Purity Evolution

The purity of a quantum system is defined as

$$P = \mathrm{tr}\,\hat{\rho}^2$$

and $\hat{\rho}$ is the Density Matrix.

A pure state have $\hat{\rho} = |\psi\rangle\langle\psi|$ and $P = 1$

A mixed state have $\hat{\rho} = \sum_i P_i |\psi_i\rangle\langle\psi_i|$ and

$$P = \sum_{ij} P_i P_j |\langle\psi_i|\psi_j\rangle|^2 \leq \sum_{ij} P_i P_j = \left(\sum_i P_i\right)^2 = 1$$

where $=$ holds when all $\langle\psi_i|\psi_j\rangle = e^{i\varphi_{ij}}$ then the state is indeed a pure st

According the Liouville evolution P is a constant of motion i.e.

$$\frac{dP}{dt} = 0$$

proof:

$$\frac{dP}{dt} = \mathrm{tr}\,\dot{\rho}\rho + \rho\dot{\rho} = \frac{1}{i\hbar}\mathrm{tr}\left([H,\rho]\rho + \rho[H,\rho]\right)$$

(A B B A)

by the cyclic property of the trace $\mathrm{tr}AB = \mathrm{tr}BA$

$$\frac{dP}{dt} = \frac{2}{i\hbar} \operatorname{tr}[H,\rho]\rho = \frac{2}{i\hbar} \operatorname{tr} H\rho^2 - \rho H\rho = 0$$

(cyclic)

Reduced Purity

$P^{(S)} = \operatorname{tr}_S \hat{\rho}^{(S)2}$ where $\hat{\rho}^{(S)} = \operatorname{tr}_B \hat{\rho}$ is the reduced Density Matrix of the System which obey the BBGKY equation

$$\frac{\partial \rho^{(S)}}{\partial t} = \frac{1}{i\hbar}[H_S, \hat{\rho}^{(S)}] + \frac{1}{i\hbar} \operatorname{tr}_B [H_{SB}, \rho]$$

(Liouvillian evolution; "collision" term)

and $H = H_S + H_B + H_{SB}$

$$\frac{dP^{(S)}}{dt} = \operatorname{tr}_S\left(\dot{\rho}^{(S)}\rho^{(S)} + \rho^{(S)}\dot{\rho}^{(S)}\right) = 2\operatorname{tr}_S \rho^{(S)}\dot{\rho}^{(S)}$$

by the cyclic property

$$\frac{dP^{(S)}}{dt} = \frac{2}{i\hbar} \operatorname{tr}_S \rho^{(S)}[H_S, \rho^{(S)}] + \frac{2}{i\hbar} \operatorname{tr}_S \rho^{(S)} \operatorname{tr}_B [H_{SB}, \rho]$$

("collision" term in purity evolution)

$\operatorname{tr}_S \rho^{(S)}[H_S, \rho^{(S)}] = 0$ ← as Liouvillian evolution gives $dP/dt = 0$

the second term on the r.h.s. is not generally 0

$$\operatorname{tr}_S \rho^{(S)} \operatorname{tr}_B H_{SB}\rho - \operatorname{tr}_S \rho^{(S)} \operatorname{tr}_B \rho H_{SB} =$$

$$= \operatorname{tr}_S\left(\operatorname{tr}_B \rho\right) \operatorname{tr}_B H_{SB}\rho - \operatorname{tr}_S\left(\operatorname{tr}_B \rho\right) \operatorname{tr}_B \rho H_{SB}$$

Indeed $\mathrm{tr}_S(\mathrm{tr}_B \rho)\,\mathrm{tr}_B H_{SB}\rho \neq \mathrm{tr}_S \mathrm{tr}_B \rho H_{SB}\rho$

However for a Disentangled S/B the collision term in purity evolution $\dot{s} = 0$

$$\rho = \rho^{(S)} \otimes \rho^{(B)} \quad \text{disentagled S/B}$$

$$\mathrm{tr}_S(\mathrm{tr}_B \rho)\,\mathrm{tr}_B H_{SB}\rho - \mathrm{tr}_S(\mathrm{tr}_B \rho)\,\mathrm{tr}_B \rho H_{SB} =$$

$$= \mathrm{tr}_S \rho^{(S)} (\underbrace{\mathrm{tr}_B \rho^{(B)}}_{=1})\,\mathrm{tr}_B H_{SB}\rho^{(S)}\rho^{(B)} -$$

$$- \mathrm{tr}_S \rho^{(S)}\,\mathrm{tr}_B \rho^{(S)}\rho^{(B)} H_{SB} =$$

$$= \mathrm{tr}_{S,B} \rho^{(S)} H_{SB} \underbrace{\rho^{(S)}\rho^{(B)}}_{\text{Commutes}} - \rho^{(S)2}\rho^{(B)} H_{SB} =$$

$$= \mathrm{tr}_{S,B} \rho^{(S)} H_{SB} \rho^{(B)}\rho^{(S)} - \rho^{(S)2}\rho^{(B)} H_{SB} = 0$$

cyclic

Entanglement $S+B$ $\Rightarrow$ Relaxation of System purity $\Rightarrow$ mixed System state

Let $\hat{L}^{(S)} = \frac{1}{i\hbar} \operatorname{tr}_B [\hat{H}_{SB}, \hat{\rho}]$ the "collision" part which act on system variables only

then

$$\frac{dP}{dt} = 2 \operatorname{tr}_S \hat{\rho}^{(S)} \hat{L}^{(S)}$$

$\hat{L}^{(S)}$ is Hermitian

$$\hat{L}^{(S)\dagger} = -\frac{1}{i\hbar}\left\{ \left(\operatorname{tr}_B H_{SB} \rho \right)^{\dagger} - \left(\operatorname{tr}_B \rho H_{SB} \right)^{\dagger} \right\}$$

$$\left(\operatorname{tr}_B A \right)^{\dagger} = \operatorname{tr}_B A^{\dagger} \quad = -\frac{1}{i\hbar}\left[\operatorname{tr}_B \rho H_{SB} - \operatorname{tr}_B H_{SB} \rho \right] = \hat{L}^{(S)}$$

then let $\hat{L}^{(S)} |\alpha\rangle = \lambda_\alpha |\alpha\rangle$ λ_α are real

$$\frac{dP}{dt} = 2 \sum_\alpha \underbrace{\langle \alpha | \hat{\rho}^{(S)} | \alpha \rangle}_{\text{positive}} \lambda_\alpha$$

we can have relaxation of purity if λ_α are negative.

Relaxation of purity means that reduced density matrix is not that of a pure system