Density Matrix and State Tomography

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QSIT: Student's presentation

Contents

The purpose of the density matrix formalism

So far in the lecture, we represented the state of a quantum mechanical system with its *state vector*. Nevertheless, it can be useful to represent it in a different way, such that:

- we can treat conveniently the case where the state of the system is only partially known
- we can describe subsystems of a composite quantum mechanical system
- this formalism is equivalent to the state vector/wave function formalism. In particular, it is compatible with the postulates of quantum mechanics

$\Rightarrow$ **Density matrix formalism**

Definition of the density matrix

Consider a quantum system which is in a state $|\Psi_i\rangle \in \mathcal{H}$ with probability p_i. Let's have a look at the expectation value of an arbitrary observable $\hat{A}$:

$$\left\langle \hat{A} \right\rangle = \sum_i p_i \langle \Psi_i | \hat{A} | \Psi_i \rangle .$$

Using a complete orthonormal basis $\{\varphi_i\}$, we can write

$$\left\langle \hat{A} \right\rangle = \sum_{n,m} \langle \varphi_n | \hat{A} | \varphi_m \rangle \langle \varphi_m | \left(\sum_i p_i | \Psi_i \rangle \langle \Psi_i | \right) | \varphi_n \rangle .$$

We can therefore define the *density matrix* or *density operator*

$$\hat{\rho} = \sum_i p_i | \Psi_i \rangle \langle \Psi_i | \Longrightarrow \left\langle \hat{A} \right\rangle = \mathrm{Tr}(\hat{\rho}\hat{A}).$$

Pure states and mixed states

We distinguish between two different types of states. A *pure state* can be written as $\hat{\rho} = |\Psi\rangle\langle\Psi|$, whereas a *mixed state* is expressed as

$$\hat{\rho} = \sum_i p_i |\Psi_i\rangle\langle\Psi_i| \quad , p_i < 1.$$

A mixed state is therefore a *statistical ensemble* of pure states. As a simple example, consider an ensemble of spins that can be in the states $\{ |\uparrow\rangle, |\downarrow\rangle \}$. A pure state can be expressed as $\hat{\rho}_p = |\uparrow\rangle\langle\uparrow|$, a mixed state is for instance $\hat{\rho}_m = (|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|)/2$. Explicitly, the density matrices are

$$\hat{\rho}_p = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad \hat{\rho}_m = \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}.$$

It is easy to verify that $\hat{\rho}_p$ has eigenvalues 0 and 1, whereas $\hat{\rho}_m$ has eigenvalues 1/2 and 1/2. Furthermore, we have $\mathrm{Tr}(\hat{\rho}_p) = \mathrm{Tr}(\hat{\rho}_m) = 1$ but $\mathrm{Tr}(\hat{\rho}_p^2) = 1$, $\mathrm{Tr}(\hat{\rho}_m^2) = 1/2$.

A further example of a density matrix with basis change

Consider two states in the basis $\{ |0\rangle , |1\rangle \}$. We now change the basis and go to: $|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}$. We can define in the new basis the following state: $\hat{\rho}_p = |+\rangle \langle +|$, which can be explicitly written in the basis $\{ |+\rangle , |-\rangle \}$

$$\hat{\rho}_p = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}.$$

In the $\{ |0\rangle , |1\rangle \}$ basis, the density operators can be explicitly written as

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

$$\Rightarrow \hat{\rho}_p = \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix}.$$

Measurements on a quantum system

In quantum mechanics, measurements are performed through *measurement operators* M_m. For a system in the initial state $|\Psi_i\rangle$, the probability to get an outcome m is

$$p(m|i) = \langle\Psi_i| M_m^\dagger M_m |\Psi_i\rangle = \mathrm{Tr}(M_m^\dagger M_m |\Psi_i\rangle\langle\Psi_i|).$$

Therefore, the probability to get an outcome m after the measurement is

$$p(m) = \sum_i p_i \langle\Psi_i| M_m^\dagger M_m |\Psi_i\rangle = \mathrm{Tr}(M_m^\dagger M_m \hat{\rho})$$

and the state after measuring m becomes

$$|\Psi_i^m\rangle = \frac{M_m |\Psi_i\rangle}{\sqrt{\langle\Psi_i| M_m^\dagger M_m |\Psi_i\rangle}} \Rightarrow \hat{\rho}_m = \frac{M_m \hat{\rho} M_m^\dagger}{\mathrm{Tr}(M_m^\dagger M_m \hat{\rho})}.$$

Example of a measurement operator

As an example, consider the operator $M_1 = |1\rangle\langle 1|$ for the density matrix $\hat{\rho} = a|0\rangle\langle 0| + b|1\rangle\langle 1|$. The probability to measure the state $|1\rangle$ is

$$p(1) = \mathrm{Tr}(M_1^\dagger M_1 \hat{\rho}) = \mathrm{Tr}(|1\rangle \underbrace{\langle 1||1\rangle}_{\mathrm{I}} \langle 1| (p_0 |0\rangle\langle 0| + p_1 |1\rangle\langle 1|)).$$

$$\Rightarrow p(1) = \mathrm{Tr}(|1\rangle\langle 1| p_1) = p_1.$$

Some properties of the density matrix

Using the definition of the density matrix, it is easy to show the following properties:

- $Tr(\hat{\rho}) = 1$
- $\hat{\rho}$ *is positive definite*
- $\hat{\rho} = \hat{\rho}^\dagger$
- $Tr(\hat{\rho}^2) \leq 1$

