# Open quantum systems:

So far, we have considered isolated quantum systems that do not interact with their environment. In reality, quantum systems often interact with an environment, and these interactions may "kill" quantum effects. To describe such open quantum systems, we introduce the density operator.

To this end, we first consider a quantum system which is prepared in the state $|\Psi\rangle$. The expectation value of an observable $\hat{A}$ is then

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

Next, consider a quantum system, which is prepared in one of the states $|\Psi_n\rangle$ with probability $p_n$, where $\sum_n p_n = 1$. In this case, the expectation value should be

$$\langle \hat{A} \rangle = \sum_n p_n \langle \Psi_n | \hat{A} | \Psi_n \rangle$$

This can be written as

$$\langle \hat{A} \rangle = \mathrm{Tr}\{\hat{A}\hat{\rho}\}$$

in terms of the density matrix

$$\hat{\rho} \equiv \sum_n p_n |\Psi_n\rangle\langle\Psi_n|$$

To see this, we write

$$\langle \hat{A} \rangle = \sum_m \langle \Psi_m | \hat{A} \sum_n p_n |\Psi_n\rangle \underbrace{\langle\Psi_n|\Psi_m\rangle}_{\delta_{n,m}}$$

$$= \sum_m p_m \langle \Psi_m | \hat{A} | \Psi_m \rangle \checkmark$$

A few properties of $\hat{\rho}$ are:

1. Self-adjointness:

$$\hat{\rho}^\dagger = \sum_n p_n^* |\Psi_n\rangle\langle\Psi_n| = \hat{\rho}, \text{ since } p_n \in [0,1]$$

2. Positivity:

$$\langle \Psi | \hat{\rho} | \Psi \rangle = \sum_n p_n \langle \Psi | \Psi_n \rangle\langle \Psi_n | \Psi \rangle$$

$$= \sum_n p_n |\langle \Psi | \Psi_n \rangle|^2 \geq 0 \ \forall |\Psi\rangle$$

3. Normalization

$$\mathrm{Tr}\{\hat{\rho}\} = \sum_m \langle \Psi_m | \sum_n p_n |\Psi_n\rangle \underbrace{\langle\Psi_n|\Psi_m\rangle}_{\delta_{n,m}}$$

$$= \sum_m p_m = 1 \checkmark$$

- $\hat{\rho}^2 = \sum_m p_m |\Psi_m\rangle\langle\Psi_m| \sum_n p_n |\Psi_n\rangle\langle\Psi_n|$

$$= \sum_n p_n^2 |\Psi_n\rangle\langle\Psi_n| = \hat{\rho} \text{ if pure state,}$$

i.e. $p_k = 1$ others $= 0$

- $\mathrm{Tr}\{\hat{\rho}^2\} = \sum_m \langle\Psi_m| \sum_n p_n^2 |\Psi_n\rangle\langle\Psi_n|\Psi_m\rangle$

$$= \sum_n p_n^2 = \begin{cases} 1, & \text{if pure state} \\ <1, & \text{otherwise} \end{cases}$$

- Example:

Consider the spin of an electron. The Hilbert space can be spanned by the states $|\uparrow\rangle$ and $|\downarrow\rangle$. Some possible density matrices are

$$\hat{\rho}_1 = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}; \quad \hat{\rho}_2 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}; \quad \hat{\rho}_3 = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

Q: Which density matrices correspond to pure/mixed states?

A: $\hat{\rho}_1 = \underbrace{\frac{1}{2}}_{p_\uparrow} |\uparrow\rangle\langle\uparrow| + \underbrace{\frac{1}{2}}_{p_\downarrow} |\downarrow\rangle\langle\downarrow| \rightsquigarrow$ mixed state

$\hat{\rho}_2 = 1\, |\uparrow\rangle\langle\uparrow| \rightsquigarrow$ pure state $|\uparrow\rangle$

Since $\mathrm{Tr}\{\hat{\rho}_3\} = 1$ and $\det\{\hat{\rho}_3\} = 0$, $\hat{\rho}_3$ has the eigenvalues $0$ & $1$.

The corresponding eigenvectors are

$$\underbrace{\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}}_{|1\rangle} \quad \text{and} \quad \underbrace{\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}}_{|0\rangle}$$

thus,

$$\hat{\rho}_3 = 1\,|1\rangle\langle 1| + 0\,|0\rangle\langle 0| = |1\rangle\langle 1|$$

$$= \begin{pmatrix}\frac{1}{2} & \frac{1}{2}\\ \frac{1}{2} & \frac{1}{2}\end{pmatrix} \checkmark$$

Therefore, $\hat{\rho}_3$ corresponds to the pure state

$$|1\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right)$$

Q: Both for $\hat{\rho}_1$ and $\hat{\rho}_3$, the probability to find the system in the state $|\uparrow\rangle$ is ½. How are $\hat{\rho}_1$ and $\hat{\rho}_3$ different?

