# An introduction to quantum information and computation

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## Lecture 5: Decoherence and density matrix.

### 1) The ensemble interpretation of quantum mechanics.

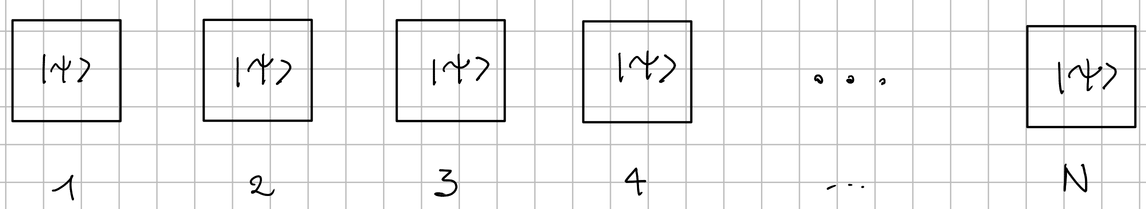
So far we have considered a qubit and have written its state as $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$. Let us pause for a second to think at what this means.

We know experimentally something on a quantum system only when we measure it. How can we use the theoretical knowledge on $|\psi\rangle$ to predict the outcome of the measurement? In general quantum mechanics returns the probability of obtaining a given result after a measurement. If for instance we consider the observable

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{with eigenvector/values} \quad \begin{matrix} \{|0\rangle, +1\} \\ \{|1\rangle, -1\} \end{matrix}$$

we obtain the state $|0\rangle$ with probability $|\alpha|^2$ and the state $|1\rangle$ with probability $|\beta|^2$.

If I want to understand whether my theory is correct, performing one measurement is not sufficient.
I need an ensemble of experimental setups which are prepared in the same initial conditions and that we believe are described by the same state vector $|\psi\rangle$.



We perform the measurement, in $N_0$ setups we obtain $|0\rangle$ and in $N_1$ setups we obtain $|1\rangle$, with $N_0 + N_1 = N$. If $N \gg 1$, then

$$\frac{N_0}{N} \sim |\alpha|^2 \qquad \text{and} \qquad \frac{N_1}{N} \sim |\beta|^2 .$$

Now it is possible to compare the experimental results to the theoretical predictions.
For this reason we say that $|\psi\rangle$ describes an ensemble of experiments. It does not make much sense to say that $|\psi\rangle$ describes a single experiment performed only once.

Note that the ensemble of experiments does not need to be a realistic set of $N \gg 1$ experiments. It could also just be a single experimental apparatus where many experiments are repeated in sequence.

## 2) Statistical mixtures.

Let us now consider our ensemble with N experiments and let us assume that they have all been prepared in the state $|0\rangle$.

| | | | | | | |
|---|---|---|---|---|---|---|
| $\boxed{\|0\rangle}$ | $\boxed{\|0\rangle}$ | $\boxed{\|0\rangle}$ | $\boxed{\|0\rangle}$ | $\boxed{\|0\rangle}$ | $\cdots$ | $\boxed{\|0\rangle}$ |
| 1 | 2 | 3 | 4 | 5 | ... | N |

If all the qubits are well isolated from the rest of the universe, nothing is supposed to happen.
In reality, this is never the case and the quantum system will be in contact with an external system, that from now on we will call *the environment*.

Physical example: an atom is kept levitating in a vacuum chamber. The vacuum is never perfect: there are always residual particles that interact with the atom. The atom levitates because it is trapped by an electromagnetic field. It is also an environment.

The environment can modify the state in an uncontrolled and undesired way. For instance, let us imagine that at a rate $\gamma$ the qubit is flipped. In the language of quantum information, the environment creates a "not" error.