The time evolution of the density matrix is obtained by applying the Schroedinger equation to the definition of $\hat{\rho}$. One obtains the *Liouville-von Neumann equation*:

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho} = \left[\hat{H}, \hat{\rho}\right].$$

Reduced density matrix

Suppose we have systems A and B described by the density matrix $\hat{\rho}_{AB}$. Then, we can obtain the *reduced density matrix* by taking the *partial trace* of $\hat{\rho}_{AB}$, e.g.

$$\hat{\rho}_A = \mathrm{Tr}_B(\hat{\rho}_{AB}),$$

where we extracted the information about system A. The partial trace operation is defined as

$$\mathrm{Tr}_B(|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|) = |a_1\rangle\langle a_2| \,\mathrm{Tr}(|b_1\rangle\langle b_2|).$$

Example: consider two-level system in excited state (e.g. an atom). We have the systems: A: atomic state, B: photon-field state. Given we have no knowledge about the photon state, we get the density matrix of the atom by taking the partial trace over B of the density matrix of the full system.

The postulates of Quantum Mechanics in the Density Matrix formalism

We find that the four following postulates are compatible with the ones given in lecture:

1. *States:* The states of a physical system are represented as density operators acting on a Hilbert space $\mathcal{H}$.
2. *Evolution:* The Liouville-von Neumann equation governs the dynamics of the quantum system.
3. *Measurement:* Measurements on a quantum system are represented by measurement operators, acting on the state space of the system being measured.
4. *Composition:* The states of a composite quantum system with state spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ are represented as density operators on $\mathcal{H}_A \otimes \mathcal{H}_B$

QUANTUM STATE TOMOGRAPHY

Quantum state Tomography

- Classical tomography
- QM tomography
- Tools: Stokes Parameters
- Different Approaches for tomography:
  - Quantum tomography
  - Maximum likelihood estimation (MLE)
  - Applications:
  - Quantum process tomography
- Examples of physical implementation
- Conclusion

Classical Tomography

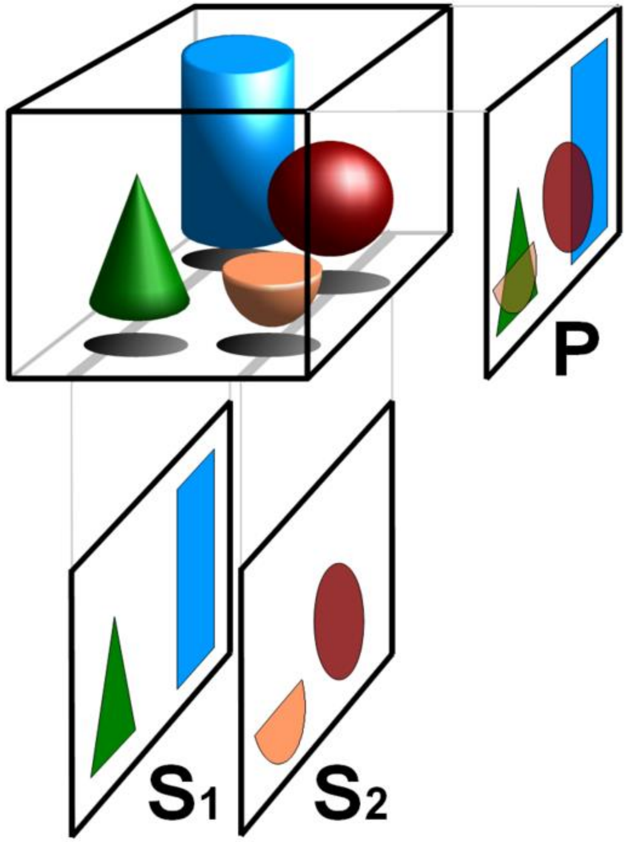


Fig.1 Basic principle of tomography – projected plane image of the original object [1]

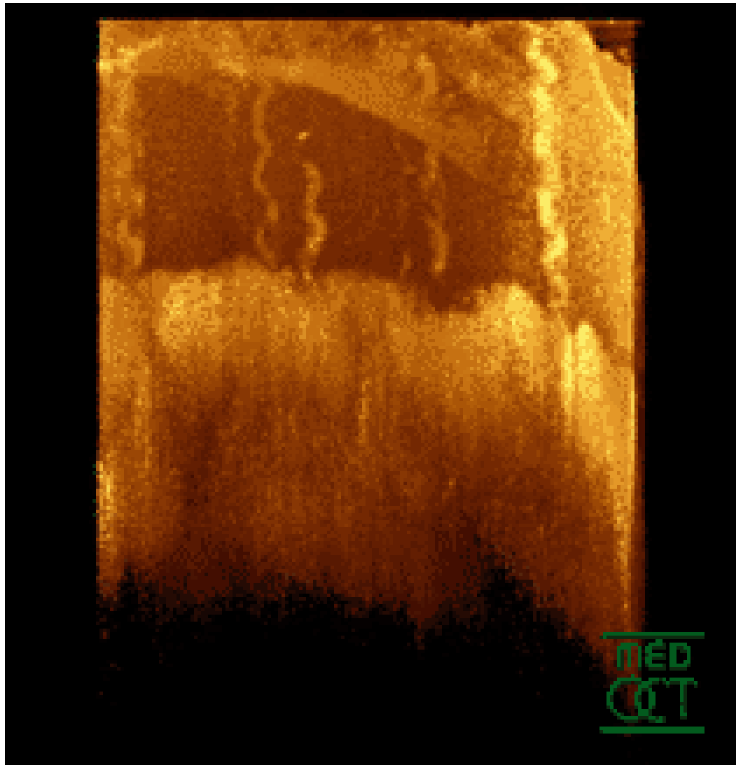


Fig.2 Optical coherence reconstruction of a fingertip [2]

- Tomography: Derived from Ancient Greeks, τόμος γράφω *tomos*, "slice, section" and *graphō*, "to write"
- By collecting many 2D sectional images→ reconstruct the appearance of the object.
- Classical system: robust against measurements.

