DENSITY MATRIX & PARTIAL DENSITY MATRIX.

I. STATISTICAL MIXTURES

The density matrix generalises the notion of state vector $|\psi\rangle \in \mathcal{H}$. It is needed in two physical settings:

1) To describe statistical mixtures.
2) To describe part of a system, in other words to describe a part which is not isolated.

We first introduce the first setting. In order to go to the second setting we will have to make a mathematical digression to the notion of partial trace.

Statistical mixtures.

Imagine a collection of N particles (or N quantum degrees of freedom, qubits, photon polarisations, spins, ...) found in possible states

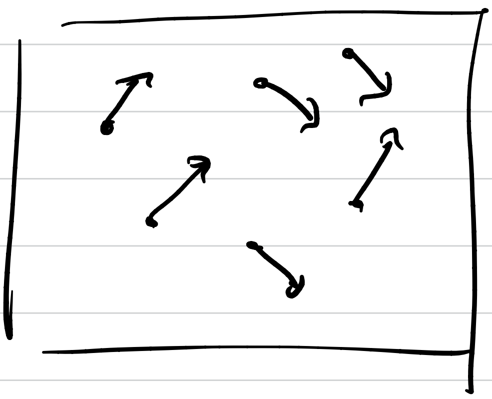
$$|\varphi_1\rangle, |\varphi_2\rangle, \dots, |\varphi_K\rangle \in \mathcal{H}$$

in corresponding proportions (fractions)

$$p_1, p_2, \dots, p_K.$$

Here $0 \leq p_i \leq 1$, $\sum_{i=1}^{K} p_i = 1$ are probabilities.

In other words we imagine a "gas" with:



$p_1 N$ particles in state $|\varphi_1\rangle$

$p_2 N$ " " $|\varphi_2\rangle$

$\vdots$

$p_K N$ " " $|\varphi_K\rangle$

This is called a <u>statistical mixture</u> and is described by the convex sum:

$$\rho = \sum_{i=1}^{K} p_i \underbrace{|\varphi_i\rangle\langle\varphi_i|}$$

$\left.\begin{matrix}\text{ket - bra}\\ \text{column - line}\end{matrix}\right)$ matrix.

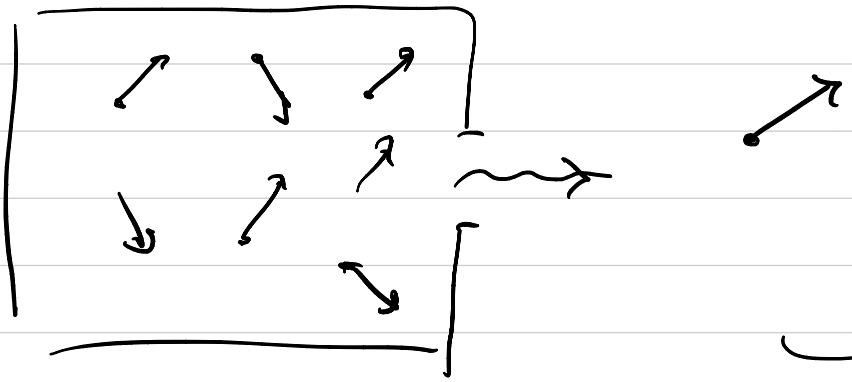
projection matrix on state vector $|\varphi_i\rangle$

Note $(|\varphi_i\rangle\langle\varphi_i|)|\psi\rangle = |\varphi_i\rangle \underbrace{\langle\varphi_i|\psi\rangle}_{\mathbb{C}.}$

projection matrix $\qquad \propto |\varphi_i\rangle$.

$\boxed{\text{$\rho$ is the density matrix describing the statistical mixture. All information that can be retrieved from experiments is contained in ρ.}}$

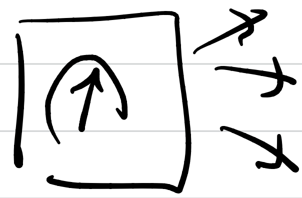
In order to get an intuition on the last statement imagine the following experiment.



