique element $\phi \in H$ such that $\lim_{i\to\infty} ||\phi - \phi_i|| = 0$. 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. (For example, surprisingly, $l_2 \simeq L_2$—Riesz-Fischer Theorem .)*

For each ϕ of a Hilbert space H the mapping $f_\phi : H \to \mathbf{C}$ defined by

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

is a linear mapping on H in the sense that $f_\phi(c\psi) = cf_\phi(\psi)$ and $f_\phi(\psi_1 + \psi_2) = f_\phi(\psi_1) + f_\phi(\psi_2)$. One can even show that we get all linear mappings from H to $\mathbf{C}$ by this construction. Namely, it holds:

Theorem 0.3 *To each continuous linear mapping $f : H \to \mathbf{C}$ there exists a unique $\phi_f \in H$ such that $f(\psi) = \langle\phi_f|\psi\rangle$ for any $\psi \in H$.*

The space of all linear mappings (called also **functionals**) of a Hilbert space H forms again a Hilbert space, the so-called **dual Hilbert space** (or **conjugate Hilbert space**) H^* with the inner product $\langle f|g\rangle = \langle\phi_f|\phi_g\rangle$, for $f, g \in H^*$.

BASIC EXAMPLES of HILBERT SPACES

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

Example 0.4 (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.*

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

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

Example 0.5 (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]

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

[3] Hilbert 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.

[4] To 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).

ORTHOGONALITY of STATES

Two vectors $|\phi\rangle$ and $|\psi\rangle$ are called **orthogonal** if $\langle\phi|\psi\rangle = 0$. Physically are fully distinguishable only orthogonal vectors (states).

A **basis** $\mathcal{B}$ of H_n is any set of n vectors $|b_1\rangle, |b_2\rangle, \ldots, |b_n\rangle$ of the norm 1 which are 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 nutually 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

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

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

QUBITS

A **qubit** is a quantum state in H_2

$$|\phi\rangle = \alpha|0\rangle + \beta|1\rangle$$

where $\alpha, \beta \in \mathbf{C}$ are such that $|\alpha|^2 + |\beta|^2 = 1$ and

$$\{|0\rangle, |1\rangle\} \quad \text{is a } \textbf{(standard) basis} \text{ of } \ H_2$$

EXAMPLE: Representation of qubits by

(a) electron in a Hydrogen atom

(b) a spin-$\frac{1}{2}$ particle

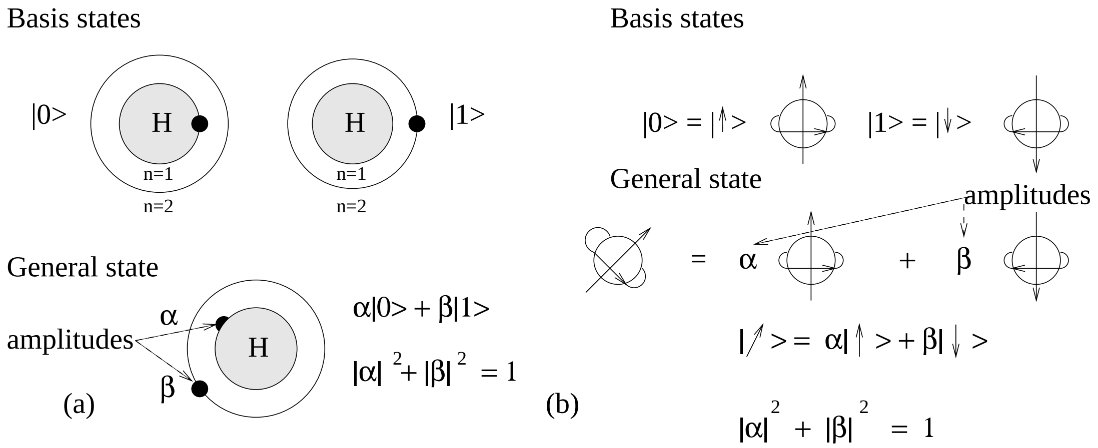

Figure 1: Qubit representations by energy levels of an electron in a hydrogen atom and by a spin-$\frac{1}{2}$ particle. The condition $|\alpha|^2 + |\beta|^2 = 1$ is a legal one if $|\alpha|^2$ and $|\beta|^2$ are to be the probabilities of being in one of two basis states (of electrons or photons).

