General characteristics of multi-partite quantum systems (Lecture of the Quantum Information class of the Master in Quantum Science and Technology)

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20, 24, 27, 31 January, 2025

Outline

1. **General characteristics of multi-partite quantum systems**
   - A. Classical bits
   - B. Quantum bit - pure states
   - C. Multi-qubit systems - pure states
   - D. Measurement
   - E. Mixed states and the density matrix
   - F. Geometry of quantum states
     - A single qubit
     - A single qudit (qunit):*d*-dimensional systems
   - G. Two or more qubits: reduced states
   - H. Bipartite systems: Schmidt decomposition
   - I. Purifications
   - J. Purity
   - K. Entropy
     - Shannon entropy, von Neumann entropy
     - Quantum conditional entropy, q. mutual information, q. relative entropy
     - Linear entropy
   - L. Fidelity
   - M. Distances

A single classical bit

- A classical bit can be either 0 or 1. Can we still use it to describe a real number between 0 and 1?
- For that, we need an ensemble of several classical bits

$$\{b_k\}_{k=1}^{M}, \tag{1}$$

where $b_k = 0$ or 1

- We can interpret the average value and the variance. That is,

$$\langle b \rangle = \frac{1}{M} \sum_k b_k, \tag{2}$$

and

$$(\Delta b)^2 = \frac{1}{M} \sum_k (b_k - \langle b \rangle)^2. \tag{3}$$

A single classical bit II

- This can also be given with probabilities:
- Let P_0 and P_1 be the probabilities of having a 0 or a 1.
- The expectation value and the variance are the function of P_0 and P_1. Since $P_0 + P_1 = 1$, we have a **single real degree of freedom** that describes the statistical properties of an ensemble of bits.
- Hence,

  $$\langle b \rangle = P_1 \tag{4}$$

  and

  $$(\Delta b)^2 = P_0(0 - P_1)^2 + P_1(1 - P_1)^2. \tag{5}$$

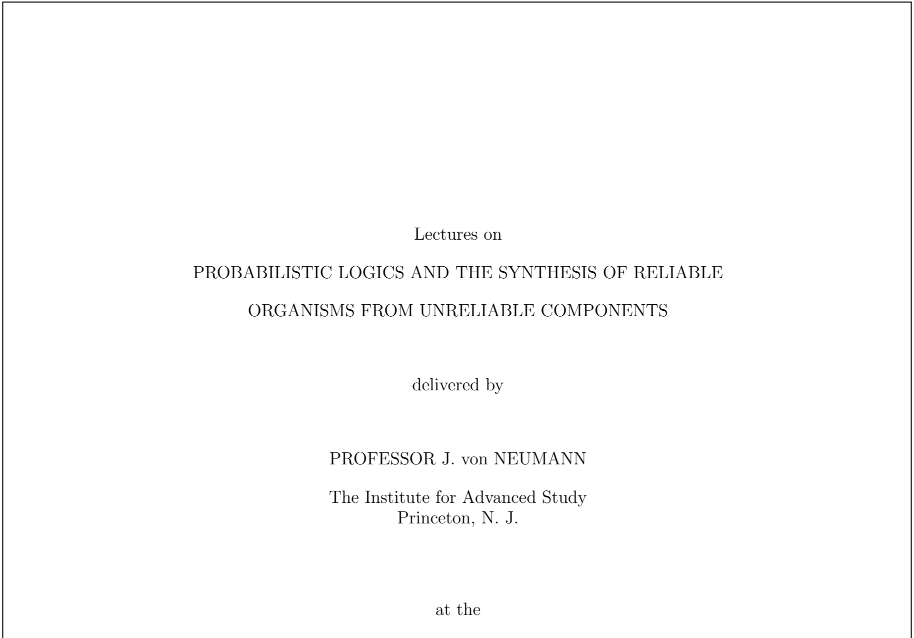
Stochastic computing

- Stochastic computing uses random bits to calculate (John von Neumann, 1953).
- A random bit represents a real number between 0 and 1. Two random bits can easily be multiplied.

$$\langle b_1 b_2 \rangle = \langle b_1 \rangle \langle b_2 \rangle. \tag{6}$$

- We need many samples to get the average with small error.

Stochastic computing II



Lectures on

PROBABILISTIC LOGICS AND THE SYNTHESIS OF RELIABLE
ORGANISMS FROM UNRELIABLE COMPONENTS

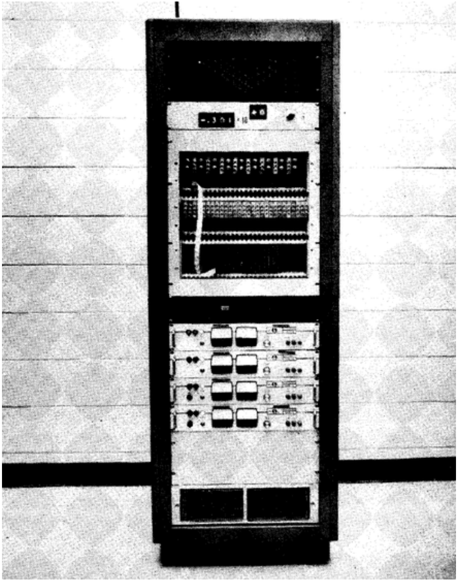
delivered by

PROFESSOR J. von NEUMANN

The Institute for Advanced Study
Princeton, N. J.

at the

Stochastic computing III



The RASCEL stochastic computer, circa 1969, Wikipedia.

Stochastic computing IV

Multiplication is possible with an AND gate.

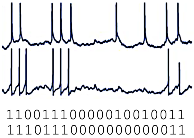


Figure 1.2: Similarity of biological signals and stochastic numbers; information is carried via pulses.

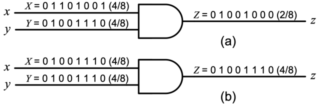


Figure 1.3: Stochastic multiplication: (a) accurate result with uncorrelated inputs; (b) inaccurate result due to correlated inputs.