After a time $t$, some qubits have changed:

| | | | | | | |
|---|---|---|---|---|---|---|
| $\boxed{\|0\rangle}$ | $\boxed{\|1\rangle}$ | $\boxed{\|0\rangle}$ | $\boxed{\|1\rangle}$ | $\boxed{\|1\rangle}$ | $\cdots$ | $\boxed{\|0\rangle}$ |
| 1 | 2 | 3 | 4 | 5 | ... | N |

In this simple situation, we can model the dynamical effect of the environment with two coupled differential equations:

$$\begin{cases} \dot{N}_0(t) = -\gamma N_0(t) + \gamma N_1(t) \\ \dot{N}_1(t) = -\gamma N_1(t) + \gamma N_0(t) \end{cases}$$

The solution is simple. $\frac{d}{dt}(N_0 + N_1) = 0 \rightarrow N_0(t) + N_1(t) = N$

$$\frac{d}{dt}(N_0 - N_1)(t) = -2\gamma (N_0 - N_1)(t)$$

$$\hookrightarrow N_0(t) - N_1(t) = \left(N_0(0) - N_1(0)\right) e^{-2\gamma t}$$

In our case, $N_0(0) = N$ and $N_1(0) = 0$.

Using $-N_1(t) = N_0(t) - N$ we get:

$$N_0(t) = \frac{1}{2} N \left(1 + e^{-2\gamma t}\right)$$

$$N_1(t) = \frac{1}{2} N \left(1 - e^{-2\gamma t}\right)$$

At large times I have $N_0(\infty) = N_1(\infty) = N/2$.

How can I predict the outcome of a measurement performed on this ensemble at time $t$?

I have to weight it. For the specific observable $Z$ that we discussed above,

$\{+1, |0\rangle\}$ with probability $\frac{N_0(t)}{N} = \frac{1}{2}\left(1 + e^{-2\gamma t}\right)$

$\{-1, |1\rangle\}$ with probability $\frac{N_1(t)}{N} = \frac{1}{2}\left(1 - e^{-2\gamma t}\right)$

We can also consider a more generic observable $\hat{A}$ with eigenvalues $\{a_1, a_2\}$ and eigenvectors $\{|a_1\rangle, |a_2\rangle\}$.

The probability of measuring $a_i$ at time $t=0$ is:

$$p_{a_1}(t=0) = |\langle a_1|0\rangle|^2 \qquad p_{a_2}(t=0) = |\langle a_2|0\rangle|^2$$

and the expectation value of $\langle A\rangle$ is

$$\langle A\rangle = |\langle a_1|0\rangle|^2 \times a_1 + |\langle a_2|0\rangle|^2 \times a_2 .$$

At time $t>0$, this expectation value must be weighted by the fact that $N_0(t)$ experiments are described by $|0\rangle$ and $N_1(t)$ experiments are described by $|1\rangle$. Hence:

$$\langle A\rangle = \frac{N_0(t)}{N}\left(|\langle a_1|0\rangle|^2 \times a_1 + |\langle a_2|0\rangle|^2 \times a_2\right) +$$

$$+ \frac{N_1(t)}{N}\left(|\langle a_1|1\rangle|^2 \times a_1 + |\langle a_2|1\rangle|^2 \times a_2\right).$$

In summary, at time $t>0$ the ensemble is not described anymore by the pure state $|0\rangle$. What is the theoretical object that describes the ensemble?

The strong temptation is to say that we need a new conceptual tool. Indeed, we know that the ensemble is not anymore composed of identical experiments. We thus introduce the writing

$$\left\{ \frac{N_0(t)}{N}, |0\rangle \quad ; \quad \frac{N_1(t)}{N}, |1\rangle \right\}$$

and we call this situation a statistical mixture.

## 3) Statistical mixtures are different from pure states.

What we have presented before shows very clearly the difference of an ensemble described by a pure state from an ensemble described by a statistical mixture.

Let us try to revert the question: given an ensemble over which I can perform measurements, can I tell the difference between a statistical mixture and a pure state?
The goal here is to give an operational viewpoint on statistical mixtures.

Let us consider the statistical mixture that is produced at $t \to \infty$ where $N_0 = N_1 = N/2$.
If I perform a measurement of $Z$ in this ensemble, I will get

- $|0\rangle$ for $N/2$ experiments
- $|1\rangle$ for $N/2$ experiments.

This is not sufficient to tell us that we have a statistical mixture.
For instance, a quantum state of the form

$$|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle + e^{i\varphi}\frac{1}{\sqrt{2}}|1\rangle$$

is compatible with this result.
How can I operationally distinguish the statistical mixture from $|\psi\rangle$?