X

OPERATORS of HILBERT SPACES

A linear operator on a Hilbert space H is a linear mapping $A : H \to H$.

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 $|\psi\rangle \in H$.

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.

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

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

A linear operator A is called **bounded** if its norm $||A||$ 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.

Self-adjoint operators

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 $|\phi\rangle$.

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

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

TRACE of OPERATORS

Definition 0.6 *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 $M : \mathcal{H} \to \mathcal{H}$ is defined by*

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

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

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

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.
- $Tr(A + B) = Tr(A) + Tr(B)$.
- $Tr(AB) = Tr(BA)$; $Tr(A \otimes B) = Tr(A)\,Tr(B)$.
- $Tr(\alpha A) = \alpha\, Tr(A)$.
- $Tr(|\psi\rangle\langle\phi|) = \langle\phi|\psi\rangle$.

SELF-ADJOINT OPERATOS — HERMITIAN MATRICES

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

Theorem 0.7 *Hermitian matrices have the following properties.*

1. *All eigenvalues of a Hermitian matrix are real.*
2. *The determinant of a Hermitian matrix equals the product of its eigenvalues.*
3. *The* **trace** *(the sum of diagonal elements) of a Hermitian matrix A, notation* Tr(A), *equals the sum of its eigenvalues .*

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

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

where P_i is the projection operator into the subspace of H spanned by the eigenvectors corresponding to λ_i.

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

$$\text{exp}_{\psi}(A) = \sum_{i=1}^{k} \lambda_i \text{prob}_{\psi}(\lambda_i).$$

it can be shown that

$$mboxExp_{\psi}(A) = \langle \psi | A \psi \rangle$$

$$\text{Exp}_{\psi}(A) = \text{Tr}(P_{\psi} A).$$

QUANTUM (PROJECTION) MEASUREMENTS

Informally, a quantum state $|\psi\rangle$ is observed (measured) with respect to an **observable** — a decomposition of a given Hilbert space into orthogonal subspaces (such that each vector can be uniquely represented as a sum of vectors of these subspaces) being eigenspaces represented to eigenvalues of a self-adjoint operator A.

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

1. Information into which subspace projection of $|\phi\rangle$ was made.
2. Resulting projection (a new 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.

PROBABILITIES

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

In quantum mechanics we used to consider the measurement of states mainly with respect to sharp observables. The numerical outcome of the measurement of a pure state $|\psi\rangle$ with respect to an observable A is one of the eigenvalues of A and the side 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

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

On a more general level let A be a self-adjoint operator, $|\psi\rangle$ a state, and Δ be an interval on the real line. To Δ corresponds a subspace L^A_Δ of those states $|\psi\rangle$ measurement of which with respect to A gives a value from Δ with certainty. Let P^A_Δ be the projection operator into the subspace L^A_Δ. In such a case the probability that mesasurement of a state $|\psi\rangle$ provides a value from Δ is

$$\langle\psi|P^A_\Delta\psi\rangle.$$

MEASUREMENT of PURE STATES

Projectors form

Let

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

be the spectral decomposition of an observable A, where $\{\lambda_i\}_{i=1}^{k}$ are eigenvalues of A, and P_i is the projection operator into the subspace L_i spanned by eigenvectors corresponding to the eigenvalue λ_i.

Measurement of a pure state $|\psi\rangle$ with respect to A is with probability

$$\langle\psi|P_i\psi\rangle = ||\langle|\psi|P_i\psi\rangle||^2$$

the state $P_i|\psi\rangle$ on quantum level and the eigenvalue λ_i on classical level.