A: Consider the expectation value of an observable $\hat{O}$:

$$\langle\hat{O}\rangle_1 = \mathrm{Tr}\{\hat{O}\hat{\rho}_1\}$$

$$= \sum_{\sigma=\uparrow,\downarrow}\langle\sigma|\,\hat{O}\,\frac{1}{2}\left(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|\right)|\sigma\rangle$$

$$= \frac{1}{2}\langle\uparrow|\hat{O}|\uparrow\rangle + \frac{1}{2}\langle\downarrow|\hat{O}|\downarrow\rangle$$

$$\langle\hat{O}_3\rangle = \mathrm{Tr}\{\hat{O}\hat{\rho}_3\} = \langle 1|\hat{O}|1\rangle$$

$$= \frac{1}{2}\left(\langle\uparrow| + \langle\downarrow|\right)\hat{O}\left(|\uparrow\rangle + |\downarrow\rangle\right)$$

$$= \frac{1}{2}\langle\uparrow|\hat{O}|\uparrow\rangle + \frac{1}{2}\langle\downarrow|\hat{O}|\downarrow\rangle + \underbrace{\mathrm{Re}\langle\uparrow|\hat{O}|\downarrow\rangle}_{\text{interference term!}}$$

## The density matrix for a spin:

The density matrix for a spin-1/2 particle is a $2\times 2$ matrix, which can be expanded by the Pauli matrices. Specifically, we can write

$$\hat{\rho} = \frac{1}{2}\left(\mathbb{I} + \underline{a}\cdot\hat{\underline{\sigma}}\right)$$

$$= \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} + \frac{a_x}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} + \frac{a_y}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} + \frac{a_z}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},$$

where $\underline{a} = (a_x, a_y, a_z)$ is the Pauli vector.

Since $\hat{\rho}$ is hermitian, $\hat{\rho}^\dagger = \hat{\rho}$, we have

$$\hat{\rho}^\dagger = \frac{1}{2}\left(\mathbb{I} + \underline{a}^*\cdot\hat{\underline{\sigma}}\right) = \frac{1}{2}\left(\mathbb{I} + \underline{a}\cdot\hat{\underline{\sigma}}\right),$$

so that $\underline{a}^* = \underline{a}$ must be real. We also see that

$$\mathrm{Tr}\{\hat{\rho}\} = \frac{1}{2}\mathrm{Tr}\{\mathbb{1}\} + 0 = \frac{1}{2}\times 2 = 1 \checkmark$$

Moreover, for a pure state, we have

$$\mathrm{Tr}\{\hat{\rho}^2\} = \lambda_1^2 + \lambda_2^2 = 1/2\left(1 + |a|^2\right) = 1,$$

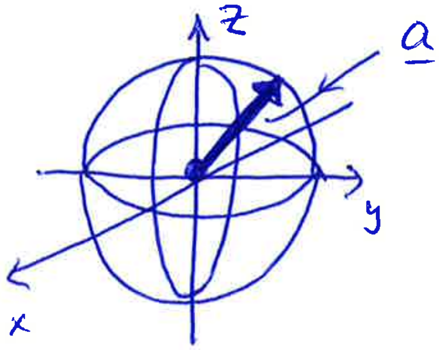
so that $|a| = 1$ for a pure state.

Here, we have used that

$$\det\left(\underline{a}\cdot\hat{\underline{\sigma}}\right) = \begin{vmatrix}a_z & a_x - ia_y\\ a_x + ia_y & -a_z\end{vmatrix} = -|a_z|^2 - |a_y|^2 - |a_x|^2 = -|a|^2$$

and $\mathrm{Tr}\{\underline{a}\cdot\hat{\underline{\sigma}}\} = 0$, implying that $\underline{a}\cdot\hat{\underline{\sigma}}$ has the eigenvalues $\pm|a|$.

Thus, as we have already seen, the pure states of a two-level system "live" on the surface of the Bloch sphere.