What is Quantum tomography?

- QM tomography is a process which reconstructs the state of an unknown quantum source by repeated measurements.
- 3rd QM postulate: Collapse Rule → Must prepare many copies of the same state for repeated measurements.
- Perfect identified state is said to form "quorum"
- In real experiment, measurements are non-ideal.
- Always subject to noise.

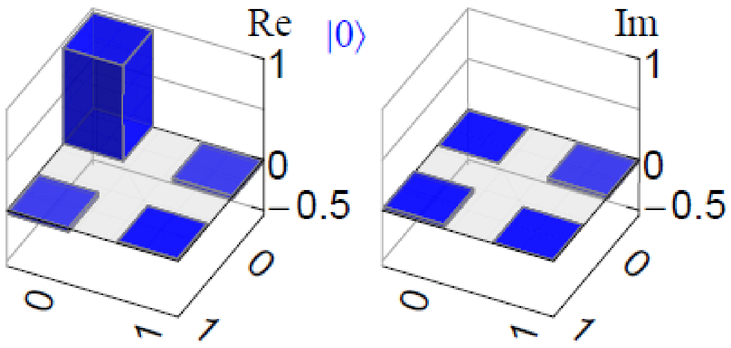


Fig.3 Reconstruction of density matrix [3]

Tools : Stokes parameters

Density matrix for single qubit relate to Stokes parameter by:

$$\hat{\rho} = \frac{1}{2}\sum_{i=0}^{3} S_i \hat{\sigma}_i$$

$$\hat{\rho} = \sum_i P_i |\psi_i\rangle\langle\psi_i| = \begin{matrix} & \langle 0| & \langle 1| \\ |0\rangle & A & Ce^{i\phi} \\ |1\rangle & Ce^{-i\phi} & B \end{matrix}$$

$$\hat{\sigma}_0 \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \hat{\sigma}_1 \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \hat{\sigma}_2 \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \hat{\sigma}_3 \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

σ_i: Pauli matrices

Stokes (S) parameter are defined by: $|H\rangle = |0\rangle, |V\rangle = |1\rangle$

$$S_i \equiv \mathrm{Tr}\{\hat{\sigma}_i \hat{\rho}\}$$

$$S_0 = P_{|0\rangle} + P_{|1\rangle}$$
$$S_1 = P_{\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)} - P_{\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)}$$
$$S_2 = P_{\frac{1}{\sqrt{2}}(|0\rangle+i|1\rangle)} - P_{\frac{1}{\sqrt{2}}(|0\rangle-i|1\rangle)}$$
$$S_3 = P_{|0\rangle} - P_{|1\rangle},$$

where $P_{|\psi\rangle}$ is the probability to measure the state $|\psi\rangle$

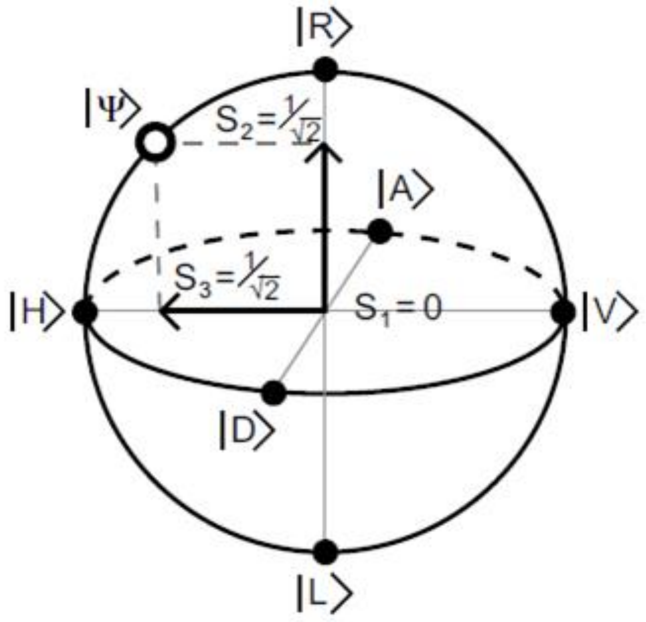


Fig.4 The Bloch Poincaré sphere, equivalent to a rotated Bloch sphere for a qubit [4]

Example of photon case : Single Qubit tomography

Stokes parameter fully characterize the polarization of the light [4]

Eg. Consider an input state $|H\rangle = |0\rangle$

$$\begin{aligned} S_0 &= \text{Tr}\{\sigma_0 \rho_H\} = 1 \\ S_1 &= \text{Tr}\{\sigma_1 \rho_H\} = 0 \\ S_2 &= \text{Tr}\{\sigma_2 \rho_H\} = 0 \\ S_3 &= \text{Tr}\{\sigma_3 \rho_H\} = 1, \end{aligned} \longrightarrow \rho_H = (\sigma_0 + \sigma_3) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