Slightly differently are sometime treated the so-called **selective measurement operator** or **filtration operator**

$$|\psi\rangle\langle\psi|$$

If this filtration operator is applied on a state $|\phi\rangle$ the outcome is the state $|\psi\rangle$ with probability

$$|\langle\psi|\phi\rangle|$$

and with probability $1 - |\langle|\psi|\phi\rangle|$ the outcome is no quantum state.

For example if photon in the state $\alpha|0\rangle + \beta|1\rangle$ is sent through a horizontal (vertical) filter – corresponding to the state $|0\rangle(|1\rangle)$,then the outcome is with probability $|\alpha|^2$ ($|\beta|^2$ a photon with horizontal (vertical) polarization and with the remaining probability no photon gets through.

CLASSICAL versus QUANTUM MECHANICS

A crucial difference between quantum theory and classical mechanics is perhaps this: whereas classical states are essentially **descriptive**, quantum states are essentially **predictive**; they encapsulate predictions concerning the values that measurements of physical quantities will yield, and these predictions are in terms of probabilities.

The state of a classical particle is given by its position $q = (q_x, q_y, q_z)$ and momentum $p = (p_x, p_y, p_z)$.

The state of n particles is therefore given by $6n$ numbers.

Hamiltonian, or total energy $H(p, q)$ of a system of n particles is then a function of $3n$ coordinates p^i_u, $i = 1, \ldots,$, $u \in \{x, y, z\}$ and $3n$ coordinates q^i_u.

Evolution of such a system is then described by a system of $3n$ pairs of equations

$$\frac{dq^i_u}{dt} = \frac{\partial H}{\partial p^i_u} \qquad \frac{dp^i_u}{dt} = \frac{\partial H}{\partial q^i_u}$$

TENSOR PRODUCTS

of vectors

$$(x_1, \ldots, x_n) \otimes (y_1, \ldots, y_m) = (x_1y_1, \ldots, x_1y_m, x_2y_1, \ldots, x_2y_m, \ldots, x_ny_1, \ldots, x_ny_m$$

of matrices $$A \otimes B = \begin{pmatrix} a_{11}B & \ldots & a_{1n}B \\ \vdots & & \vdots \\ a_{n1}B & \ldots & a_{nn}B \end{pmatrix}$$

where $$A = \begin{pmatrix} a_{11} & \ldots & a_{1n} \\ \ldots & & \ldots \\ a_{n1} & \ldots & a_{nn} \end{pmatrix}$$

Example

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & 0 & 0 \\ a_{21} & a_{22} & 0 & 0 \\ 0 & 0 & a_{11} & a_{12} \\ 0 & 0 & a_{21} & a_{22} \end{pmatrix}$$

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} a_{11} & 0 & a_{12} & 0 \\ 0 & a_{11} & 0 & a_{12} \\ a_{21} & 0 & a_{22} & 0 \\ 0 & a_{21} & 0 & a_{22} \end{pmatrix}$$

of Hilbert spaces $H_1 \otimes H_2$ is the complex vector space spanned by tensor products of vectors from H_1 and H_2, that corresponds to the quantum system composed of the quantum systems corresponding to Hilbert spaces H_1 and H_2.

An important difference between classical and quantum systems

A state of a compound classical (quantum) system can be (cannot be) always composed from the states of the subsystems.

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 $\{(p_i,\phi_i)\,|\,1\leq i\leq k\}$ on pure states $\{\phi_i\}_{i=1}^k$, with probabilities $0<p_i\leq 1$, $\Sigma_{i=1}^k\, p_i=1$ is called a **mixed state** or **mixture**, and denoted by $[\psi\rangle=\{(p_i,\phi_i)\,|\,1\leq i\leq k\}$ or

$$[\psi\rangle=(p_1,\phi_1)\oplus\ldots\oplus(p_k,\phi_k). \tag{1}$$

where $\oplus$ symbol is used just to separate particular pure states and their probabilities.

