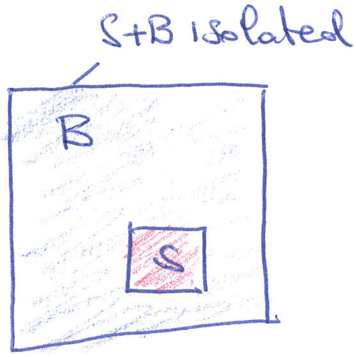
Evolution of Reduced Density Matrix

For an isolated system with Hamiltonian H

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}]$$



Let's consider the partition with S subsystem of $S+B$ then

$$\hat{H} = \hat{H}_S + \hat{H}_B + \hat{H}_{SB}$$

interaction

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar}[\hat{H}_S, \hat{\rho}] + $$

$$-\frac{i}{\hbar}[\hat{H}_B, \hat{\rho}] +$$

$$-\frac{i}{\hbar}[\hat{H}_{SB}, \hat{\rho}]$$

Define reduced density matrix for system S

$\hat{\rho}^{(S)} = \mathrm{tr}_B\, \hat{\rho}$ ← trace over the B degree of freedom

taking the trace

$$\frac{\partial \hat{\rho}^{(S)}}{\partial t} = +\underbrace{\frac{i}{\hbar}[\hat{\rho}^{(S)}, \hat{H}_S]}_{(A)} \underbrace{- \frac{i}{\hbar}\mathrm{tr}_B\left([\hat{H}_B, \hat{\rho}]\right)}_{(B)} \underbrace{- \frac{i}{\hbar}\mathrm{tr}_B\left([H_{SB}, \hat{\rho}]\right)}_{(C)}$$

the term (B) is zero

$$\mathrm{tr}_B [\hat{H}_B, \hat{\rho}] = \sum_\alpha \left(\langle\alpha|\hat{H}_B \hat{\rho}|\alpha\rangle - \langle\alpha|\hat{\rho}\,\hat{H}_B|\alpha\rangle \right)$$

let $|\alpha\rangle$ eigenstates of $\hat{H}_B$

$\hat{H}_B|\alpha\rangle = E_\alpha^{(B)}|\alpha\rangle$ then $\langle\alpha|\hat{H}_B = \langle\alpha|E_\alpha^{(B)}$

and (B) is zero c. v. d.

$$\boxed{\frac{\partial \rho^{(s)}}{\partial t} + \frac{i}{\hbar}[\hat{H}_s, \hat{\rho}^{(s)}] = -\frac{i}{\hbar}\mathrm{tr}_B\left([\hat{H}_{SB}, \hat{\rho}]\right)}$$

evolution of reduced density matrix

in absence of interaction ($\hat{H}_{SB} = 0$)
the evolution of ρ is Unitary i.e.

$$\hat{\rho}^{(s)}(t) = e^{-\frac{i}{\hbar}\hat{H}_s t}\, \hat{\rho}_s(0)\, e^{\frac{i}{\hbar}\hat{H}_s t}$$

proofs by substitution ...

if $[H_{SB}, H_s] = 0$ there exists a basis in which

both H_{SB} & H_s are diagonal ...

Purity

Purity P is defined as

$$P \stackrel{def}{=} tr\hat{\rho}^2$$

a) for a pure state $P = 1$

b) for a mixture $P \leq 1$

a) $\rho = |\psi\rangle\langle\psi|$ $\quad \rho^2 = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = \hat{\rho}$

$$tr\hat{\rho}^2 = tr\hat{\rho} = 1$$

b) $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ $\quad \rho^2 = \sum_{ij} p_i p_j |\psi_i\rangle\langle\psi_i|\psi_j\rangle\langle\psi_j|$

$$P = \sum_{ij} p_i p_j \sum_\alpha \langle\alpha|\psi_i\rangle\langle\psi_i|\psi_j\rangle\langle\psi_j|\alpha\rangle =$$

$$= \sum_{ij} p_i p_j \langle\psi_i|\psi_j\rangle\langle\psi_j|\psi_i\rangle = \sum_{ij} p_i p_j |\langle\psi_i|\psi_j\rangle|^2$$

now $|\langle\psi_i|\psi_j\rangle|^2 \leq 1$

$$P \leq \left(\sum_i p_i\right)^2 = 1$$

time evolution of purity

$$\frac{dP}{dt} = \frac{d}{dt} \operatorname{tr} \hat{\rho}\hat{\rho} = \operatorname{tr} \frac{\partial\hat{\rho}}{\partial t}\hat{\rho} + \hat{\rho}\frac{\partial\hat{\rho}}{\partial t} =$$

$$= -\frac{i}{\hbar}\left[\operatorname{tr}[\hat{H},\hat{\rho}]\hat{\rho} + \operatorname{tr}\hat{\rho}[\hat{H},\hat{\rho}]\right]$$

but $\operatorname{tr} \hat{A}\hat{B} = \operatorname{tr} \hat{B}\hat{A}$ cyclic property

$$\frac{dP}{dt} = -\frac{2i}{\hbar}\left(\operatorname{tr}[\hat{H},\hat{\rho}]\hat{\rho}\right) =$$

$$= -\frac{2i}{\hbar}\left(\operatorname{tr}(\hat{H}\rho^2 - \hat{\rho}\hat{H}\hat{\rho})\right)$$

but again for the cyclic property

$$\boxed{\frac{dP}{dt} = 0 \qquad P(t) = P(0)}$$

the purity of an isolated system is a

Constant of motion

Purity of a reduced system (sub system)