Generalisation to n-qubits

- Generalization to n-qubit is straight-forward, the density matrix of a n-qubit state can be written as:

$$\hat{\rho} = \frac{1}{2^n} \sum_{i_1, i_2, \ldots i_n = 0}^{3} S_{i_1, i_2, \ldots i_n} \hat{\sigma}_{i_1} \otimes \hat{\sigma}_{i_2} \otimes \ldots \otimes \hat{\sigma}_{i_n}$$

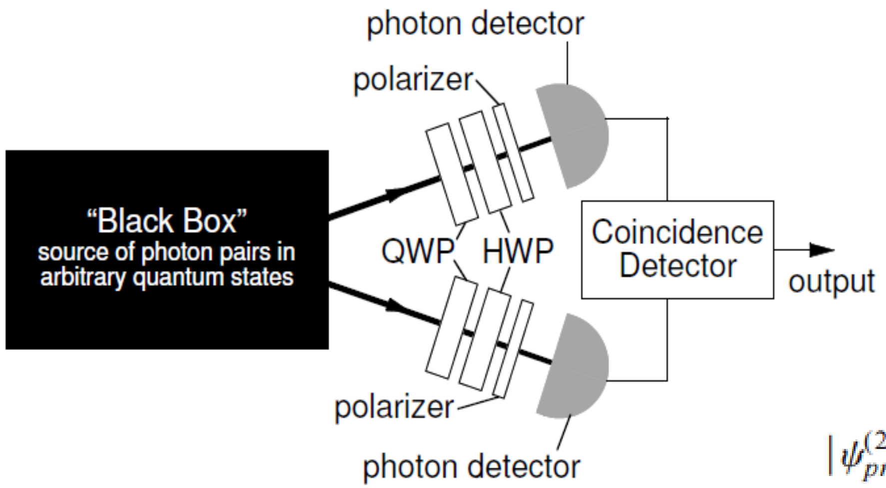
now, one would have 4^n - 1 real parameters (due to normalization).

Eg. For n =2, 4 parameters for

$$|\psi\rangle = \alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle$$

$$\hat{\rho} = \begin{matrix} & \langle HH| & \langle HV| & \langle VH| & \langle VV| \\ |HH\rangle \\ |HV\rangle \\ |VH\rangle \\ |VV\rangle \end{matrix} \begin{pmatrix} A_1 & B_1 e^{i\phi_1} & B_2 e^{i\phi_2} & B_3 e^{i\phi_3} \\ B_1 e^{-i\phi_1} & A_2 & B_4 e^{i\phi_4} & B_5 e^{i\phi_5} \\ B_2 e^{-i\phi_2} & B_4 e^{-i\phi_4} & A_3 & B_6 e^{i\phi_6} \\ B_3 e^{-i\phi_3} & B_5 e^{-i\phi_5} & B_6 e^{-i\phi_6} & A_4 \end{pmatrix}$$

Photon polarization experiment



$$\hat{U}_{QWP}(q) = \frac{1}{\sqrt{2}}\begin{pmatrix} i-\cos(2q) & \sin(2q) \\ \sin(2q) & i+\cos(2q) \end{pmatrix}$$

$$\hat{U}_{HWP}(q) = \begin{pmatrix} \cos(2h) & -\sin(2h) \\ -\sin(2h) & -\cos(2h) \end{pmatrix}.$$

$$|\psi^{(1)}_{proj}(h,q)\rangle = \hat{U}_{QWP}(q)\cdot\hat{U}_{HWP}(h)\cdot\begin{pmatrix}0\\1\end{pmatrix} = a(h,q)|H\rangle + b(h,q)|V\rangle,$$

$$\begin{aligned}|\psi^{(2)}_{proj}(h_1,q_1,h_2,q_2)\rangle &= |\psi^{(1)}_{proj}(h_1,q_1)\rangle\otimes|\psi^{(1)}_{proj}(h_2,q_2)\rangle \\ &= a(h_1,q_1)a(h_2,q_2)|HH\rangle \\ &\quad + a(h_1,q_1)b(h_2,q_2)|HV\rangle \\ &\quad + b(h_1,q_1)a(h_2,q_2)|VH\rangle \\ &\quad + b(h_1,q_1)b(h_2,q_2)|VV\rangle.\end{aligned}$$

- Black box consists of a non-linear crystal for parametric down conversion, producing photon pairs of qubits in an arbitrary state of polarization.

- Three optical elements: a polarizer (which only allows vertical light), quarter-wave plate and a half-wave plate.

- The angles of both axes in QWP and HWP on both arms provide 4 degrees of freedom (q1,q2,h1,h2), i.e. a 2 qubit state.