For example, a mixed state is created if a source produces pure state $|\phi_i\rangle$ with probability p_i and $\Sigma_{i=1}^k\, p_i=1$.

To each mixed state $[\psi\rangle$ corresponds a **density operator** $\rho_{[\psi\rangle}$.

If $[\psi\rangle=|\phi\rangle$ for a pure state $|\phi\rangle$, then $\rho_{[\phi\rangle}=|\phi\rangle\langle\phi|$.
If $[\psi\rangle=\oplus_{i=1}^k(p_i,|\phi_i\rangle)$, where $|\phi_i\rangle$ are pure states, then

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

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

EXAMPLES

The density matrix corresponding to the mixed state

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

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

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

corresponds the density matrix

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

PROPERTIES of DENSITY MATRICES

1. Any density matrix ρ is Hermitian, nonnegative, has only nonegative eigenvalues and $Tr(\rho) = 1$.
2. If ρ_1 and ρ_2 are density matrics on the same Hilbert space, then $p\rho_1 + (1-p)\rho_2$, $0 \leq p \leq 1$ is a density matrix too.
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 $Tr\rho = 1$.

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):

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

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

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

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

$$Tr_B(|\phi_1\rangle\langle|\phi_2| \otimes |\psi_1\rangle\langle\psi_2|) = |\phi_1\rangle\langle\phi_2|\, Tr(|\psi_1\rangle\langle\psi_2|) = \langle\psi_2|\psi_1\rangle|\phi_1\rangle\langle\phi_2|.$$

MEASUREMENT on MIXED STATES

Let A be an observable (self-adjoint operator), Δ an interval on real axis and P_Δ^A the projection operator into the subspace of all pure states measurement of which, with respect to A, produces with certainty a value from Δ.

The probability that measurement of a mixed state ρ with respect to an observable A produces a value from Δ, that is

$$Pr_\rho(A, \Delta)$$

equals

$$Pr_\rho(A, \Delta) = Tr(\rho P_\Delta^A)$$

and in the case ρ is a pure state, that is $\rho = |\psi\rangle\langle\psi|$ for a pure state $|\psi\rangle$, then

$$Pr_\psi(A, \Delta) = \langle\psi|P_\Delta^P\psi\rangle.$$

SUPEROPERTOTS

- A **superoperator (SO)** is a linear transformation 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 (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.

CSPO are exactly the physically allowed transformations on density matrices.

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

SUPEROPERATORS — INFORMAL VIEW

Informally, the best way is to see a superoperator S applied to a state $|\phi\rangle$ of a Hilbert space H as to take first an auxiliary state (called usually **ancilla**) of another Hilbert space H', then to apply a unitary operator U to the state $|\phi\rangle \otimes |\psi\rangle$ and, finally, to discard the H'-part of the resulting state.

QUANTUM EVOLUTION/COMPUTATION

EVOLUTION	COMPUTATION
in	in
QUANTUM SYSTEM	HILBERT SPACE

is described by

Schrödinger linear equation

$$i\hbar\frac{\partial\psi(t)}{\partial t} = H(t)\psi(t),$$

where $H(t)$ is a quantum analogue of a Hamiltonian of the classical system, from which it follows that evolution (computation) of a quantum system is performed by a **unitary operator** and a step of such an evolution we can see as a multiplication of a **unitary matrix** A with a vector $|\psi\rangle$, i.e.

$$A|\psi\rangle$$

A matrix A is **unitary** if

$$A \cdot A^* = A^* \cdot A = I$$

HAMILTONIANS

The Schrödinger equation tells us how a quantum system evolves

subject to the Hamiltonian

However, in order to do quantum mechanics, one has to know how to pick up the Hamiltonian.

The principles that tell us how to do so are real bridge principles of quantum mechanics.

Each quantum system is actually uniquely determined by a Hamiltonian.