$$P^{(S)} = \mathrm{tr}_S\, \hat{\rho}^{(S)2} = \mathrm{tr}_S \left(\mathrm{tr}_B\, \hat{\rho}\right)^2 \neq \left(\mathrm{tr}_S \mathrm{tr}_B\, \hat{\rho}\right)^2 = 1$$

$$\frac{dP^{(S)}}{dt} = \mathrm{tr}_S\left(\frac{\partial \hat{\rho}^{(S)}}{\partial t}\hat{\rho}^{(S)} + \hat{\rho}^{(S)}\frac{\partial \hat{\rho}^{(S)}}{\partial t}\right) = \mathrm{tr}_S\left\{\hat{\rho}^{(S)}, \frac{\partial \hat{\rho}^{(S)}}{\partial t}\right\}$$

$$\frac{\partial \hat{\rho}^{(S)}}{\partial t} = \underbrace{-\frac{i}{\hbar}\left[H_S, \hat{\rho}^{(S)}\right]}_{(A)} \underbrace{- \frac{i}{\hbar}\mathrm{tr}_B\left[\hat{H}_{SB}, \hat{\rho}\right]}_{(c)}$$

the (A) term gives 0 in the $\{ \,,\, \}$ because is a unitary evolution therefore

$$\frac{dP^{(S)}}{dt} = -\frac{i}{\hbar}\mathrm{tr}_S\left\{\hat{\rho}^{(S)}, \underbrace{\mathrm{tr}_B\left[\hat{H}_{SB}, \hat{\rho}\right]}_{\text{operator on } S}\right\} =$$

cyclic property

$$= -\frac{2i}{\hbar}\mathrm{tr}_S\left(\hat{\rho}^{(S)}\mathrm{tr}_B\left[\hat{H}_{SB}, \hat{\rho}\right]\right) =$$

$$= -\frac{2i}{\hbar}\mathrm{tr}_S\, \hat{\rho}^{(S)}\mathrm{tr}_B\, \hat{H}_{SB}\hat{\rho} - \hat{\rho}^{(S)}\mathrm{tr}_B\, \hat{\rho}\hat{H}_{SB}$$

$$\boxed{\frac{dP^{(S)}}{dt} = -\frac{2i}{\hbar}\mathrm{tr}_S\left(\hat{\rho}^{(S)}\left(\mathrm{tr}_B\, \hat{H}_{SB}\hat{\rho} - \mathrm{tr}_B\, \hat{\rho}\hat{H}_{SB}\right)\right)}$$

by defining the Derivative

$$\frac{D\hat{\rho}^{(s)}}{Dt} = \frac{\partial \hat{\rho}^{(s)}}{\partial t} + \frac{i}{\hbar}[\hat{H}_s, \hat{\rho}^{(s)}]$$

such that

$$\frac{D\hat{\rho}^{(s)}}{Dt} = -\frac{i}{\hbar}\operatorname{tr}_B[\hat{H}_{SB}\hat{\rho}]$$ interaction

$$\boxed{\frac{dP^{(s)}}{dt} = 2\operatorname{tr}_S \hat{\rho}^{(s)}\frac{D\hat{\rho}^{(s)}}{Dt}}$$

the r.h.s. allows for a relaxation of purity

i.e. ⇒ dissipation

⇒ decoherence

- if at any time the system S and the remaining part B are disentangled i.e.

$$\hat{\rho}(t) = \hat{\rho}^{(S)}(t) \otimes \hat{\rho}^{(B)}(t) = \hat{\rho}^{(B)} \otimes \hat{\rho}^{(s)}$$

$$\operatorname{tr}_S \hat{\rho}^{(s)}\left(\operatorname{tr}_B \hat{H}_{SB}\, \rho^{(s)} \otimes \rho^{(B)} - \operatorname{tr}_B \hat{\rho}_S \otimes \hat{\rho}_B\, \hat{H}_{SB}\right) =$$

$$= \operatorname{tr}_S \hat{\rho}^{(s)}\left(\cancel{\rho^{(s)}}\left(\operatorname{tr}_B H_{SB}\, \rho^{(B)}\right)\hat{\rho}^{(s)} - \rho^{(s)} \operatorname{tr}_B \hat{\rho}^{(B)} \hat{H}_{SB}\right)$$

$= 0$ cyclic properties

~~the one~~ we have no relaxation of purity i.e.

entanglement ⟶ relaxation

However this is not a sufficient condition to mixing i.e. $\hat{\rho}^{(s)} \to \hat{\rho}^{(s)}_{stat}$

- the forcing term of the equation of motion of P give exponential relaxation for that consider

$$\hat{L}^{(s)} = -\frac{1}{\hbar} \mathrm{tr}_B [\hat{H}_{SB}, \hat{\rho}]$$

which is an operator acting on system variables only then it is easy to see that $\hat{L}$ is Hermitian - $\hat{L}^{+} = \hat{L}$ then $\exists \{|\alpha\rangle\} \mid L|\alpha\rangle = \lambda_\alpha |\alpha\rangle$

and

$$\frac{dP}{dt} = 2\,\mathrm{tr}_S\, \hat{\rho}^{(s)} \hat{L}^{(s)} = 2 \sum_\alpha \underbrace{\langle \alpha | \rho^{(s)}(t) | \alpha \rangle}_{\text{positive}} \underbrace{\lambda_\alpha}_{\text{real}}$$

and (provided that $\lambda_\alpha < 0$) we have relaxation of purity that means that starting from a pure state (for the system) through interaction & reach a mixture hopefully giving → decoherence → dissipation