Photon polarization experiment

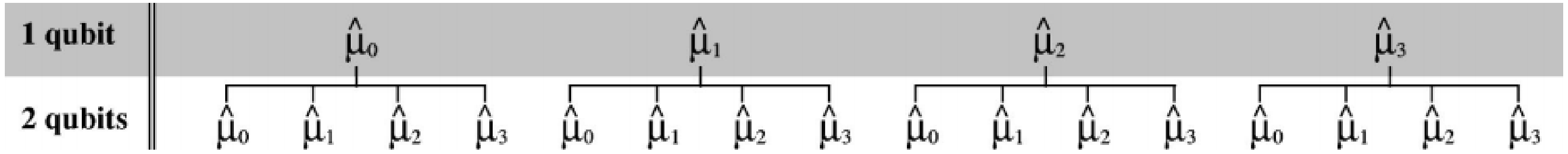
ν	Mode 1	Mode 2	h_1	q_1	h_2	q_2
1	$\|H\rangle$	$\|H\rangle$	45°	0	45°	0
2	$\|H\rangle$	$\|V\rangle$	45°	0	0	0
3	$\|V\rangle$	$\|V\rangle$	0	0	0	0
4	$\|V\rangle$	$\|H\rangle$	0	0	45°	0
5	$\|R\rangle$	$\|H\rangle$	22.5°	0	45°	0
6	$\|R\rangle$	$\|V\rangle$	22.5°	0	0	0
7	$\|D\rangle$	$\|V\rangle$	22.5°	45°	0	0
8	$\|D\rangle$	$\|H\rangle$	22.5°	45°	45°	0
9	$\|D\rangle$	$\|R\rangle$	22.5°	45°	22.5°	0
10	$\|D\rangle$	$\|D\rangle$	22.5°	45°	22.5°	45°
11	$\|R\rangle$	$\|D\rangle$	22.5°	0	22.5°	45°
12	$\|H\rangle$	$\|D\rangle$	45°	0	22.5°	45°
13	$\|V\rangle$	$\|D\rangle$	0	0	22.5°	45°
14	$\|V\rangle$	$\|L\rangle$	0	0	22.5°	90°
15	$\|H\rangle$	$\|L\rangle$	45°	0	22.5°	90°
16	$\|R\rangle$	$\|L\rangle$	22.5°	0	22.5°	90°

Measurement table of 16 measurements, in different basis.

$$S_0 = P_{|0\rangle} + P_{|1\rangle}$$
$$S_1 = P_{\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)} - P_{\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)}$$
$$S_2 = P_{\frac{1}{\sqrt{2}}(|0\rangle+i|1\rangle)} - P_{\frac{1}{\sqrt{2}}(|0\rangle-i|1\rangle)}$$
$$S_3 = P_{|0\rangle} - P_{|1\rangle},$$

$$|D\rangle \equiv (|H\rangle + |V\rangle)/\sqrt{2},$$
$$|A\rangle \equiv (|H\rangle - |V\rangle)/\sqrt{2},$$
$$|R\rangle \equiv (|H\rangle + i|V\rangle)/\sqrt{2},$$
$$|L\rangle \equiv (|H\rangle - i|V\rangle)/\sqrt{2}.$$

E.g. Measure S_2 by projecting onto $|R\rangle$ and $|L\rangle$



Coincident count for 2 qubits.

Graphical representation of QM tomography result

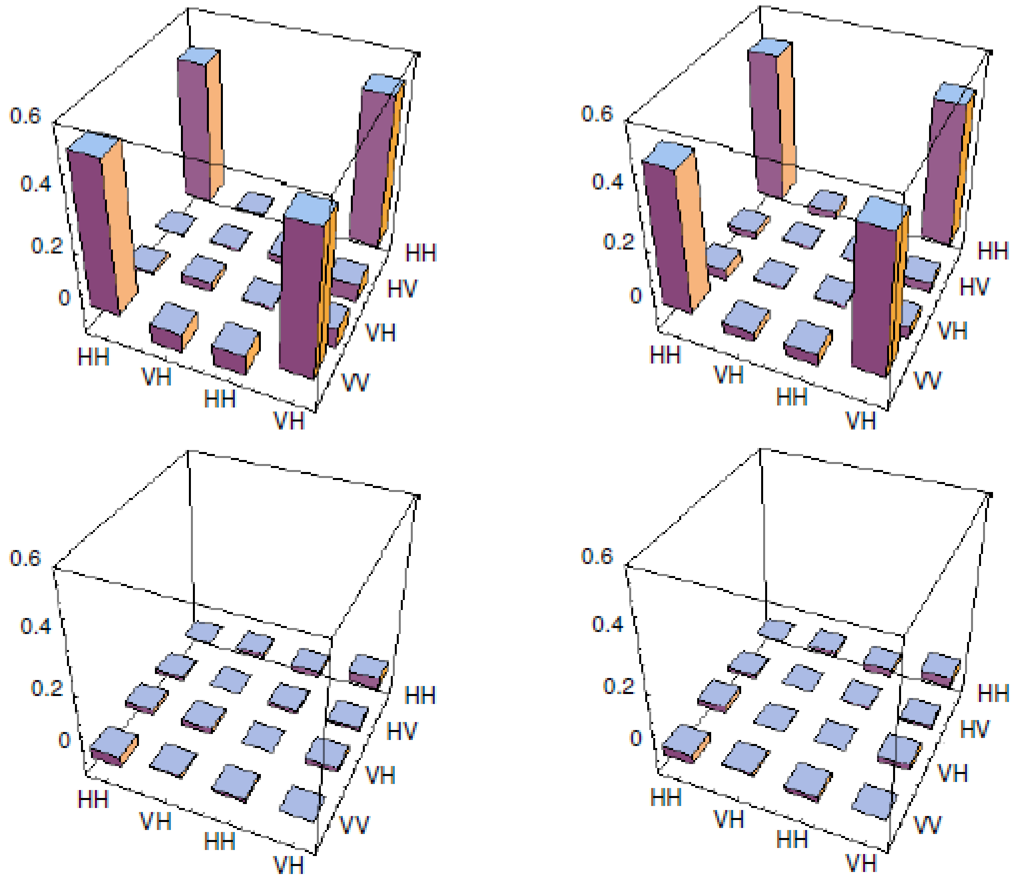


Fig.6 Graphical representation of the density matrix obtained by linear tomography and maximum likelihood technique.