We need to perform another measurement. In fact, we can be perfectly sure of the difference considering two other measurements.

Two additional observables: $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

- In order to compute the expectation values of $X$ and $Y$ on the statistical mixture, we need to know:

$$\langle 0 | X | 0 \rangle, \quad \langle 1 | X | 1 \rangle, \quad \langle 0 | Y | 0 \rangle, \quad \langle 1 | Y | 1 \rangle$$

To show this, let us get back to the formula:

$$\langle A \rangle = \frac{N_0(t)}{N} \left( |\langle a_1 | 0 \rangle|^2 \times a_1 + |\langle a_2 | 0 \rangle|^2 \times a_2 \right) +$$

$$+ \frac{N_1(t)}{N} \left( |\langle a_1 | 1 \rangle|^2 \times a_1 + |\langle a_2 | 1 \rangle|^2 \times a_2 \right).$$

We have seen many times that

$$|\langle a_1 | 0 \rangle|^2 \times a_1 + |\langle a_2 | 0 \rangle|^2 \times a_2 = \langle A \rangle_{|0\rangle} = \langle 0 | A | 0 \rangle$$

$$|\langle a_1 | 1 \rangle|^2 \times a_1 + |\langle a_2 | 1 \rangle|^2 \times a_2 = \langle A \rangle_{|1\rangle} = \langle 1 | A | 1 \rangle.$$

Hence:

$$\langle A \rangle = \frac{N_0}{N} \langle 0 | A | 0 \rangle + \frac{N_1}{N} \langle 1 | A | 1 \rangle$$

in our case

$$= \frac{1}{2} \langle 0 | A | 0 \rangle + \frac{1}{2} \langle 1 | A | 1 \rangle.$$

It does not take much time to show that

$$\langle 0 | X | 0 \rangle = 0 \qquad \langle 1 | X | 1 \rangle = 0 \qquad \langle 0 | Y | 0 \rangle = 0 \qquad \langle 0 | Y | 0 \rangle = 0$$

and thus that

$$\langle X \rangle_{\text{stat mixture}} = 0 \qquad\qquad \langle Y \rangle_{\text{stat mixture}} = 0.$$

Let us now see what happens in the case $|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}e^{i\varphi}|1\rangle$.

$$\langle A\rangle_{|\psi\rangle} = \langle\psi|A|\psi\rangle = \frac{1}{2}\langle 0|A|0\rangle + \frac{1}{2}\langle 1|A|1\rangle +$$

$$+ \frac{1}{2}e^{i\varphi}\langle 0|A|1\rangle + \frac{1}{2}e^{-i\varphi}\langle 1|A|0\rangle .$$

It is remarkable to observe that the first line coincide exactly with $\langle A\rangle_{\substack{\text{stat}\\\text{mixture}}}$.

Hence: $\langle A\rangle_{|\psi\rangle} - \langle A\rangle_{\substack{\text{stat}\\\text{mixture}}} = \frac{1}{2}e^{i\varphi}\langle 0|A|1\rangle + \text{c.c.}$

These off-diagonal matrix elements contain the information about the difference between pure state

$$|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle + e^{i\varphi}\frac{1}{\sqrt{2}}|1\rangle$$

and statistical mixture

$$\left\{\frac{1}{2}, |0\rangle \; ; \; \frac{1}{2}\, |1\rangle\right\}$$

Observables such that $\langle 0|A|1\rangle \neq 0$ are able to discriminate between the two situations here above.

# 4) The density matrix,

We have seen that the formalism of states $|\psi\rangle$ cannot describe statistical mixtures. We now introduce a formalism that can describe both situations.

To this goal, we introduce the density matrix $\rho$ associated to the vector $|\psi\rangle$

$$\rho \doteq |\psi\rangle\langle\psi|$$

- $\rho$ is a linear operator.
- $\rho$ is Hermitian.
- $\rho$ contains all the information that is in $|\psi\rangle$: of course, I am not discarding anything!