$|\varphi_i\rangle$ comes out with probability p_i

then we measure observable A

$|\varphi_i\rangle \Rightarrow$



What is the expectation value of A in this experimental setting?

$$\text{Expected value of } A = \sum_{i=1}^{N} p_i \underbrace{\langle \varphi_i | A | \varphi_i \rangle}$$

probability that state is ρ_i in statistical mixture.

expected value when state is $|\varphi_i\rangle$

(follows from Born rule see class 1)

$$\mathrm{Exp}(A) = \sum_{i=1}^{K} p_i \langle \varphi_i | A | \varphi_i \rangle$$

$$\overset{(*)}{=} \sum_{i=1}^{K} p_i \; \mathrm{Tr}\, A |\varphi_i\rangle\langle\varphi_i|$$

$$= \mathrm{Tr}\left\{ A \sum_{i=1}^{K} p_i |\varphi_i\rangle\langle\varphi_i| \right\}$$

$$= \mathrm{Tr}\, A\rho.$$

Thus expectation values of an observable are given by the very important formula

$$\boxed{\mathrm{Exp}(A) = \mathrm{Tr}\, A\rho = \mathrm{Tr}(\rho A) \in \mathbb{R}.}$$

Remark (*) we use <u>cyclicity of Trace</u> : $\mathrm{Tr}\, AB = \mathrm{Tr}\, BA$

$$\mathrm{Tr}\, \underbrace{A}_{d\times d}\underbrace{|\varphi_i\rangle}_{d\times 1}\underbrace{\langle\varphi_i|}_{1\times d} = \mathrm{Tr}\, \underbrace{\langle\varphi_i|}_{1\times d}\underbrace{A}_{d\times d}\underbrace{|\varphi_i\rangle}_{d\times 1} = \underbrace{\langle\varphi_i|A|\varphi_i\rangle}_{\substack{1\times 1\\ \text{scalar.}}}$$

Similarly we have for all higher moments of an observable:

$$\text{Exp val}(A^p) = \mathrm{Tr}(A^p \rho) = \mathrm{Tr}(\rho A^p)$$

Thus all statistical information is basically contained in ρ.

<u>Limit case of pure states:</u>

If $p_j = 1$ for some j and $p_i = 0$, $i \neq j$

then $\rho = |\varphi_j\rangle\langle\varphi_j|$

$= $ projector onto state $|\varphi_j\rangle \in \mathcal{H}$

$\text{Exp val}(A) = \mathrm{Tr}\,\rho A = \langle\varphi_j|A|\varphi_j\rangle$

We are back in the case of the usual description of a single system in state vector $|\varphi_j\rangle \in \mathcal{H}$. Such ρ's are called pure states.

Note for a pure state: $\rho^2 = \rho$ (projector).
This is a criterion for the purity of a state. If it is not satisfied we have a statistical mixture.

Properties of a density matrix:

If we have a Hilbert space $\mathcal{H}$, $\dim \mathcal{H} = d$
ρ is a square matrix satisfying

1) $\rho = \rho^{+}$ $(= \rho^{T,*})$ hermitian
2) $\rho \geqslant 0$ semi-definite positive matrix
3) $\mathrm{Tr}\rho = 1$ normalization condition.

Proof

1) Obvious from $\rho = \sum_{i=1}^{K} p_i |\varphi_i\rangle\langle\varphi_i|$
since $p_i \in \mathbb{R}$ & $(|\varphi_i\rangle\langle\varphi_i|)^{+} = |\varphi_i\rangle\langle\varphi_i|$.