This figure represents a bell-state.

Quantum tomography

- Using ideal quantum tomography, If a measurement $P = \{\hat{E}_1 \ldots \hat{E}_N\}$ is performed on a system in state ρ, then the probability of observing $\hat{E}_i$ is $p_i = Tr(\hat{E}_i \rho)$[5]
- No measurement can reveal the true probability of each event, but the frequencies of occurrence by performing repeated measurements
- In the ideal case, gather enough statistics $N \rightarrow \infty$ → form a quorum.

$$\mathrm{Tr}\left(\hat{\rho}_{\mathrm{tomo}} E_i\right) = \frac{n_i}{N}$$

- Subject to noise → Negative eigenvalues (Physical system must be a positive definite matrix!), same problem exist in MLE.
- Problems get worse for larger Hilbert space

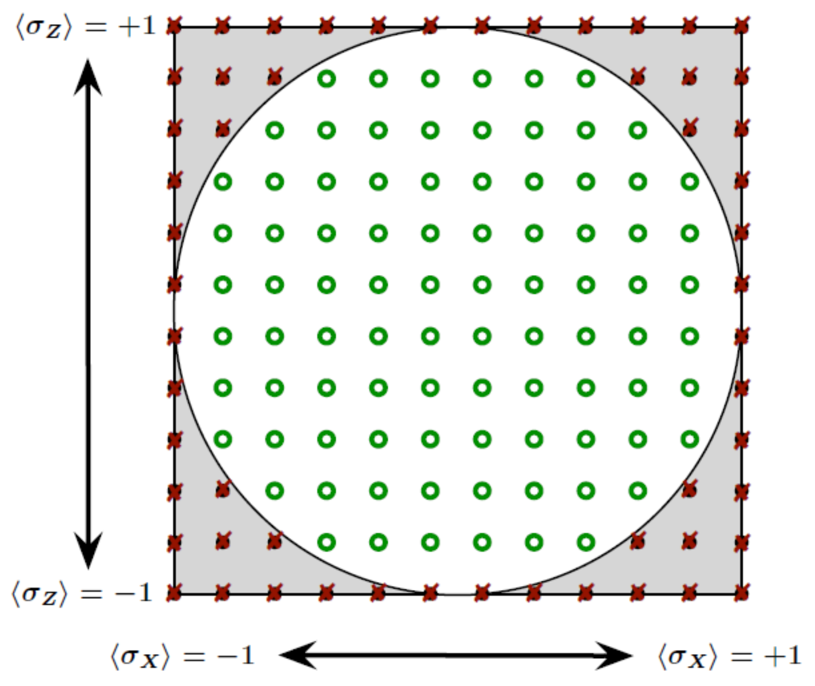


Fig.4 A cross section of the Bloch cube, green dots represent positive physical states of 144 ρ_{tomo}, red spots are unphysical, N = 11 measurements.

Example – extreme case

If Alice only perform measurement of along each polarization basis, i.e. alternating between horizontal $|H\rangle$, right circular $|R\rangle$ and diagonal $|D\rangle$ polarization, and imagine she obtained:

$$|D\rangle \equiv (|H\rangle + |V\rangle)/\sqrt{2},$$
$$|A\rangle \equiv (|H\rangle - |V\rangle)/\sqrt{2},$$
$$|R\rangle \equiv (|H\rangle + i|V\rangle)/\sqrt{2},$$
$$|L\rangle \equiv (|H\rangle - i|V\rangle)/\sqrt{2}.$$

Expectation of the outcome: $\langle\sigma_x\rangle = \langle\sigma_y\rangle = \langle\sigma_z\rangle = 1$

$$\hat{\rho}_{\text{tomo}} = \begin{pmatrix} 1 & \frac{1+i}{2} \\ \frac{1-i}{2} & 0 \end{pmatrix}$$

More qubits ? ⟶

Eigenvalue: $\lambda = \frac{1-\sqrt{2}}{2} \approx -0.207$

Negative eigenvalue ! (unphysical)

- This demonstrates that tomography only matches the observed frequency of each measurement outcome, and pays no respect to positivity, physical state.

Problem gets worse in larger Hilbert Space!, probability of at least one negative eigenvalue scales with dimension d !

Discussion

- Up to now, the tools developed so far implicity allow infinitely set of ideal data set. When applying this linear tomography technique, the probabilities obtained in real experiment can be contradictory and even physically impossible → necessary to adopt a new approach to return a legitimate density matrix !

- Which can include experimental errors, and deal with the unphysical negative eigenvalues.

Maximum likelihood Estimation Algorithm [6]

(i) Generate a density matrix that must be positive, Hermitian to be physical

(ii) Introduce a likelihood function which quantifies how "good" the density matrix fits the data

(iii) Optimize the likelihood function with standard numerical technique, e.g. Monte Carlo method.