A. Alaghi, The Logic of Random Pulses: Stochastic Computing,
Ph.D. Thesis, University of Michigan, 2015.

Several classical bits

- N classical bits can be in one of the 2^N binary states. For example, for $N = 2$, these are 00, 01, 10 and 11.

- For $N = 2$, these are

$$P_{00}, P_{01}, P_{10}, P_{11}. \tag{7}$$

- The ensemble of the N-bit units can be described by the 2^N probabilities.

- Since, again, the sum of all the probablities is 1, **we need** $2^N - 1$ **real degrees of freedom** to describe the statistical properties of such an ensemble.

Several classical bits II

- Let us consider some function of N bits $f(k)$, where k is now an N bit number.
- Then, the expectation value of f is

$$\langle f \rangle = \sum_{k=0}^{2^N-1} p_k f(k) = \vec{p}\vec{f}, \tag{8}$$

where k is an N-bit number, i.e., an integer between 0 and $2^N - 1$. We put the $f(k)$'s into a vector $\vec{f}$. We also put the p_k probabilities into $\vec{p}$.

Several classical bits III

- We can also write

  $$\langle f^2 \rangle = \sum_k p_k [f(k)]^2 \tag{9}$$

  Hence,

  $$(\Delta f)^2 = \sum_k p_k [f(k)]^2 - \left(\sum_k p_k f(k) \right)^2 . \tag{10}$$

  These were relevant, since in the quantum case, we will have similar expressions.

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Quantum bit - pure states

- A quantum bit (=two-state system, spin-$\frac{1}{2}$ particle) can be in a pure state

$$|q\rangle = \alpha|0\rangle + \beta|1\rangle, \tag{11}$$

  where α and β are complex numbers, and the normalisation condition $|\alpha|^2 + |\beta|^2 = 1$.

- Note that the overall phase does not matter, thus a pure quantum bit is described by two degrees of freedom.

- The two complex coefficients have **4 real degrees of freedom.**

- However, due to the normalisation condition and the arbitrariness of the overall phase we are left with **two degrees of freedom.**)

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Multi-qubit systems - pure states

- What about a two-qubit system? What kind of states it can be in? One could think on qubit 1 in state

$$|q_1\rangle = \alpha_1|0\rangle + \beta_1|1\rangle, \tag{12}$$

  and qubit 2 in state

$$|q_2\rangle = \alpha_2|0\rangle + \beta_2|1\rangle. \tag{13}$$

- However, we all know that the general state of the two-qubit system can be given as

$$|q_{12}\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|00\rangle + \alpha_{11}|01\rangle. \tag{14}$$

Multi-qubit systems - pure states II

- In general, for N qubits we need N complex numbers. Again the state has to be normalized and the overall phase does not matter, thus this means $2 \times 2^N - 2$ real degrees of freedom.
- We can place the coefficients in a vector, called state vector and write

$$|\Psi\rangle = \begin{pmatrix} \alpha_{00} \\ \alpha_{01} \\ \alpha_{10} \\ \alpha_{11} \end{pmatrix}. \tag{15}$$

- The properties of the state vector are: it is normalized

$$\langle\Psi|\Psi\rangle = 1. \tag{16}$$

Multi-qubit systems - pure states III

- An overall phase does not matter:

$$e^{-i\theta}|\Psi\rangle \tag{17}$$

  describes the same state for any θ.

- The expectation value of an operator for a pure state can be obtained as

$$\langle A\rangle = \langle\Psi|A|\Psi\rangle = \mathrm{Tr}(A|\Psi\rangle\langle\Psi|). \tag{18}$$

Outline

Measurement

- The von Neumann measuement in the z basis results is eithet 0 or 1. If the state was $\alpha|0\rangle + \beta|1\rangle$, then we get a statistical mixture of 0 and 1, with the probabilities

  $$P_0 = |\alpha|^2, \tag{19}$$

  and

  $$P_1 = |\beta|^2. \tag{20}$$

  That is, from an ensemble of quantum bits we get an ensemble of classical bits.
- If we measure in the x basis, we get another classical ensemble.
- For a multi-qubit system, if we measure in the some basis (e.g., x, y or z), we get an ensemble of N-bit systems. However, for exach choice of basis we get a different classical ensemble.

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Mixed states and the density matrix

- So far we were talking about pure states.
- In reality, in an experiment we do not have a situation where a machine always produces the $|\Psi_1\rangle$ state.
- Sometimes it makes mistakes, and produces the $|\Psi_k\rangle$ states for $k = 2, 3, ...$ How to describe such a situation?

$\lvert\Psi_1\rangle$	p_1
$\lvert\Psi_2\rangle$	p_2
$\lvert\Psi_3\rangle$	p_3
...	...

Mixed states and the density matrix

- What is the expectation value of an operator in such a system? We can write it as

$$\langle A \rangle = \sum_k p_k \langle \Psi_k | A | \Psi_k \rangle = \mathrm{Tr}\left(A \sum_k p_k |\Psi_k\rangle\langle\Psi_k| \right). \tag{21}$$

- This can be rewritten as

$$\langle A \rangle = \mathrm{Tr}(\varrho A), \tag{22}$$

where

$$\varrho = \sum_k p_k |\Psi_k\rangle\langle\Psi_k| \tag{23}$$

is the density matrix (Neumann, Landau).

- Note that if ϱ is diagonal, we obtain

$$\langle A \rangle = \mathrm{Tr}(\varrho A) = \sum_k \varrho_{kk} A_{kk}. \tag{24}$$

That is, A is written in the eigenbasis of ϱ. This is the scalar product of two vectors as in $\langle f \rangle = \vec{p}\vec{f}$ [given in Eq. (8)].