2) A matrix $M = M^\dagger$ is positive semi-definite iff for any vector $|\psi\rangle$,

$$\langle\psi|M|\psi\rangle \geq 0$$

Here $\langle\psi|\rho|\psi\rangle = \sum_{i=1}^{K} p_i \langle\psi|\varphi_i\rangle\langle\varphi_i|\psi\rangle$

$$= \sum_{i=1}^{K} p_i |\langle\varphi_i|\psi\rangle|^2$$

$$\geq 0.$$

Note: this could be $= 0$ if $|\psi\rangle$ is $\perp$ to all $|\varphi_i\rangle$, $i = 1 \dots K$.

(the $|\varphi_i\rangle$ do not necessarily form a basis)

3) The normalization condition is easy:

$$\mathrm{Tr}\,\rho = \mathrm{Tr} \sum_{i=1}^{K} p_i |\varphi_i\rangle\langle\varphi_i|$$

$$= \sum_{i=1}^{K} p_i \underbrace{\mathrm{Tr}\,|\varphi_i\rangle\langle\varphi_i|}_{\mathrm{Tr}\,\langle\varphi_i|\varphi_i\rangle = 1} = \sum_{i=1}^{K} p_i = 1.$$

by cyclicity

Theorem. Any matrix that satisfies

$$\rho = \rho^{\dagger}, \quad \rho \geq 0, \quad \mathrm{Tr}\,\rho = 1$$

is a density matrix.

Proof. By the spectral theorem we have for an hermitian matrix

$$\rho = \sum_{i=1}^{d} \lambda_i \, |u_i\rangle\langle u_i|$$

where $\rho|u_i\rangle = \lambda_i |u_i\rangle$ & $|u_i\rangle$ form a basis ($\perp$)

Since $\rho \geq 0$ we must have $\lambda_i \geq 0$.

Also $\mathrm{Tr}\,\rho = 1 \Rightarrow \sum_{i=1}^{d} \lambda_i = 1$

Thus also $0 \leq \lambda_i \leq 1$ and they are probabilities. ∎

Remark: the spectral thm gives a special decomposition s.t $|u_i\rangle$ form an $\perp$ basis, But there are other decompositions of ρ if we relax orthogonality. In particular the "physical" one may be with non-ortho states.

II. PARTIAL TRACES

Now in order to introduce the second point of view (of density matrices as description of non-isolated systems) we have to make a mathematical digression on partial traces.

Let $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ be a tensor product Hilbert space. Take a basis

$|v_1\rangle \ldots |v_{d_A}\rangle$ for $\mathcal{H}_A$

$|w_1\rangle \ldots |w_{d_B}\rangle$ for $\mathcal{H}_B$

A basis of $\mathcal{H}_A \otimes \mathcal{H}_B$ is:

$|v_i\rangle \otimes |w_j\rangle$ $\qquad d_A d_B$ basis vectors.

A general matrix can be represented as

$$M = \sum_{i,j,k,l} \underbrace{M_{ijkl}}_{d_A d_B \times d_A d_B \text{ matrix.}} \left(|v_i\rangle \otimes |w_j\rangle\right)\left(\langle v_k| \otimes \langle w_l|\right)$$

We define partial trace as :

$$\mathrm{Tr}_{\mathcal{H}_A} M = \sum_{i,j,k,l} M_{ijkl} \langle v_k | v_i \rangle \, |w_j\rangle\langle w_l|$$

$$= \sum_{j,l} \left(\sum_{i,k} M_{ijkl} \langle v_k | v_i \rangle \right) |w_j\rangle\langle w_l|$$

$$= d_B \times d_B \text{ matrix.}$$

$$\mathrm{Tr}_{\mathcal{H}_B} M = \sum_{ijkl} M_{ijkl} \langle w_l | w_j \rangle \, |v_i\rangle\langle v_k|$$

$$= \sum_{i,k} \left(\sum_{j,l} M_{ijkl} \langle w_l | w_j \rangle \right) |v_i\rangle\langle v_k|$$

$$= d_A \times d_A \text{ matrix.}$$

Note: $\mathrm{Tr}_{\mathcal{H}} M = \mathrm{Tr}_{\mathcal{H}_A} \mathrm{Tr}_{\mathcal{H}_B} M = \mathrm{Tr}_{\mathcal{H}_B} \mathrm{Tr}_{\mathcal{H}_A} M$.