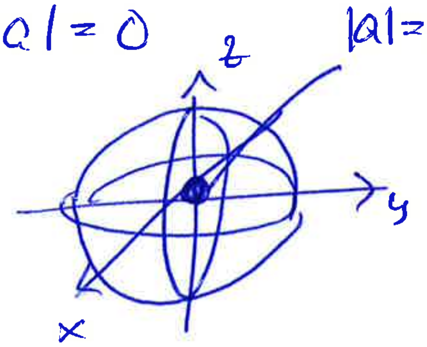



By contrast, for a non-pure state, we have

$$\mathrm{Tr}\{\hat{\rho}^2\} = \frac{1}{2}(1+|a|^2) < 1 \Rightarrow |a|^2 < 1$$
$$\Rightarrow \underline{|a|<1}$$

For example, for a system in a complete statistical mixture with $\hat{\rho} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$, we have

$$\mathrm{Tr}\{\hat{\rho}^2\} = \mathrm{Tr}\begin{Bmatrix} \frac{1}{4} & 0 \\ 0 & \frac{1}{4} \end{Bmatrix} = \frac{1}{2} \Rightarrow |a| = 0$$




__Time-evolution:__

The equation of motion for the density matrix reads

$$i\hbar\,\partial_t\,\hat{\rho}(t) = i\hbar\,\partial_t \sum_n p_n |\psi_n\rangle\langle\psi_n|$$
$$= \sum_n p_n \left[\left(i\hbar\,\partial_t|\psi_n\rangle\right)\langle\psi_n| + |\psi_n\rangle\left(i\hbar\,\partial_t\langle\psi_n|\right)\right]$$

Using the Schrödinger equation, we have

$$i\hbar\,\partial_t |\psi_n\rangle = \hat{H}|\psi_n\rangle$$

and $\quad -i\hbar\,\partial_t \langle\psi_n| = \langle\psi_n|\hat{H}.$

Thus, we find

$$\begin{aligned} i\hbar\,\partial_t \hat{\rho}(t) &= \sum_n p_n \left(\hat{H}|\psi_n\rangle\langle\psi_n| - |\psi_n\rangle\langle\psi_n|\hat{H}\right) \\ &= \hat{H}\Big(\sum_n p_n |\psi_n\rangle\langle\psi_n|\Big) - \Big(\sum_n p_n|\psi_n\rangle\langle\psi_n|\Big)\hat{H} \\ &= [\hat{H},\hat{\rho}] \end{aligned}$$

$$\rightsquigarrow \boxed{i\hbar\,\partial_t \hat{\rho}(t) = [\hat{H},\hat{\rho}(t)]}$$ von Neumann equation.

Example: Spin precession:

Let us revisit the problem of spin precession in a constant magnetic field, described by the Hamiltonian $\hat{\mathcal{H}} = \frac{\hbar\omega_0}{2}\hat{\sigma}_z$ (B-field pointing in z-direction). Since the density matrix can be written as

$$\hat{\rho}(t) = \frac{1}{2}\left(\mathbb{1} + \underline{a}(t)\cdot\hat{\underline{\sigma}}\right),$$

we get

$$i\hbar\,\partial_t \hat{\rho}(t) = \frac{i\hbar}{2}\,\partial_t\left(\underline{a}(t)\cdot\hat{\underline{\sigma}}\right)$$

$$= \left[\frac{\hbar\omega_0}{2}\hat{\sigma}_z\,;\ \frac{1}{2}\,\underline{a}(t)\cdot\hat{\underline{\sigma}}\right]$$

$$= \frac{\hbar\omega_0}{4}\left[\hat{\sigma}_z,\ a_x\hat{\sigma}_x + a_y\hat{\sigma}_y + a_z\hat{\sigma}_z\right]$$

$$= \frac{\hbar\omega_0}{4}\left(a_x\left[\hat{\sigma}_z,\hat{\sigma}_x\right] + a_y\left[\hat{\sigma}_z,\hat{\sigma}_y\right] + 0\right)$$

$$= \frac{\hbar\omega_0}{4}\left(a_x\, 2i\hat{\sigma}_y - a_y\, 2i\sigma_x\right)$$

$$= i\,\frac{\hbar\omega_0}{2}\left(a_x\hat{\sigma}_y - a_y\hat{\sigma}_x\right)$$

$a_z =$ const.