Mixed states and the density matrix II

- The density matrix describes the state completely. Now we see, why the overall phase does not matter:

$$e^{-i\theta}|\Psi_k\rangle\langle\Psi_k|e^{+i\theta} = |\Psi_k\rangle\langle\Psi_k|. \tag{25}$$

- The properties of the density matrix are

$$\begin{aligned} \varrho &= \varrho^\dagger, \\ \varrho &\geq 0, \\ \mathrm{Tr}(\varrho) &= 1. \end{aligned} \tag{26}$$

- **A** $2^N \times 2^N$ **density matrix has** $4^N - 1$ **real parameters.**

- For $N = 1$, this means 3 real parameters, corresponding to the three coordinates of the Bloch vector. For r $N = 2$, this means 8 real parameters.

Mixed states and the density matrix III

- We can also say that
$$\mathrm{Tr}(\varrho^2) \leq 1. \tag{27}$$
It is one only for pure (rank-1) states.

- The density matrix can be decomposed into the sum of pure states in many ways. The decomposition
$$\varrho = \sum_k p_k |\Psi_k\rangle\langle\Psi_k| \tag{28}$$
is not unique, i.e., it is not necessarily an eigendecomposition. This has a large importance for entanglement theory.

Mixed states and the density matrix IV

Summary:

	N bits	N qubits
Number of DOF	$2^N - 1$	$4^N - 1$
Description	$\vec{p}$	ϱ
Expectation value	$\vec{f}\vec{p}$	$\mathrm{Tr}(A\varrho)$
Normalization	$\sum_k p_k = 1$	$\mathrm{Tr}(\varrho) = 1$

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Bloch vector

- For a single qubit, **the density matrix has three real parameters.** It can be written as

$$\varrho = \frac{1}{2}\left(\mathbb{1} + \sum_{l=x,y,z} v_l \sigma_l\right), \tag{29}$$

  where σ_l are the Pauli spin matrices.

- Using $\mathrm{Tr}(\sigma_k \sigma_l) = 2\delta_{kl}$, we can write

$$\mathrm{Tr}(\varrho^2) = \frac{1}{2} + \frac{1}{2}\sum_{l=x,y,z} v_l^2. \tag{30}$$

  That is, the Bloch vector has a maximal length for pure states.

Bloch vector II

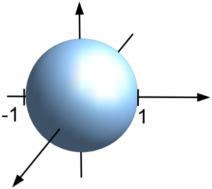
- From $\mathrm{Tr}(\varrho^2) \leq 1$, the condition for being physical is Eq. (26), which is equvalent to

  $$\sum_{l=x,y,z} |v_l|^2 \leq 1. \tag{31}$$

  The three-element vector is called the Bloch vector.

Bloch vector III

- Let us identify the points in (v_x, v_y, v_z) corresponding to physical states. They are in a ball.
- The pure states are on the surface.
- Mixed states are inside the Ball. This is because $\mathrm{Tr}(\varrho^2)$ is directly related to the length of the Bloch vector.
- The $|0\rangle$ and $|1\rangle$ correspond to the North and South Pole.
- $|0\rangle + \exp(-i\phi)|1\rangle$ correspond to points on the equator.



Set of physical quantum states for a single qubit. The axes correspond to v_l for $l = x, y, z$. Pure states correspond to points on the surface, mixed states correspond to internal points.

A single qudit (qunit):*d*-dimensional systems

- For higher dimensional systems the picture is much more complicated. Let us consider qudits with dimension d.

- Similarly to the case before, **a** $d \times d$ **Hermitian matrix with a unit trace has** $d^2 - 1$ **degrees of freedom.**

- Hence, we can write a density matrix as a linear combination of $d^2 - 1$ SU(d) generators as

$$\varrho = \frac{1}{d}\mathbb{1} + \frac{1}{2}\sum_{l=1}^{d^2-1} v_l g_l. \tag{32}$$

Here,

$$\mathrm{Tr}(g_k g_l) = 2\delta_{kl}. \tag{33}$$

(Like for the Pauli matrices. Thus, we have something like the generalized Pauli matrices. $d = 3$: Gell-Mann matrices.)

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- Like for the Pauli matrices. Thus, we have something like the generalized Pauli matrices. $d = 3$: for instance, Gell-Mann matrices.

A single qudit (qunit):*d*-dimensional systems II

- Gell-Mann matrices:

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}$$

$$\lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad \lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}.$$

There are other possibilities: J. Lawrence, quant-ph/0403095.

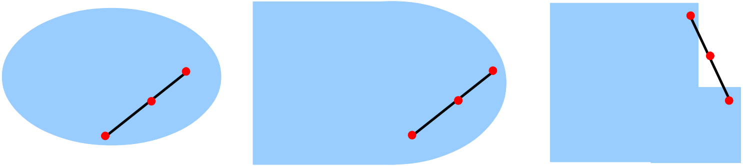
A single qudit (qunit): d-dimensional systems III

- Let us again look at the points $(v_1, v_2, ..., v_{d^2-1})$ corresponding to physical states.

- First note that the set of convex. This is because mixing two physical states ϱ_1 and ϱ_2, we always get a physical state

$$\varrho = p\varrho_1 + (1-p)\varrho_2. \tag{36}$$

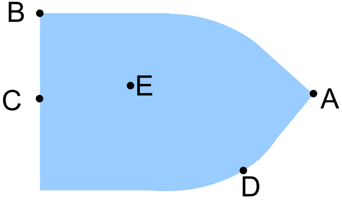
A single qudit (qunit): d-dimensional systems IV



Two convex objects and one that is not convex.

A single qudit (qunit):*d*-dimensional systems V

- On the next figure we will show the set of quantum states.
- The cooridnate axis could be the v_l, for example.
- Inside the set there are the density matrices with full rank.
- On the boundary there are the states with less than full rank, such as for example rank-1 states, which are pure states.



Set of physical quantum states. Note that the set is convex.
A,B,D: rank-1 states. C: rank-2 state. E: full rank states.