Examples:

$$|\psi\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \to \rho = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$|\psi\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \to \rho = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$|\psi\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \to \rho = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \end{pmatrix} = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$$

$$|\psi\rangle = \cos\theta\,|0\rangle + e^{i\varphi}\sin\theta\,|1\rangle$$

$$\hookrightarrow \rho = \begin{pmatrix} \cos\theta \\ e^{i\varphi}\sin\theta \end{pmatrix} \begin{pmatrix} \cos\theta & e^{-i\varphi}\sin\theta \end{pmatrix} = \begin{pmatrix} \cos^2\theta & e^{-i\varphi}\cos\theta\sin\theta \\ e^{i\varphi}\cos\theta\sin\theta & \sin^2\theta \end{pmatrix}$$

# General properties of $\rho$.

- $\text{Tr}\,\rho = 1$ To prove it, consider a O.N. basis $\{|i\rangle\}$.

$$\text{Tr}\,\rho = \sum_i \rho_{ii} = \sum_i \langle i|\rho|i\rangle = \sum_i \langle i|\psi\rangle\langle\psi|i\rangle$$

diagonal matrix elements.

$$= \sum_i \langle\psi|i\rangle\langle i|\psi\rangle = \langle\psi|\Big(\sum_i |i\rangle\langle i|\Big)|\psi\rangle$$

Here we use the completeness relation.

$$= \langle\psi|\psi\rangle = 1$$

- $\rho = \rho^+$ — $\rho$ is Hermitian, obvious.

- $\rho$ is positive : $\rho \geq 0$.

By definition, it means that $\langle\phi|\rho|\phi\rangle \geq 0 \quad \forall|\phi\rangle$,

Indeed : $\langle\phi|\rho|\phi\rangle = \langle\phi|\psi\rangle\langle\psi|\phi\rangle = |\langle\phi|\psi\rangle|^2$.

## How can I use the density matrix?

Given an observable $\hat{A}$, the expectation value of A reads:

$$\langle\hat{A}\rangle = \langle\psi|\hat{A}|\psi\rangle = \text{tr}[\rho A]$$

To show this last equality:

$$\text{tr}[\rho\hat{A}] = \text{tr}[|\psi\rangle\langle\psi|\hat{A}] = \sum_i \langle i|\psi\rangle\langle\psi|\hat{A}|i\rangle$$

$$= \sum_i \langle\psi|\hat{A}|i\rangle\langle i|\psi\rangle = \langle\psi|\hat{A}\Big(\sum_i |i\rangle\langle i|\Big)|\psi\rangle$$

$$= \langle \Psi | \hat{A} | \Psi \rangle$$

So far, the density matrix is just a formal way of rewriting $|\Psi\rangle$.
The interest of this conceptual tool lies in the fact that it can also represent statistical mixture.

CLAIM The statistical mixture $\left\{ \frac{1}{2}, |0\rangle ; \frac{1}{2}, |1\rangle \right\}$ is represented by the density matrix

$$\rho = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}.$$

In order to show it, let us consider an observable $\hat{A}$:

$$\langle A \rangle_{\substack{\text{stat} \\ \text{mixture}}} = \mathrm{Tr}\left[ A \rho \right] = \sum_{i=0,1} \langle i | \hat{A} \rho | i \rangle$$

What is $\rho |i\rangle$?

- $\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$
- $\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

It is $\frac{1}{2} |i\rangle$

Hence: $\langle A \rangle_{\substack{\text{stat} \\ \text{mixture}}} = \frac{1}{2} \sum_{i=0,1} \langle i | A | i \rangle = \frac{1}{2} \langle 0 | \hat{A} | 0 \rangle + \frac{1}{2} \langle 1 | \hat{A} | 1 \rangle$

which is exactly the formula we had before. Nice!

What are the formal properties that $\rho = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$ shares with $\rho = |\Psi\rangle\langle\Psi|$?

- $\mathrm{tr}\,\rho = 1$
- $\rho = \rho^{\dagger}$
- $\rho \geq 0$

In the light of this observation, scientists have reformulated quantum mechanichs using the notion of density matrix. An ensemble of quantum experiments is always described by a density matrix $\rho$ that has

$$\bullet\ \mathrm{tr}\,\rho = 1 \qquad \bullet\ \rho = \rho^{\dagger} \qquad \bullet\ \rho \geq 0$$

and such that $\langle A \rangle = \mathrm{tr}[\rho A]$.