$\Downarrow$

$$\Rightarrow \quad \frac{d}{dt}a_x = -\omega_0 a_y\,;\quad \frac{d}{dt}a_y = \omega_0 a_x\,;\quad \frac{d}{dt}a_z = 0$$

$$\Rightarrow \quad \frac{d}{dt}\begin{pmatrix} a_x \\ a_y \end{pmatrix} = +\omega_0\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} a_x \\ a_y \end{pmatrix} = -i\omega_0\underbrace{\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}}_{\underline{\underline{\sigma}}_y}\begin{pmatrix} a_x \\ a_y \end{pmatrix}$$

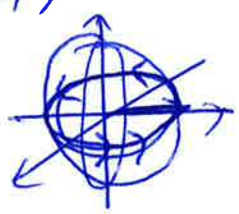
$$\Rightarrow \quad \begin{pmatrix} a_x(t) \\ a_y(t) \end{pmatrix} = e^{-i\omega_0\underline{\underline{\sigma}}_y t}\begin{pmatrix} a_x(0) \\ a_y(0) \end{pmatrix}$$

$$= \left[\mathbb{I}\cos(\omega_0 t) - i\,\underline{\underline{\sigma}}_y\sin(\omega_0 t)\right]\begin{pmatrix} a_x(0) \\ a_y(0) \end{pmatrix}$$

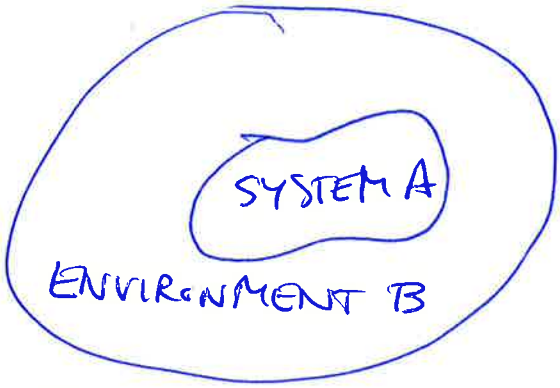
$$= \begin{pmatrix} \cos(\omega_0 t) & -\sin(\omega_0 t) \\ \sin(\omega_0 t) & \cos(\omega_0 t) \end{pmatrix}\begin{pmatrix} a_x(0) \\ a_y(0) \end{pmatrix}$$

$$= \underline{\underline{R}}(\omega_0 t)\begin{pmatrix} a_x(0) \\ a_y(0) \end{pmatrix}$$

counterclockwise rotation by $\omega_0 t$



## Reduced density matrices:




Non-pure states can arise if we trace out the degrees of freedom associated with the environment of a quantum system.

Specifically, the expectation value of an observable in A is

$$\langle \hat{O}_A \rangle = \mathrm{Tr}\{\hat{O}_A \hat{\rho}\}$$

$$= \sum_{n_A, n_B} \langle n_B | \langle n_A | \hat{O}_A \hat{\rho} | n_A \rangle | n_B \rangle$$

$$= \sum_{n_A, n_B} \langle m_B | \langle n_A | \hat{O}_A \underbrace{\Big( \sum_{m_A, m_B} | m_A \rangle | m_B \rangle \langle m_B | \langle m_A | \Big)}_{=1} \hat{\rho} | n_A \rangle | n_B \rangle$$

$$= \sum_{\substack{n_A, n_B \\ m_A, m_B}} \langle m_A | \hat{O}_A | m_A \rangle \underbrace{\langle n_B | m_B \rangle}_{\delta_{n_B m_B}} \langle m_B | \langle m_A | \hat{\rho} | n_A \rangle | n_B \rangle$$

$$= \sum_{n_A, m_A} \langle n_A | \hat{O}_A | m_A \rangle \underbrace{\sum_{n_B} \langle n_B | \langle m_A | \hat{\rho} | n_A \rangle | n_B \rangle}_{:= \langle m_A | \hat{\rho}_A | n_A \rangle}$$

$$= \sum_{n_A, m_A} \langle n_A | \hat{O}_A | m_A \rangle \langle m_A | \hat{\rho}_A | n_A \rangle = \sum_{n_A} \langle m_A | \hat{O}_A \hat{\rho}_A | n_A \rangle$$

$$= \mathrm{Tr}_A \{\hat{O}_A \hat{\rho}_A\} \quad //$$

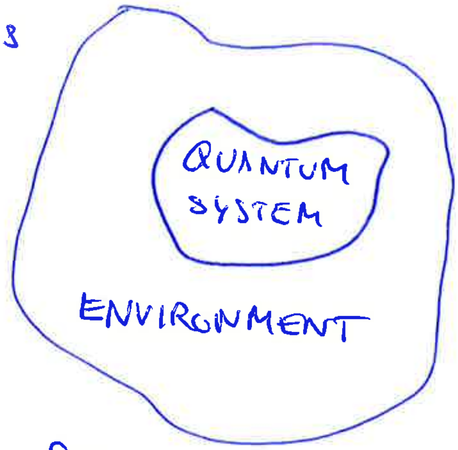
Here we have defined the reduced density matrix in A:

$\hat{\rho}_A = \mathrm{Tr}_B\{\hat{\rho}\}$, with the partial trace defined as

$$\langle m_A | \hat{\rho}_A | n_A \rangle \equiv \sum_{n_B} \langle n_B | \langle m_A | \hat{\rho} | n_A \rangle | n_B \rangle \quad //$$

# Lindblad equation for an open quantum system:

In many cases, the interactions of a quantum system with its environment, can be described by a Liouville-von Neumann (or Lindblad) equation of the form




$$\frac{d}{dt}\hat{\rho} \equiv \mathcal{L}\hat{\rho} \equiv \frac{1}{i\hbar}[\hat{H},\hat{\rho}] + \mathcal{D}\hat{\rho},$$

where $\hat{\rho}$ is the reduced density matrix of the quantum system with Hamiltonian $\hat{H}$, and $\mathcal{D}$ is a Lindblad dissipator of the form

$$\mathcal{D}\hat{\rho} = \gamma\left(\hat{L}\hat{\rho}\hat{L}^{\dagger} - \frac{1}{2}\{\hat{L}^{\dagger}\hat{L},\hat{\rho}\}\right)$$

for some operator $\hat{L}$. The generator of the time evolution $\mathcal{L}$ is known as the Liouvillean. Above, the commutator $[\hat{H},\hat{\rho}]$ describes the unitary evolution of the quantum system, if it was isolated, while the Lindblad dissipator accounts for the interactions with the environment.

## Example: Pure dephasing

Let us consider a spin-½ particle that processes in an external magnetic field. However, due to fluctuations in the environment the magnetic field is not constant in time. This situation can be described by a Hamiltonian of the form

$$\hat{H}(t) = \frac{\hbar}{2}\left(\omega_0 + \delta\omega_0(t)\right)\hat{\sigma}_z,$$

where the random variable $\delta\omega_0(t)$ describes the fluctuations of the field. We assume that it vanishes on average; $\langle\delta\omega_0(t)\rangle = 0$, and the fluctuations are Gaussian with a variance that we denote by $\gamma$. Under these assumptions, one can formulate a Lindblad equation reading (here we do not show the derivation)

$$\frac{d}{dt}\hat{\rho} = \frac{1}{i\hbar}\left[\hbar\omega_0 \frac{1}{2}\hat{\sigma}_z, \hat{\rho}\right] + \gamma/2\left(\hat{\sigma}_z\hat{\rho}\hat{\sigma}_z^{+} - \frac{1}{2}\left\{\hat{\sigma}_z^{+}\hat{\sigma}_z, \hat{\rho}\right\}\right)$$

$$= -i\frac{\omega_0}{2}\left[\hat{\sigma}_z, \hat{\rho}\right] + \gamma/2\left(\hat{\sigma}_z\hat{\rho}\hat{\sigma}_z - \hat{\rho}\right),$$

since $\hat{\sigma}_z^{+} = \hat{\sigma}_z$, and $\hat{\sigma}_z^{2} = 1$

Using again that $\hat{\rho}(t) = \frac{1}{2}(\mathbb{1} + \underline{a}(t)\cdot\hat{\underline{\sigma}})$, we find

$$\frac{d}{dt}\left(\underline{a}(t)\cdot\hat{\underline{\sigma}}\right) = -\frac{i\omega_0}{2}\left[\hat{\sigma}_z, \underline{a}(t)\cdot\hat{\underline{\sigma}}\right] + \frac{\gamma}{2}\left(\hat{\sigma}_z(\underline{a}(t)\cdot\hat{\underline{\sigma}})\hat{\sigma}_z - \underline{a}(t)\cdot\hat{\underline{\sigma}}\right)$$

$$= -\frac{i\omega_0}{2}\left(a_x(t)[\hat{\sigma}_z,\hat{\sigma}_x] + a_y(t)[\hat{\sigma}_z,\hat{\sigma}_y] + 0\right)$$

$$+ \frac{\gamma}{2}\Big(a_x(t)\underbrace{\hat{\sigma}_z\hat{\sigma}_x\hat{\sigma}_z}_{-\hat{\sigma}_x} + a_y(t)\underbrace{\hat{\sigma}_z\hat{\sigma}_y\hat{\sigma}_z}_{-\sigma_y} + a_z(t)\hat{\sigma}_z$$