A single qudit (qunit):d-dimensional systems VI

- **Observation.** The following inequality is true

$$\lambda_{\min}(A+B) \geq \lambda_{\min}(A) + \lambda_{\min}(B). \tag{37}$$

Proof. Let us consider that for a Hermitian matrix X we have

$$\lambda_{\min}(X) = \min_{\psi} \langle \psi | X | \psi \rangle. \tag{38}$$

Then, for A and B Hermitian matrices we have

$$\begin{aligned} \lambda_{\min}(A+B) &= \min_{\psi} \langle \psi | A+B | \psi \rangle \geq \min_{\psi} \langle \psi | A | \psi \rangle + \min_{\psi} \langle \psi | B | \psi \rangle \\ &= \lambda_{\min}(A) + \lambda_{\min}(B). \end{aligned} \tag{39}$$

□

We can prove similarly that

$$\lambda_{\max}(A+B) \leq \lambda_{\max}(A) + \lambda_{\max}(B). \tag{40}$$

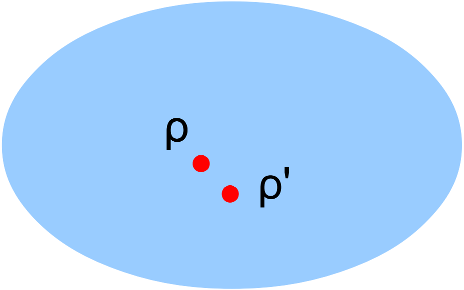
Full rank states

- Using this, we can say the following.
- **Observation.** Full-rank states are inside the set.
  Proof. If the state is full rank, it means that for some small ϵ

  $$\varrho' = \varrho + \epsilon H \tag{41}$$

  is also physical, where H is a trace 0 Hermitian matrix. Why is that? See also the next figure.

Full rank states II



We take an internal state ϱ and consider the states ϱ' in its neighborhood.

Full rank states III

- It is physical since
  1. Trace is 1.
  2. Hermitian.
  3. Full rank means that

$$\lambda_{\min}(\varrho) > 0, \qquad \lambda_{\max}(\varrho) < 1. \tag{42}$$

Eigenvalues are nonzero for small ϵ. This is because

$$\lambda_{\max}(\varrho) + \lambda_{\max}(\epsilon H) \geq \lambda_k(\varrho') \geq \lambda_{\min}(\varrho) + \lambda_{\min}(\epsilon H). \tag{43}$$

Here we have

$$\lambda_{\min}(\epsilon H) = \begin{cases} +\epsilon\lambda_{\min}(H), & \text{if } \epsilon \geq 0, \\ -|\epsilon|\lambda_{\max}(H), & \text{if } \epsilon < 0. \end{cases} \tag{44}$$

Similar statement holds for $\lambda_{\max}(\epsilon H)$. □

Non-full-rank states

- **Observation.** Non-full-rank states are on the surface of the set.

- *Proof.* If the state is not full rank, then it has zero eigenvalues. Thus, there is an H such that ϱ' is aphisical for any $\epsilon > 0$ or any $\epsilon < 0$.

- To be more explicit, let us write

$$\varrho = UDU^{\dagger}, \tag{45}$$

such that D contains the eigenvalues. Here,

$$D = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3, ..., \lambda_d), \tag{46}$$

and the eigenvectors are

$$U = [|\Psi_1\rangle, |\Psi_2\rangle, |\Psi_3\rangle, ..., |\Psi_d\rangle]. \tag{47}$$

Non-full-rank states II

- Assume that $\lambda_d = 0$. Then,

  $$\varrho' = \varrho + \epsilon(|\Psi_d\rangle\langle\Psi_d| - \mathbb{1}/d) \tag{48}$$

  has a negative eigenvalue for any $\epsilon < 0$. The Identity is needed to make the expression zero-trace.

- This is because the eigenvalues of this matrix are

  $$D' = \mathrm{diag}(\lambda_1 - \epsilon/d, \lambda_2 - \epsilon/d, \lambda_3 - \epsilon/d, ..., \lambda_d + \epsilon(1 - 1/d)). \tag{49}$$

  $\square$

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Two or more qubits: reduced states

- How can one see the state of a qubit, if it is the part of an entangled state?

- A reduced state of a bipartite system can be obtained after tracing out one of the subsystems. Let us consider a two-qubit system and write the density matrix in the basis $|00\rangle, |01\rangle, |10\rangle, |11\rangle$. Then, denote the elements of the density matrix by

  $$\varrho_{ij,kl}, \tag{50}$$

  where $i, j, k, l = 0, 1$. In other words, it looks like

  $$\varrho = \begin{array}{c} \\ |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{array} \begin{array}{c} \begin{array}{cccc} |00\rangle & |01\rangle & |10\rangle & |11\rangle \end{array} \\ \left(\begin{array}{cccc} \varrho_{00,00} & \varrho_{00,01} & \varrho_{00,10} & \varrho_{00,11} \\ \varrho_{01,00} & \varrho_{01,01} & \varrho_{01,10} & \varrho_{01,11} \\ \varrho_{10,00} & \varrho_{10,01} & \varrho_{10,10} & \varrho_{10,11} \\ \varrho_{11,00} & \varrho_{11,01} & \varrho_{11,10} & \varrho_{11,11} \end{array} \right) \end{array} . \tag{51}$$

  Thus, the size of the density matrix is 4x4.

Two or more qubits: reduced states II

- To become familiar with bras and kets, one can even use the completeness relation

  $$\mathrm{Identity} = \sum_{ij} |ij\rangle\langle ij|. \tag{52}$$

  Then, one obtains

  $$\mathrm{Identity} \times \varrho \times \mathrm{Identity} = \sum_{ijkl} |ij\rangle(\langle ij|\varrho|kl\rangle)\langle kl|, \tag{53}$$

  where the expression in the bracket is just the matrix element of the density matrix

  $$\varrho_{ij,kl} = \langle ij|\varrho|kl\rangle. \tag{54}$$

  Hence, the density matrix can be written as

  $$\varrho = \sum_{ijkl} \varrho_{ij,kl}|ij\rangle\langle kl|. \tag{55}$$

Two or more qubits: reduced states III

- Then, tracing out the second subsystem gives the reduced state

  $$\mathrm{Tr}_2(\varrho) = \varrho_{\mathrm{red}}, \tag{56}$$

  which is given as

  $$\varrho_{\mathrm{red,ik}} = \sum_m \varrho_{im,km}. \tag{57}$$

  This is a 2x2 density matrix of a qubit. With this, for any A

  $$\langle A \otimes \mathbb{1} \rangle_{\varrho} = \langle A \rangle_{\varrho_{\mathrm{red}}} \tag{58}$$