Let us now get back to the example we discussed regarding similarities and differences between:

$$|\psi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ e^{i\varphi} \end{pmatrix} \qquad \text{and} \qquad \left\{ \tfrac{1}{2}, |0\rangle \,;\, \tfrac{1}{2}, |1\rangle \right\}$$

The associated density matrices are:

$$\rho = \frac{1}{2}\begin{pmatrix} 1 & e^{-i\varphi} \\ e^{i\varphi} & 1 \end{pmatrix} \qquad\qquad \rho = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

The difference is that in one case you have the off-diagonal matrix elements and in the other case they disappeared.

The off-diagonal matrix elements of $\rho$ are said COHERENCES.
The interaction with an environment has the tendency to bring the coherences to zero. For this reason, this process is called DECOHERENCE.

What is the physical interpretation of the diagonal matrix elements? If we introduce for instance the observable

$\hat{P}_{|0\rangle} = |0\rangle\langle 0|$ such that $\langle \hat{P}_{|0\rangle} \rangle$ is the probability of measuring a $|0\rangle$ state then

$$\mathrm{Tr}[\rho P_{|0\rangle}] = \langle 0|\rho|0\rangle = \rho_{00} \quad \text{diagonal matrix elements.}$$

Hence, the diagonal matrix elements are interpreted as probabilities.

In summary

$$\rho = \begin{pmatrix} p_0 & c \\ c^* & p_1 \end{pmatrix}$$

where $p_0$ and $p_1$ are the probabilities of measuring the sistem in $|0\rangle$ or $|1\rangle$, and $c$ is the coherence.

Important physical interpretation: $\mathrm{Tr}[\rho] = p_0 + p_1 \stackrel{!}{=} 1$ !

Moreover, since $\rho = \rho^\dagger \Rightarrow$ then $p_0, p_1 \in \mathbb{R}$.

Moreover, positivity $\rho \geq 0 \Rightarrow p_0, p_1 \geq 0$.

Thus

$$0 \leq p_0, p_1 \leq 1 \quad \text{and} \quad p_0 + p_1 = 1.$$

When $\rho \propto \mathbb{1}$, namely $\rho = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ all quantum states are equiprobable. Given a state $|\phi\rangle$, the probability of measuring it with an apparatus modeled by $|\phi\rangle\langle\phi|$ is $1/2$, independently from the state $|\phi\rangle$.

The difference between the density matrix associated to a pure state $|\psi\rangle$ and that of a statistical mixture can be quantified looking at the eigenvalues.

For $\rho = |\psi\rangle\langle\psi|$ I have $\lambda_1 = 1$ and $\lambda_2 = 0$

For $\rho = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$ I have $\lambda_1 = 1/2$ and $\lambda_2 = 1/2$

In both cases $\lambda_1 + \lambda_2 = 1$ because $\mathrm{Tr}\,\rho = 1$.

The situation is different if we take

$$\lambda_1^2 + \lambda_2^2 = \begin{cases} 1 & \text{in the } |\psi\rangle \text{ case} \\ \frac{1}{2} & \text{for the statistical mixture.} \end{cases}$$

I claim that $\mathrm{tr}[\rho^2] = \lambda_1^2 + \lambda_2^2$

How to prove that? $\rho$ is hermitian, hence there is a orthonormal basis of eigenvectors of $\rho$.

$$\rho|\lambda_1\rangle = \lambda_1|\lambda_1\rangle \qquad \text{and} \qquad \langle\lambda_i|\lambda_j\rangle = \delta_{ij}$$
$$\rho|\lambda_2\rangle = \lambda_2|\lambda_2\rangle \qquad \sum_i |\lambda_i\rangle\langle\lambda_i| = \mathbb{1}.$$