In particular if the basis chosen are orthonormal:

$$\operatorname{Tr}_{\mathcal{H}_A} M = \sum_{j,l} \Big(\sum_i M_{\underbrace{ij}\, il} \Big) |w_j\rangle\langle w_l|$$

$= d_B \times d_B$ matrix with elements (jl)

$$= \sum_i M_{ijil}$$

$$\operatorname{Tr}_{\mathcal{H}_B} M = \sum_{i,k} \Big(\sum_j M_{ijkj} \Big) |v_i\rangle\langle v_k|$$

$= d_A \times d_A$ matrix with elements (ik)

$$= \sum_j M_{ijkj} .$$

<u>Nice property.</u>

If $M = A \otimes B$ we have $M_{ijkl} = A_{ik} B_{jl}$

$\Rightarrow \operatorname{Tr}_{\mathcal{H}_A} M = (\operatorname{Tr} A) . B$, $\operatorname{Tr}_{\mathcal{H}_B} M = A (\operatorname{Tr} B)$.

In practice this nice property will suffice most of the time because we can decompose M as a sum of terms of the form $A \otimes B$.

III. PARTIAL DENSITY MATRICES.

Let $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ and ρ be a density matrix describing a system in $\mathcal{H}$. We only assume $\rho = \rho^\dagger$, $\rho \geq 0$, $\mathrm{Tr}\, \rho = 1$.

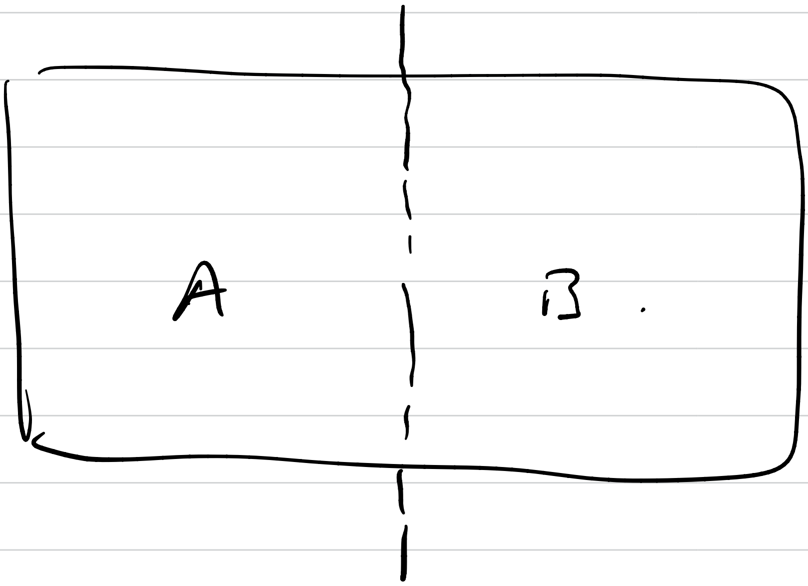
We define:

Partial or reduced DM of parts A & B:

$$\rho_A = \mathrm{Tr}_{\mathcal{H}_B}\, \rho$$

$$\rho_B = \mathrm{Tr}_{\mathcal{H}_A}\, \rho.$$

These matrices describe all local properties in parts A and B.