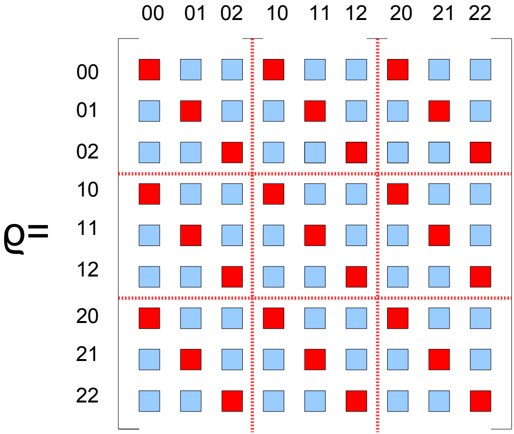
  holds.

- Graphical representation: in the blockdiagonal representation, we sum the elements in the diagonal of the small matrices.

- Tracing out for pure states:

  $$\mathrm{Tr}_2\left(\sum_k \alpha_k |\psi_k\rangle|\phi_k\rangle\right) = \sum_k |\alpha_k|^2 |\psi_k\rangle\langle\psi_k|. \tag{59}$$

Two or more qubits: reduced states IV



ϱ=

	00	01	02	10	11	12	20	21	22
00	🟥	🟦	🟦	🟥	🟦	🟦	🟥	🟦	🟦
01	🟦	🟥	🟦	🟦	🟥	🟦	🟦	🟥	🟦
02	🟦	🟦	🟥	🟦	🟦	🟥	🟦	🟦	🟥
10	🟥	🟦	🟦	🟥	🟦	🟦	🟥	🟦	🟦
11	🟦	🟥	🟦	🟦	🟥	🟦	🟦	🟥	🟦
12	🟦	🟦	🟥	🟦	🟦	🟥	🟦	🟦	🟥
20	🟥	🟦	🟦	🟥	🟦	🟦	🟥	🟦	🟦
21	🟦	🟥	🟦	🟦	🟥	🟦	🟦	🟥	🟦
22	🟦	🟦	🟥	🟦	🟦	🟥	🟦	🟦	🟥

Partial trace in a 3 × 3 system according to the second subsystem.

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Bipartite systems: Schmidt decomposition

- Any bipartite pure state can be given as

$$|\Psi_{AB}\rangle = \sum_k \lambda_k |k\rangle_A |k\rangle_B, \tag{60}$$

  where $|k\rangle_A$ are pairwise orthogonal with each other, and $|k\rangle_B$ are also pairwise orthogonal with each other. λ_k are real and $\lambda_k \geq 0$.

- It cannot be generalized easily to multipartite systems. There is no Schmidt decomposition for tripartite systems.

- The reduced states are

$$\varrho_A = \sum_k \lambda_k^2 |k\rangle\langle k|_A, \qquad \varrho_B = \sum_k \lambda_k^2 |k\rangle\langle k|_B. \tag{61}$$

Bipartite systems: Schmidt decomposition II

- If λ_k are different from each other then the Schmidt decomposition is unique. If some of the λ_k's are equal to each other then the decomposition is not unique.
- For example, let us assume that $\lambda_1 = \lambda_2$. Then,

$$\lambda_1|1\rangle_A|1\rangle_B + \lambda_2|2\rangle_A|2\rangle_B = \lambda_1|+\rangle_A|+\rangle_B + \lambda_2|-\rangle_A|-\rangle_B, \tag{62}$$

where for both A and B we define

$$|\pm\rangle = \frac{1}{\sqrt{2}}(|1\rangle \pm |2\rangle). \tag{63}$$

Outline

1 General characteristics of multi-partite quantum systems

Purifications

- The pure state Ψ_{AB} state is the purification of the mixed state ϱ_A if

$$\mathrm{Tr}_B(|\Psi_{AB}\rangle\langle\Psi_{AB}|) = \varrho_A. \tag{64}$$

  Note that $|\Psi_{AB}\rangle$ on subsystems A and B, while ϱ_A lives on subsystem A only.

- Let us assume that a density matrix is defined as

$$\varrho_A = \sum_k p_k |\phi_k\rangle\langle\phi_k|_A. \tag{65}$$

- Then, a purification can be a pure state

$$|\Psi\rangle_{AB} = \sum_k \sqrt{p_k} |\phi_k\rangle_A \otimes |k\rangle_B, \tag{66}$$

  where $|k\rangle_B$ denotes an orthonormal basis of the subsystem B.

Purifications II

- If $|\Psi\rangle_{AB}$ is a purification then

$$|\Psi\rangle'_{AB} = \mathbb{1}_A \otimes U_B |\Psi\rangle_{AB}, \tag{67}$$

  is also a purification.

Purifications III

- Purification of the eigendecomposition,

$$\varrho_A = \sum_k \lambda_k |\phi_k\rangle\langle\phi_k|_A. \tag{68}$$

  Then,

$$|\Psi\rangle_{AB} = \sum_k \sqrt{\lambda_k} |\phi_k\rangle_A \otimes |k\rangle_B. \tag{69}$$

  If ϱ_A is full rank then the size of B is the same of the size of A.

- In general, B can also have a larger dimension that A.

- For instance,

$$|\Psi\rangle_{AB} = \sum_k \sqrt{\lambda_k} |\phi_k\rangle_A \otimes |\phi_k\rangle_B. \tag{70}$$

  is also a purification.

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Purity

- Defined as

$$\mathrm{Tr}(\varrho^2). \tag{71}$$

- 1 for pure states.
- $1/d$ for the completely mixed state.