I evaluate $\mathrm{tr}\,\rho^2$ using this basis:

$$\mathrm{tr}\,\rho^2 = \langle\lambda_1|\rho^2|\lambda_1\rangle + \langle\lambda_2|\rho^2|\lambda_2\rangle = \lambda_1^2\langle\lambda_1|\lambda_1\rangle + \lambda_2^2\langle\lambda_2|\lambda_2\rangle = \lambda_1^2 + \lambda_2^2$$

Since $0 \leq \lambda_i \leq 1$ I can conclude that $\lambda_i^2 \leq \lambda_i$ hence

$$0 \leq \mathrm{tr}\,\rho^2 \leq \mathrm{tr}\,\rho = 1$$

I have the equality $\mathrm{tr}\,\rho^2 = 1$ when $\lambda_1 = 1$ and $\lambda_2 = 0$. This means that $\rho$ must have the form

$$\rho = |\lambda_1\rangle\langle\lambda_1|$$

It describes the situation where the ensemble is described by the vector state $|\lambda_1\rangle$.

We can conclude that:

$\text{tr}\,\rho^2 = 1 \iff$ Description with a vector $|\psi\rangle$ $\rightarrow$ We call this situation PURE STATE

$\text{Tr}\,\rho^2 < 1 \iff$ Description with a statistical mixture $\rightarrow$ We call this situation MIXED STATE

The value of $\text{tr}\,\rho^2$ is called Purity of the density matrix $\rho$.

## 5) Decoherence process.

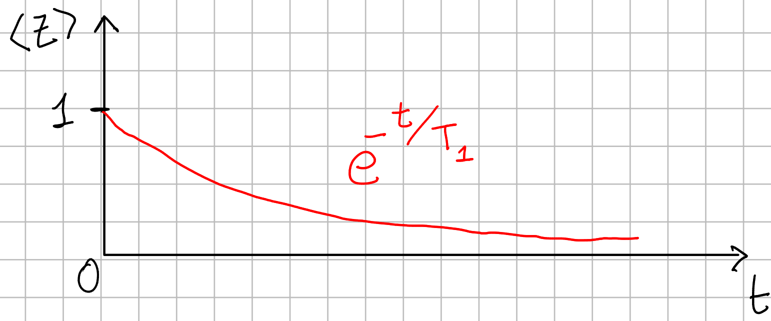
In general terms, the action of the environment is that to cause decoherence

| Initial time | $\xrightarrow[\text{acting for a time } t]{\text{Environment}}$ | At time $t>0$ |
|---|---|---|
| $\rho$ is pure $\lvert\psi\rangle$ | | $\rho$ is mixed |

In general the action of the environment is a complex beast but there are some general quantities that characterize a physical qubit:

- $T_1$, the relaxation time

  You initialize the qubit in $|0\rangle$ and one detects the expectation value of $Z$ as a function of time.




  In general at long times $\langle Z\rangle = 0$, that is $|0\rangle$ and $|1\rangle$ are equiprobable. $T_1$ is the typical time of this relaxation. It concerns only the diagonal parts of the density matrix.

- $T_2$ the coherence time

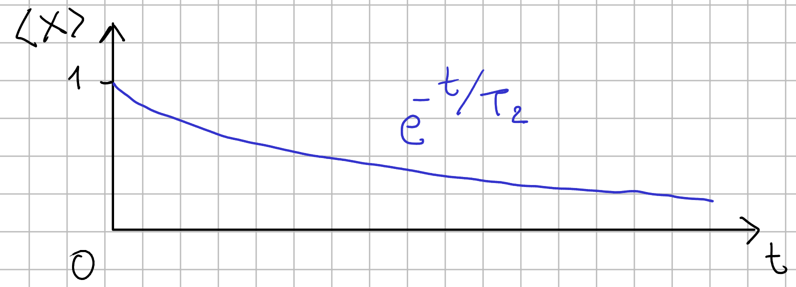
  You initialize the qubit in $|+\rangle$, described by

$$\rho = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$$

At long times it becomes $\rho = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$.

You look at the off-diagonal matrix element, that is $\langle X \rangle$

and you study its decay in time:




$T_2$ is the typical time of this relaxation process.
It concerns the off-diagonal part of the density matrix, its coherences.