Indeed suppose we make an experiment to measure an observable "supported" on part A. This observable is a hermitian matrix of the form

$$M_A \otimes \mathbb{1}_B .$$

$d_A \times d_A$ matrix

$d_B \times d_B$ identity matrix

$$\text{Exp val}(M_A \otimes \mathbb{1}_B) = \mathrm{Tr}(\rho \; M_A \otimes \mathbb{1}_B)$$

$$= \mathrm{Tr}_{\mathcal{H}_A} \mathrm{Tr}_{\mathcal{H}_B} (\rho \; M_A \otimes \mathbb{1}_B)$$

$$= \mathrm{Tr}_{\mathcal{H}_A} \left(M_A \underbrace{\mathrm{Tr}_{\mathcal{H}_B} \rho \, \mathbb{1}_B} \right)$$

$$= \mathrm{Tr}_{\mathcal{H}_A} (M_A \, \rho_A).$$

Similarly:

$$\text{Exp val}(\mathbb{1}_A \otimes M_B) = \mathrm{Tr}(\rho \; \mathbb{1}_A \otimes M_B)$$

$$= \mathrm{Tr}_{\mathcal{H}_B} \mathrm{Tr}_{\mathcal{H}_A} (\rho \; \mathbb{1}_A \otimes M_B)$$

$$= \mathrm{Tr}_{\mathcal{H}_B} \left((\mathrm{Tr}_{\mathcal{H}_A} \rho \, \mathbb{1}_A) \; M_B \right)$$

$$= \mathrm{Tr}_{\mathcal{H}_B} (\rho_B \, M_B)$$

V. QUANTUM DESCRIPTION OF A NON-ISOLATED SYSTEM.

A very common situation is a system S that we study but which is not isolated and interacts with an Environment $\mathcal{E}$.

Then S cannot be described by state vectors (at least if interaction with $\mathcal{E}$ cannot be neglected).

<u>The question adressed here is; **how should we modify "postulate 1" to describe S ?**</u>

Well, $S \cup \mathcal{E}$ is isolated (say $\mathcal{E}$ is the rest of the universe except S). Then if we assume postulate 1 for an isolated system we assume a state vector $|\psi\rangle \in \mathcal{H}_S \otimes \mathcal{H}_\mathcal{E}$ for $S \cup \mathcal{E}$. This corresponds to a "pure" density matrix (projector):

$$\rho_{S\cup\mathcal{E}} = \underbrace{|\psi\rangle\langle\psi|}_{d_S d_\mathcal{E} \times d_S d_\mathcal{E} \text{ matrix}}.$$

From discussion in previous paragraph we have to describe S to take the RDM:

$$\boxed{\rho_S = \mathrm{Tr}_\mathcal{E}\, \rho_{S\cup\mathcal{E}} = \underbrace{\mathrm{Tr}_\mathcal{E}\, |\psi\rangle\langle\psi|}_{d_S \times d_S \text{ matrix}}.}$$

For all observables concerning S only we will have

$$\boxed{\mathrm{Expval}\,(A_S \otimes \mathbb{1}_\mathcal{E}) = \mathrm{Tr}_{\mathcal{H}_S}\, A_S\, \rho_S.}$$

This shows that a density matrix is not only useful to describe statistical mixtures (there is no stat mixture here) but is also a useful concept to describe NON-ISOLATED systems.

This point of view was introduced by Landau. The point of view of mixtures was introduced by von Neumann.

V. DENSITY MATRICES OF QUBITS.

For $\mathcal{H} = \mathbb{C}^2$, qubits or two level systems (like spin 1/2 say, or two level atom, or superconducting qubits, ...) the density matrices take a particularly simple form.

We can also generalize the "Bloch sphere" description of $|\psi\rangle \in \mathbb{C}^2$ to the whole "Bloch ball" for DM's.

We can decompose any 2×2 matrix in Pauli basis

$$\rho = b_0 \mathbb{1} + b_x \sigma_x + b_y \sigma_y + b_z \sigma_z$$

$$\mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Since $\rho = \rho^{\dagger}$ we must have $b_0, b_x, b_y, b_z \in \mathbb{R}$.