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Shannon entropy

- There is a source that outputs an integer number between 1 and d.
- The Shannon entropy is given as

$$H = -\sum_{k=1}^{d} p_k \log p_k. \tag{72}$$

Shannon entropy II

- Properties
  - Classical, not quantum.
  - The source can have *d* possible outputs with some probability.
  - In information theory, the entropy of a random variable is the average level of "information", "surprise", or "uncertainty" inherent in the variable's possible outcomes (Wikipedia).
  - There is a clear relation to compression of data. If the entropy is lower, one can compress the data to a smaller space.

Shannon entropy III

- Further properties
  - $H = 0$ if $p_1 = 1$, all other $p_k = 0$. $\vec{p} = (1, 0, 0, 0, ...)$. The output is always the same. No information is provided.
  - Comment: we can show that, using L'Hospitals rule,

$$\lim_{x \to 0} (x \log x) = \lim_{x \to 0} \frac{\log x}{1/x} = \lim_{x \to 0} \frac{1/x}{-1/x^2} = -\lim_{x \to 0} x = 0. \tag{73}$$

  - $H = \log d$ (maximal) if $p_k = \frac{1}{d}$. $\vec{p} = (\frac{1}{d}, \frac{1}{d}, \frac{1}{d}, \frac{1}{d}, ...)$. All outputs are equally probable, a lot of information is provided.

Von Neumann entropy

- Von Neumann entropy for a quantum state is defined as

$$S(\varrho) = -\mathrm{Tr}(\varrho \log \varrho) \equiv -\langle \log \varrho \rangle. \tag{74}$$

- Note: matrix logarithm! It can be written with the eigenvalues of the density matrix as

$$S(\varrho) = -\sum_{k=1}^{d} \lambda_k \log \lambda_k. \tag{75}$$

Von Neumann entropy II

- Properties

  - Quantum. "Quantum version" of the Shannon entropy.
  - For a pure state we have $\lambda_k = \{1, 0, 0, ..., 0\}$, and thus it is zero.
  - Its maximal is for the completely mixed state for which $\lambda_k = \{\frac{1}{d}, \frac{1}{d}, \frac{1}{d}, ..., \frac{1}{d}\}$, and its value is $\log_2 d$.
  - Invariant under change of basis:

$$S(\varrho) = S(U\varrho U^\dagger). \tag{76}$$

  - Concave, i.e.,

$$S(p\varrho_1 + (1-p)\varrho_2) \geq pS(\varrho_1) + (1-p)S(\varrho_2). \tag{77}$$

Von Neumann entropy III

- Concavity (continued)
  - Let us prove the concavity. We need Klein's inequality. f is a convex function. Then,

    $$\mathrm{Tr}[f(A) - f(B)] \geq \mathrm{Tr}[(A - B)f'(B)]. \tag{78}$$

    Special case, $f(t) = t \ln t$. Then, $f'(t) = 1 + \ln t$. Hence,

    $$\mathrm{Tr}[A \ln A - B \ln B] \geq \mathrm{Tr}[(A - B) \ln B] + \mathrm{Tr}(A - B). \tag{79}$$

    Hence,

    $$\mathrm{Tr}[A \ln A - A \ln B] \geq \mathrm{Tr}(A - B) \tag{80}$$

    with equality if and only if $A = B$.

Von Neumann entropy III

- Concavity (continued)
  - Let us take $A = \varrho_1$ and ϱ_2 and $B = \varrho$. Then, we have

$$\mathrm{Tr}(\varrho_1 \ln \varrho_1 - \varrho_1 \ln \varrho) \geq \mathrm{Tr}(\varrho_1 - \varrho) = 0, \tag{81}$$

and

$$\mathrm{Tr}(\varrho_2 \ln \varrho_2 - \varrho_2 \ln \varrho) \geq \mathrm{Tr}(\varrho_2 - \varrho) = 0. \tag{82}$$

  - Then, we can write that

$$\begin{aligned} \mathrm{Tr}(\varrho \ln \varrho) &= p\mathrm{Tr}(\varrho_1 \ln \varrho) + (1-p)\mathrm{Tr}(\varrho_2 \ln \varrho) \\ &\leq p\mathrm{Tr}(\varrho_1 \ln \varrho_1) + (1-p)\mathrm{Tr}(\varrho_2 \ln \varrho_2). \end{aligned} \tag{83}$$

  - We used the book "Geometry of quantum states." ☐

Von Neumann entropy IV

- Further property
  - Additive for independent systems.

$$S(\varrho_1 \otimes \varrho_2) = S(\varrho_1) + S(\varrho_2). \tag{84}$$

Let us prove it. First we need that This can be shown as follows

$$\begin{aligned}
\log(\varrho_1 \otimes \varrho_2) &= \log\left(\sum_k \lambda_k |\Psi_k\rangle\langle\Psi_k| \otimes \sum_l \sigma_l |\Phi_l\rangle\langle\Phi_l|\right) \\
&= \sum_k \sum_l \log(\lambda_k \sigma_l) |\Psi_k\rangle\langle\Psi_k| \otimes |\Phi_l\rangle\langle\Phi_l| \\
&= \sum_k \sum_l [\log(\lambda_k) + \log(\sigma_l)] |\Psi_k\rangle\langle\Psi_k| \otimes |\Phi_l\rangle\langle\Phi_l| \\
&= \sum_k \log(\lambda_k) |\Psi_k\rangle\langle\Psi_k| \otimes \sum_l |\Phi_l\rangle\langle\Phi_l| \\
&+ \sum_k |\Psi_k\rangle\langle\Psi_k| \otimes \sum_l \log(\sigma_l) |\Phi_l\rangle\langle\Phi_l| \\
&= \log(\varrho_1) \otimes \mathbb{1} + \mathbb{1} \otimes \log(\varrho_2).
\end{aligned} \tag{85}$$

Von Neumann entropy V

- Additive for independent systems (continued)
- Thus, we have just derived that

$$\log(\varrho_1 \otimes \varrho_2) = \log(\varrho_1) \otimes \mathbb{1} + \mathbb{1} \otimes \log(\varrho_2). \tag{86}$$