$$- a_x(t)\hat{\sigma}_x - a_y(t)\hat{\sigma}_y - a_z(t)\hat{\sigma}_z\Big)$$

$$= -\frac{i\omega_0}{2}\left(a_x(t)\,2i\hat{\sigma}_y - a_y(t)\,2i\hat{\sigma}_x\right) - \gamma\left(a_x(t)\hat{\sigma}_x + a_y(t)\hat{\sigma}_y\right)$$

$$= \omega_0\left(a_x(t)\hat{\sigma}_y - a_y(t)\hat{\sigma}_x\right) - \gamma\left(a_x(t)\hat{\sigma}_x + a_y(t)\hat{\sigma}_y\right)$$

$$\overset{!}{=} \dot{a}_x(t)\hat{\sigma}_x + \dot{a}_y(t)\hat{\sigma}_y + \dot{a}_z(t)\hat{\sigma}_z$$

$$\Rightarrow \quad \frac{d}{dt}\begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} = \begin{pmatrix} -\gamma & -\omega_0 & 0 \\ \omega_0 & -\gamma & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix}$$

$\Rightarrow$ $a_z(t) = a_z(0) = \text{const.}$ &

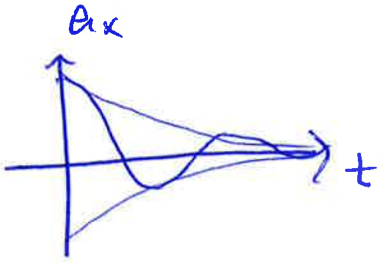
$$\frac{d}{dt}\begin{pmatrix} a_x \\ a_y \end{pmatrix} = \left(-i\omega_0\underline{\underline{\sigma}}_y - \gamma\mathbb{1}\right)\begin{pmatrix} a_x \\ a_y \end{pmatrix}$$

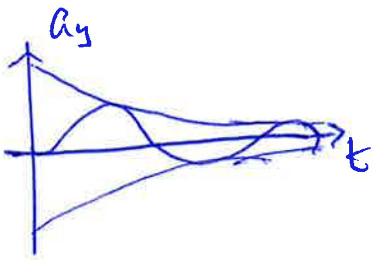
$$\Rightarrow \quad \begin{pmatrix} a_x \\ a_y \end{pmatrix} = e^{-\gamma\mathbb{1}t}\, e^{-i\omega_0\underline{\underline{\sigma}}_y t}\begin{pmatrix} a_x \\ a_y \end{pmatrix}$$

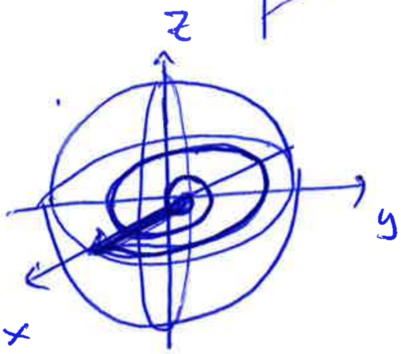
$$\begin{pmatrix} a_x(t) \\ a_y(t) \end{pmatrix} = e^{-\gamma t} \left( \cos(\omega_0 t)\, \mathbb{1} - \sin(\omega_0 t)\, \hat{\sigma}_y \right) \begin{pmatrix} a_x(0) \\ a_y(0) \end{pmatrix}$$

$$= e^{-\gamma t} \left( \begin{pmatrix} \cos(\omega_0 t) & 0 \\ 0 & \cos(\omega_0 t) \end{pmatrix} + \begin{pmatrix} 0 & -\sin(\omega_0 t) \\ \sin(\omega_0 t) & 0 \end{pmatrix} \right) \begin{pmatrix} a_x(0) \\ a_y(0) \end{pmatrix}$$

$$= \underbrace{e^{-\gamma t}}_{\to\, 0 \text{ for } t \to \infty} \begin{pmatrix} \cos(\omega_0 t) & -\sin(\omega_0 t) \\ \sin(\omega_0 t) & \cos(\omega_0 t) \end{pmatrix} \begin{pmatrix} a_x(0) \\ a_y(0) \end{pmatrix}$$




Thus, as time goes, we end up in $\hat{\rho} = \frac{1}{2}\left(\mathbb{1} + \underline{a}(t) \cdot \underline{\hat{\sigma}}\right)$

$$\to \frac{1}{2}\mathbb{1} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$$

which is a completely classical, statistical mixture!