Since $\operatorname{Tr}\rho = 1$, and $\operatorname{Tr}\sigma_x = \operatorname{Tr}\sigma_y = \operatorname{Tr}\sigma_z = 0$

we must have $b_0 = \frac{1}{2}$. So we write:

$$\rho = \frac{1}{2}\left(\mathbb{1} + a_x \sigma_x + a_y \sigma_y + a_z \sigma_z \right)$$

Now we must implement $\rho \geq 0$.

We must have $\lambda_1 \geq 0$, $\lambda_2 \geq 0$ for the eigenvalues

But $\lambda_1 + \lambda_2 = \operatorname{Tr}\rho = 1$ & $\lambda_1 \lambda_2 = \det\rho$.

Thus <u>it is sufficient</u> to check that

$$\det\rho \geq 0.$$

$$\rho = \frac{1}{2}\begin{pmatrix} 1 + a_z & a_x - i a_y \\ a_x + i a_y & 1 - a_z \end{pmatrix}$$

$$\Rightarrow \det\rho = \frac{1}{4}\left\{ (1 - a_z^2) - (a_x^2 + a_y^2) \right\}$$
$$= \frac{1}{4}\left\{ 1 - \|\vec{a}\|^2 \right\}$$

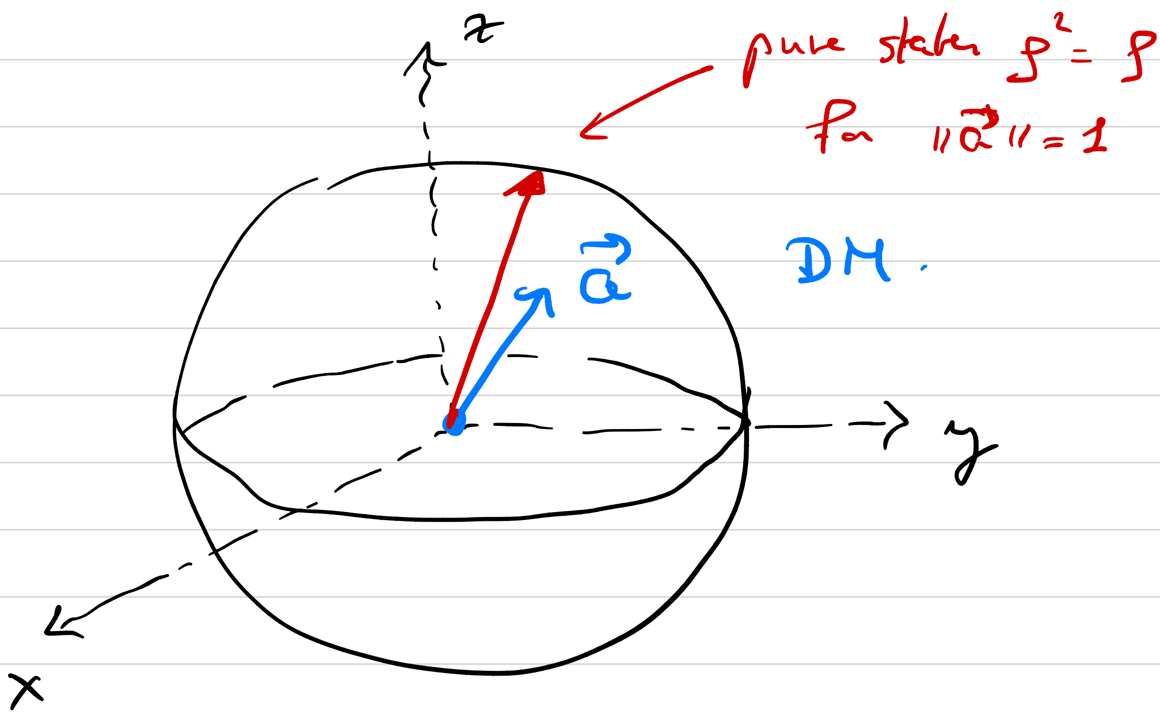
for $\vec{a} = (a_x, a_y, a_z)$.