- Hence,

$$\begin{aligned} S(\varrho_1 \otimes \varrho_2) &= -\mathrm{Tr}[\varrho_1 \otimes \varrho_2 \log(\varrho_1 \otimes \varrho_2)] \\ &= -\mathrm{Tr}\{\varrho_1 \otimes \varrho_2[\log(\varrho_1) \otimes \mathbb{1} + \mathbb{1} \otimes \log(\varrho_2)]\} \\ &= \mathrm{Tr}(\varrho_2) S(\varrho_1) + \mathrm{Tr}(\varrho_1) S(\varrho_2) \\ &= S(\varrho_1) + S(\varrho_2). \end{aligned} \tag{87}$$

□

Von Neumann entropy VI

- Properties (continued)
  - Subadditive,

$$S(\varrho_{12}) \leq S(\varrho_1) + S(\varrho_2) \equiv S(\varrho_1 \otimes \varrho_2). \tag{88}$$

  - Proof with Klein's inequality. [See "Geometry of quantum states"]
  - $A = \varrho_{12}$ and $B = \varrho_1 \otimes \varrho_2$ and we use again

$$\mathrm{Tr}(A \ln A - A \ln B) \geq \mathrm{Tr}(A - B). \tag{89}$$

Hence,

$$\mathrm{Tr}[\varrho_{12} \ln \varrho_{12} - \varrho_{12} \ln(\varrho_1 \otimes \varrho_2)] \geq \mathrm{Tr}(\varrho_{12} - \varrho_1 \otimes \varrho_2) = 0. \tag{90}$$

Hence,

$$\begin{aligned} \mathrm{Tr}(\varrho_{12} \ln \varrho_{12}) &\geq \mathrm{Tr}[\varrho_{12} \ln(\varrho_1 \otimes \varrho_2)] \\ &= \mathrm{Tr}\{\varrho_{12}[\ln(\varrho_1 \otimes \mathbb{1}) + \ln(\mathbb{1} \otimes \varrho_2)]\} \\ &= \mathrm{Tr}[\varrho_1 \ln(\varrho_1)] + \mathrm{Tr}[\varrho_2 \ln(\varrho_2)]. \end{aligned} \tag{91}$$

□

Von Neumann entropy VII

- Properties (continued)
  - Araki-Lieb inequality

$$|S(\varrho_1) - S(\varrho_2)| \leq S(\varrho_{12}). \tag{92}$$

  - Strongly subadditive,

$$S(\varrho_{123}) + S(\varrho_2) \leq S(\varrho_{12}) + S(\varrho_{23}). \tag{93}$$

    The matrices ϱ_1, ϱ_{12}, etc. reduced states.

  - Often used in condensed matter physics and field theory. See block entropy depending on the block size.

Von Neumann entropy VIII

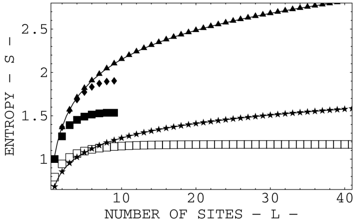

FIG. 1. *Noncritical entanglement* is characterized by a *saturation* of S_L as a function of the block size L: noncritical Ising chain (empty squares), $H_{XY}(a = 1.1, \gamma = 1)$; noncritical XXZ chain (filled squares), $H_{XXZ}(\Delta = 2.5, \lambda = 0)$. Instead, the entanglement of a block with a chain in a *critical* model displays a *logarithmic divergence* for large L: $S_L \sim \log_2(L)/6$ (stars) for the critical Ising chain, $H_{XY}(a = 1, \gamma = 1)$; $S_L \sim \log_2(L)/3$ (triangles) for the critical XX chain with no magnetic field, $H_{XY}(a = \infty, \gamma = 0)$; in a finite XXX chain of $N = 20$ spins without magnetic field (diamonds), $H_{XXZ}(\Delta = 1, \lambda = 0)$, S_L combines the critical logarithmic behavior for low L with a finite-chain saturation effect. We have also added the lines $[(c + \bar{c})/6][\log_2(L) + \pi]$ [cf. Eq. (12)] both for free conformal bosons (critical XX model) and free conformal fermions (critical Ising model) to highlight their remarkable agreement with the numerical diagonalization.

Figure from G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Entanglement in quantum critical phenomena, Phys. Rev. Lett. **90**, 227902 (2003).

Quantum conditional entropy

- Quantum conditional entropy ist is a generalization of the conditional entropy of classical information theory.

  $$S(A|B) = S(\varrho_{AB}) - S(\varrho_B). \tag{94}$$

  It can be negative, unlike in the classical case.

- If it is negative then the quantum state is entangled. Proof: for product states, we have

  $$S(A|B) = S(\varrho_A \otimes \varrho_B) - S(\varrho_B) = S(\varrho_A) + S(\varrho_B) - S(\varrho_B) = S(\varrho_B) \geq 0. \tag{95}$$

  For a mixture of product states (=separable states), we also have $S(A|B) \geq 0$ since $S(A|B)$ is concave in the state. If it is negative, then the state is not separable. In other words, the state is entangled.

Quantum mutual information

- Quantum mutual information is a measure of correlation between subsystems of a quantum state:

  $$I(A:B) = S(\varrho_A) + S(\varrho_B) - S(\varrho_{AB}) = S(\varrho_{AB} \| \varrho_A \otimes \varrho_B). \qquad (96)$$

  For product states, it is zero. It its non-negative due to the subadditivity of the entropy.