EVOLUTION and MEASUREMENT of DENSITY OPERATORS

Schrödinger equation has in terms of density operators the form

$$i\hbar\frac{\partial\rho}{\partial t} = [H,\rho] = H\rho - \rho H.$$

If a unitary transformation U is the solution of the standard Schr̈dinger equation $i\frac{\bar{U(t)}}{\partial t} = HU(t)$, then the evolution of ρ is according to the rule

$$\rho \rightarrow U\rho U^*.$$

If a density operator is measured with respect to an observable A with the spectral form $A = \Sigma_{i=1}^{k}\lambda_i P_i$, then with probability

$$Pr(\rho P_i)$$

the classical outcome is λ_i

and the state ρ collapses into the state

$$\frac{P_i\rho P_i}{Tr(\rho P_i)}.$$

SCHRÖDINGER versus HEISENBERG PICTURE

An understanding of quantum evolution in terms of states and unitary operators, at which a quantum state $|\phi\rangle$ is changed by the rule

$$|\phi\rangle \to U|\phi\rangle$$

in the case of pure states $|\phi\rangle$ or by the rule

$$\rho \to U^*\rho U$$

in the case of mixed state ρ, where U is a unitary transformation, is called (at first sight quite puzzling)

Schrödinger picture

because it represents Schrödinger's view of the quantum world.

At Schrödinger picture operators are stationary and states keep changing.

In an equivalent Heisenberg's view of the quantum world, called

Heisenberg picture,

the observables A keep changing under the rule

$$A \to U^*AU$$

and the (initial) states keep being stationary.

The equation for the change of observables has the form

$$i\hbar\frac{\partial A}{\partial t} = [A, H] = AH - HA.$$

TRACE COMPUTATION

The very basic and useful fact is that for a general form of a density operator ρ over a tensor product $H^{(1)} \otimes H^{(2)}$

$$\rho = \sum_k \alpha_k |\phi_{1,k}\rangle\langle\psi_{2,k}|,$$

where $|\phi_{1,k}\rangle \in H^{(1)}$, $|\psi_{2,k}\rangle \in H^{(2)}$ is that it holds

$$Tr(\rho) = \sum_k \alpha_k \langle\psi_{2,k}|\phi_{1,k}\rangle$$

That is in order to determine trace of ρ the outer product has been replaced by the inner product.
The above method can be generalized for partial trace as follows:

SOLVING SCHRÖDINGER EQUATION

For the Hamiltonian

$$H = \frac{\pi\hbar}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & 1 \end{pmatrix} = \frac{\pi\hbar}{2}U$$

the Schödinger equation

$$i\hbar\frac{\partial U(t)}{\partial t} = HU(t)$$

has the solution

$$U(t) = e^{-\frac{i}{\hbar}Ht} = \sum_{i=1}^{\infty}\frac{(-\frac{i\pi}{2})^k V^k t^k}{k!} = I + \frac{1}{2}\sum_{i=0}^{\infty}\frac{(-\pi i t)^k}{k!}V$$

and therefore for $t = 1$,

$$e^{-\frac{i\pi}{2}V} = I + \frac{1}{2}(e^{-i\pi} - 1)V = I - V = XOR.$$

LOGARITHM of MATRICES

If ρ is a matrix, then we define

$$\lg \rho = \frac{1}{\ln 2}\sum_{n=1}^{\infty}(-1)^{n+1}\frac{(\rho - I)^n}{n}$$

converges provided ρ is close to the identity matrix I in the sence that

$$|\rho - I|| < 1$$

what is the case if ρ is a density matrix.

In the case a density matrix is not positive-definite, only positive semi-definite (and it can have an eigenvalue 0), then $\lg \rho$ does not exist. However, in such a case there is a sequence $\{\rho_i\}_{i=1}^{\infty}$ of positive definite

Hermitian operators of trace 1 such that

$$\rho = \lim_{i\to\infty} \rho_i$$

and in such a case also the limit

$$\lim_{i\to\infty} \rho_i \lg \rho_i$$

exists. This means that von Neumann entropy is defined for all density matrices.