Example of MLE

In general, the measurement outcome follows a Gaussian distribution in large N [3]

$$p(\mathrm{m}_k|\hat{\rho}) = \frac{1}{\sqrt{2\pi}\sigma_k} e^{-\left(\mathrm{m}_k - \mathrm{Tr}(\hat{\mathcal{M}}_k \hat{\rho})\right)^2/(2\sigma_k^2)}$$

$$\hat{T}(t) = \begin{pmatrix} t_1 & 0 & 0 & 0 \\ t_5 + it_6 & t_2 & 0 & 0 \\ t_{11} + it_{12} & t_7 + it_8 & t_3 & 0 \\ t_{15} + it_{16} & t_{13} + it_{14} & t_9 + it_{10} & t_4 \end{pmatrix}$$

$$\hat{\rho}_p(t) = \hat{T}^\dagger(t)\hat{T}(t)/\mathrm{Tr}\{\hat{T}^\dagger(t)\hat{T}(t)\}$$

$$\mathcal{L} = \prod_k \frac{1}{\sqrt{2\pi}\sigma_k} e^{-(\mathrm{m}_k - \mathrm{Tr}(\hat{\mathcal{M}}_k \hat{\rho}))^2/(2\sigma_k^2)}$$

Finding the minimum of the log-likelihood function

$$\mathcal{L}_{\log} = \sum_k \frac{1}{2\sigma_k^2}(\mathrm{m}_k - \mathrm{Tr}(\hat{\mathcal{M}}_k \hat{\rho}))^2$$

$where, \widehat{M_k}$ is the $k\ th$ measurement operator, m_k is the measurement outcome.

σ_k: standard deviation suppressed as $1/\sqrt{N}$.

A convenient choice of $\hat{T}$ tridiagonal matrix, would allow the “guess” density matrix to be invertible.

Maximum likelihood Estimation (MLE) Discussion

Statistical approach [4,5]:

- Best "Fit" of the density matrix as a parameters to maximize the probabilities of observing the measured outcomes.
- i.e. Maximizing the likelihood function, where M_i = measurement operator of $i\ th$ observation, and M_i be the set of measurement frequency record.

$$\mathcal{L}(\hat{\rho}) = p(\mathcal{M}|\hat{\rho}) = \prod_i \left(\mathrm{Tr}[M_i\hat{\rho}]\right)$$

- Suffer from zero eigenvalue (inherited from quantum tomography) i.e. rank deficient.

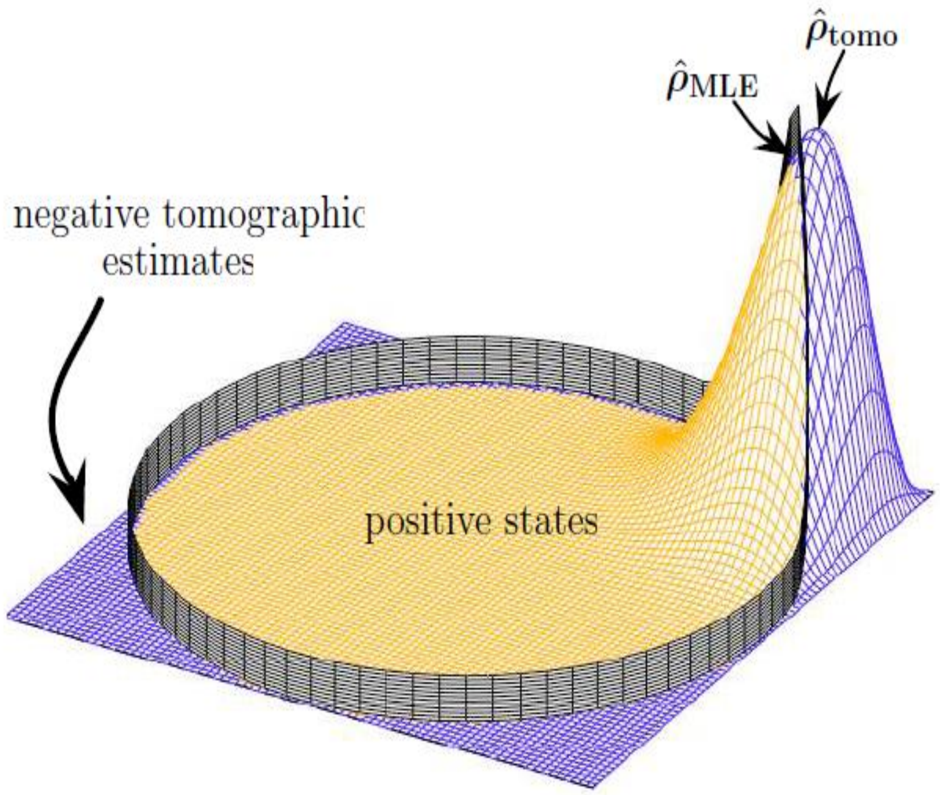


Fig.5 An example of likelihood function with constrained maximum x, z axis: $\langle\sigma_x\rangle$, $\langle\sigma_z\rangle$. [5]

Application: Quantum Process tomography

Unknown quantum operation

PREPARATION		MEASUREMENT
$\|0\rangle$	$\rightarrow$	$\chi(\|0\rangle)$
$\|1\rangle$	$\rightarrow$	$\chi(\|1\rangle)$
$\frac{1}{\sqrt{2}}(\|0\rangle + \|1\rangle)$	$\rightarrow$	$\chi\left(\frac{1}{\sqrt{2}}(\|0\rangle + \|1\rangle)\right)$
$\frac{1}{\sqrt{2}}(\|0\rangle - i\|1\rangle)$	$\rightarrow$	$\chi\left(\frac{1}{\sqrt{2}}(\|0\rangle - i\|1\rangle)\right)$

Quantum state tomography can be very useful,

- identifying an unknown quantum source
- verifying the fidelity of a known prepared state
- It can also be used to identify the quantum operation of a system.