Quantum relative entropy

- The relative entropy is given as

$$S(\varrho\|\sigma) = -\mathrm{Tr}[\varrho(\log\sigma - \log\varrho)] = -\mathrm{Tr}(\varrho\log\sigma) - S. \qquad (97)$$

- Properties
  - $S(\varrho\|\sigma) \geq 0$.
  - $S(\varrho\|\sigma) = 0$ if and only if $\varrho = \sigma$.
  - Not symmetric $S(\varrho\|\sigma) \neq S(\sigma\|\varrho)$.
  - Sort of a distance between two quantum states.
  - Invariant under simultaneous change of basis: $S(\varrho\|\sigma) = S(U\varrho U^\dagger\|U\sigma U^\dagger)$.
  - $S(\varrho_1 \otimes \varrho_2\|\sigma_1 \otimes \sigma_2) = S(\varrho_1\|\sigma_1) + S(\varrho_2\|\sigma_2)$.

Quantum relative entropy II

- Further properties
  - For the relative entropy to the completely mixed state

    $$\varrho_{\text{completely mixed}} = \mathbb{1}/d \tag{98}$$

    we have

    $$S(\varrho||\varrho_{\text{completely mixed}}) = \log(d) - S(\varrho). \tag{99}$$

  - Monotonicity under CP maps (completely positive maps = physical maps). ϱ and σ evolves under the same CP map. $S(\varrho||\sigma)$ cannot increase.

Linear entropy

- The linear entropy is defined as
$$S_{\rm lin}(\varrho) = 1 - {\rm Tr}(\varrho^2) \equiv \langle \mathbb{1} - \varrho \rangle. \tag{100}$$
- It is often easier to obtain than the von Neumann entropy.
- Its relation to von Neumann entropy via the Mercator series is
$$-\langle \log \varrho \rangle = \langle \mathbb{1} - \varrho \rangle + \langle (\mathbb{1} - \varrho)^2 \rangle / 2 + \langle (\mathbb{1} - \varrho)^3 \rangle / 3 + ... \tag{101}$$
This is based on expanding
$$\log(\mathbb{1} - (\mathbb{1} - \varrho)) \tag{102}$$
using the Mercator series
$$\log(1 + x) = x - x^2/2 + x^3/3 - +... \tag{103}$$
Note that
$$\mathbb{1} - \varrho \geq 0. \tag{104}$$
Hence,
$$S \geq S_{\rm lin}. \tag{105}$$

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Fidelity

How to measure the distance between quantum states?

- Pure states: overlap square, $\langle\psi|\phi\rangle^2$.
- $\langle\psi|\phi\rangle = 0$ if and only if $|\psi\rangle = |\phi\rangle$.
- A pure state and a mixed state:

$$\mathrm{Tr}(|\Psi\rangle\langle\Psi|\sigma) = \langle\Psi|\sigma|\Psi\rangle. \tag{106}$$

- Two mixed states: more difficult

$$F(\varrho,\sigma) = \left(\mathrm{Tr}(\sqrt{\sqrt{\varrho}\sigma\sqrt{\varrho}})\right)^2. \tag{107}$$

  - $0 \le F(\varrho,\sigma) \le 1$.
  - $F(\varrho,\sigma) = 1$ if and only if $\varrho = \sigma$.
  - $F(\varrho,\sigma) = 0$ if ϱ and σ live on orthogonal subspaces.
  - Symmetric $F(\varrho,\sigma) = F(\sigma,\varrho)$.
  - Let us check consistency. If $\rho = |\Psi\rangle\langle\Psi|$ then $\sqrt{\varrho} = \varrho = |\Psi\rangle\langle\Psi|$. Then,

$$F(\varrho,\sigma) = \mathrm{Tr}(\sqrt{|\Psi\rangle\langle\Psi|\sigma|\Psi\rangle\langle\Psi|})^2 = \langle\Psi|\sigma|\Psi\rangle\mathrm{Tr}(\sqrt{|\Psi\rangle\langle\Psi|})^2 = \langle\Psi|\sigma|\Psi\rangle. \tag{108}$$

Hence, we got back the formula for the simpler case.

Fidelity II

- Defining the Fidelity with a maximum over purifications

$$F(\varrho,\sigma) = \max_{|\Psi_\sigma\rangle} |\langle\Psi_\varrho|\Psi_\sigma\rangle|^2. \tag{109}$$

- $|\Psi_\varrho\rangle$ is a purification of ϱ, $|\Psi_\sigma\rangle$ is a purification of σ,

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Distances I

- The Bures distance is defined as We have

$$D_B(\varrho,\sigma)^2 = 2\left[1 - \sqrt{F(\varrho,\sigma)}\right], \tag{110}$$

  where F is the fidelity.

- Schatten norm

$$||A||_p = \mathrm{Tr}(|A|^p)^{\frac{1}{p}}. \tag{111}$$

  where

$$||A||_1 \geq ||A||_2. \tag{112}$$

Distances II

- The Hilbert-Schmidt norm is defined as

$$||A||_{\mathrm{HS}} = ||A||_2 = \sum_{mn} |A_{mn}|^2. \tag{113}$$

  For a Hermitian A, we have

$$||A||_{\mathrm{HS}} = \sqrt{\sum_n |\lambda_n|^2}. \tag{114}$$

- Then, the Hilbert-Schmidt distance is

$$D_{\mathrm{HS}}(\varrho, \sigma)^2 = ||\varrho - \sigma||_{\mathrm{HS}}^2 = \mathrm{Tr}[(\varrho - \sigma)^2]. \tag{115}$$

Distances III

- The trace norm is defined as

$$\|A\|_{\mathrm{tr}} = \|A\|_1 = \mathrm{Tr}(\sqrt{A^\dagger A}) = \mathrm{Tr}(|A|) = \sum_n |\lambda_n|. \tag{116}$$

For a Hermitian A, we have

$$\|A\|_{\mathrm{tr}} = \sum_n |\lambda_n|. \tag{117}$$

- Then, the trace distance is

$$D_{\mathrm{tr}}(\varrho, \sigma) = \frac{1}{2}\|\varrho - \sigma\|_{\mathrm{tr}} = \frac{1}{2}\mathrm{tr}[\|\varrho - \sigma\|]. \tag{118}$$

Hence,

$$0 \leq D_{\mathrm{tr}}(\varrho, \sigma) \leq 1. \tag{119}$$