$\det \rho \geq 0 \iff \|\vec{a}\| \leq 1$.

<u>In summary for one qubit</u>:

$$\rho = \frac{1}{2}\left(\mathbb{1} + \vec{a}\cdot\vec{\sigma}\right) = \frac{1}{2}\begin{pmatrix} 1+a_z & a_x - i a_y \\ a_x + i a_y & 1-a_z \end{pmatrix}$$

with $\|\vec{a}\| \leq 1$ in unit Ball.



Remarks: Limit cases.

- $\vec{a} = 0 \iff \rho = \frac{1}{2}\mathbb{1} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$

$\iff$ $\boxed{\text{Bernoulli random variable}}$

Let $A = |0\rangle\langle 0| - |1\rangle\langle 1| = \sigma_z$.

$$\left.\begin{aligned} \mathrm{Exp}(\sigma_z) &= \mathrm{Tr}\, \rho\sigma_z = 0 \\ \mathrm{Exp}(\sigma_z^2) &= \mathrm{Tr}\,\rho\sigma_z^2 = 1. \end{aligned}\right\}$$

$\Rightarrow \quad p(0) = \frac{1}{2}, \quad p(1) = \frac{1}{2}.$

in fact note $\begin{cases} p(0) = \mathrm{Tr}\, \rho\, |0\rangle\langle 0| = \frac{1}{2} \\ p(1) = \mathrm{Tr}\, \rho\, |1\rangle\langle 1| = \frac{1}{2}. \end{cases}$

- For $\vec{a} \parallel z$ we have $\rho = \begin{pmatrix} p & 0 \\ 0 & 1-p \end{pmatrix}$

if we measure σ_z:

$\iff$ classical R.V with $p(0) = p$, $p(1) = 1-p$.

- Of course this is also true for:

$\vec{a} \parallel x$ if we measure σ_x

$\vec{a} \parallel y$ if we measure σ_y.

- $\|\vec{a}\| = 1$. We can then check that

$$\rho^2 = \rho.$$

and thus $\rho = |\psi\rangle\langle\psi|$. with appropriate

$$|\psi\rangle = \left(\cos\frac{\theta}{2}\right)|0\rangle + \left(\sin\frac{\theta}{2}\right)e^{i\varphi}|1\rangle$$

if $\vec{a} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$

VI. TIME EVOLUTION OF DENSITY MATRICES.

From $$\rho = \sum_{i=1}^{K} p_i |\varphi_i\rangle\langle\varphi_i|$$

we infer that the correct time evolution is expressed as

$$\boxed{\rho_t = U_t \, \rho_0 \, U_t^{\dagger}}$$

(indeed $|\varphi_i\rangle\langle\varphi_i| \rightsquigarrow U_t|\varphi_i\rangle\langle\varphi_i|U_t^{\dagger}$).

From the Schroedinger equation :

$$\boxed{i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle}$$

$$i\hbar \frac{d}{dt} U(t)|\psi(0)\rangle = H\, U(t)|\psi(0)\rangle$$

$$\Leftrightarrow \quad \boxed{i\hbar \frac{d}{dt} U(t) = H\, U(t)}$$

we also get

$$\frac{d}{dt}\rho(t) = \left(\frac{d}{dt}U(t)\right)\rho(0)\,U^{+}(t)$$

$$+\; U(t)\,\rho(0)\left(\frac{d}{dt}U^{+}(t)\right)$$

$$= \frac{1}{i\hbar} H\, U(t)\,\rho(0)\,U^{+}(t)$$

$$+\; U(t)\,\rho(0)\left(-\frac{1}{i\hbar}\right)U^{+}(t)\,H$$

$$\Rightarrow \quad i\hbar \frac{d}{dt}\rho(t) = H\rho(t) - \rho(t) H$$

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

This is the Heisenberg Equation

(by definition $[A, B] = AB - BA$ for two matrices is the commutator)