Appendix

Non-orthogonal projective measurements:

Can also define a more general S-like parameter to perform non-orthogonal basis measurement:

$$T_i = \mathrm{Tr}\left\{\hat{\tau}_i \hat{\rho}\right\} \quad \text{where} \quad \hat{\tau}_i \equiv |\psi_i\rangle\langle\psi_i| - |\psi_i^{\perp}\rangle\langle\psi_i^{\perp}|$$

$$\hat{\rho} \neq \frac{1}{2}\sum_{i=0}^{3} T_i \hat{\tau}_i$$

S parameters and T parameters are related by a linear transformation

$$\begin{pmatrix} T_0 \\ T_1 \\ T_2 \\ T_3 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \mathrm{Tr}\{\hat{\tau}_0\hat{\sigma}_0\} & \mathrm{Tr}\{\hat{\tau}_0\hat{\sigma}_1\} & \mathrm{Tr}\{\hat{\tau}_0\hat{\sigma}_2\} & \mathrm{Tr}\{\hat{\tau}_0\hat{\sigma}_3\} \\ \mathrm{Tr}\{\hat{\tau}_1\hat{\sigma}_0\} & \mathrm{Tr}\{\hat{\tau}_1\hat{\sigma}_1\} & \mathrm{Tr}\{\hat{\tau}_1\hat{\sigma}_2\} & \mathrm{Tr}\{\hat{\tau}_1\hat{\sigma}_3\} \\ \mathrm{Tr}\{\hat{\tau}_2\hat{\sigma}_0\} & \mathrm{Tr}\{\hat{\tau}_2\hat{\sigma}_1\} & \mathrm{Tr}\{\hat{\tau}_2\hat{\sigma}_2\} & \mathrm{Tr}\{\hat{\tau}_2\hat{\sigma}_3\} \\ \mathrm{Tr}\{\hat{\tau}_3\hat{\sigma}_0\} & \mathrm{Tr}\{\hat{\tau}_3\hat{\sigma}_1\} & \mathrm{Tr}\{\hat{\tau}_3\hat{\sigma}_2\} & \mathrm{Tr}\{\hat{\tau}_3\hat{\sigma}_3\} \end{pmatrix} \begin{pmatrix} S_0 \\ S_1 \\ S_2 \\ S_3 \end{pmatrix}$$

Bayesian Mean Estimation (BME)

- Best estimate is an average over all states ρ consistent with the data, wighted by their likelihood. (Full rank)
- Consider all possibilities. MLE identifies the best fit to observed data, nevertheless, many nearby states are equally likely, and should be included as alternatives.
- Demand error bars, sensible choice of error bars around region of plausible states. $\hat{\rho} \pm \Delta\rho.$
- Optimize accuracy with different metrics, such as fidelity, relative entropy will favour different estimation procedures.

Bayesian Mean Estimation algorithm

- Use the measured data to generate a likelihood function $\mathcal{L}(\hat{\rho}) = p(\mathcal{M}|\hat{\rho})$ which quantifies the relative plausibility of different state assignments.
- Choose a prior distribution over states $\pi_0(\hat{\rho})\mathrm{d}\hat{\rho}$ (represent the estimator's ignorance), in general "Uniform".
- Multiply prior by likelihood, to obtain a posterior distribution.

$$\pi_f(\hat{\rho})\mathrm{d}\hat{\rho} \propto \mathcal{L}(\hat{\rho})\pi_0(\hat{\rho})\mathrm{d}\hat{\rho}$$

which represents the estimator's knowledge.

- Report the mean of this posterior

$$\hat{\rho}_{\mathrm{BME}} = \int \hat{\rho}\pi_f(\rho)\mathrm{d}\hat{\rho}$$

Linear inversion

Born 's rule states $P(E_i|\rho) = Tr(\widehat{E}_i\rho)$, $\widehat{E}_i$ being any measurement operator.

one can write density matrix e.g. 4x4 as a 16 element column vectors, with S,T being linear operators $S \cdot T = \mathrm{Tr}[S^\dagger T] = \vec{S}^\dagger \vec{T}$

$$A\vec{\rho} = \begin{pmatrix} E_1^\dagger \vec{\rho} \\ E_2^\dagger \vec{\rho} \\ E_3^\dagger \vec{\rho} \\ \vdots \end{pmatrix} = \begin{pmatrix} E_1 \cdot \rho \\ E_2 \cdot \rho \\ E_3 \cdot \rho \\ \vdots \end{pmatrix} = \begin{pmatrix} \mathrm{P}(E_1|\rho) \\ \mathrm{P}(E_2|\rho) \\ \mathrm{P}(E_3|\rho) \\ \vdots \end{pmatrix} \approx \begin{pmatrix} p_1 \\ p_2 \\ p_3 \\ \vdots \end{pmatrix} = \vec{p}$$

$$A^T A\vec{\rho} = A^T\vec{p}$$

$$\vec{\rho} = (A^T A)^{-1} A^T \vec{p}$$

Problem amounts to inverting this matrix

$$(A^T A)^{-1}$$

Reference

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