Density Matrix & Quantum Ensembles

for a pure (single) state DM is

$\hat{\rho} = |\psi\rangle\langle\psi|$ in the schrödinger representation

therefore

$\langle x|\hat{\rho}|x\rangle = |\psi(x)|^2$

a statement which hold in any representation

- $\hat{\rho}$ is Hermitian $(\hat{\rho}^{\dagger} = |\psi\rangle\langle\psi| = \hat{\rho})$
  → therefore has real eigenvalues

- ρ is positive definite
  → has ~~all~~ eigenvalues positive
  $\hat{\rho}|\lambda\rangle = \lambda|\lambda\rangle$ but $|\psi\rangle\langle\psi|\lambda\rangle = \lambda \cancel{|\psi\rangle\langle\psi|}|\lambda\rangle$
  has solution for $\langle\psi|\lambda\rangle \neq 0$ only for $\lambda = 1$ and $|\lambda\rangle = |\psi\rangle$
  pure state

- $tr\,\hat{\rho} = 1$ for any complete set $\{|n\rangle\}$

$\Sigma_n \langle n|\hat{\rho}|n\rangle = \Sigma_n \langle n|\psi\rangle\langle\psi|n\rangle = \Sigma_n |c_n|^2 = 1$

Ensembles in QM

take an ensemble of M initial data

$\{|\psi_i\rangle\}$ where $\langle\psi_i|\psi_j\rangle$ not necessarily

perpendicular (i.e. δ_{ij})

define

$$\hat{\rho} = \sum_i P_i |\psi_i\rangle\langle\psi_i|$$

with P_i probability of having the initial state i

then if $\sum_i P_i = 1$ and $\langle\psi_i|\psi_i\rangle = 1$ $\Rightarrow$ $\mathrm{tr}\,\hat{\rho} = 1$

$$\mathrm{tr}\,\hat{\rho} = \sum_n \sum_i P_i \langle n|\psi_i\rangle\langle\psi_i|n\rangle =$$

$$= \sum_i P_i \underbrace{\sum_n \langle\psi_i|n\rangle\langle n|\psi_i\rangle}_{\langle\psi_i|\psi_i\rangle} = 1$$

Ensemble Average

$$\langle\hat{A}\rangle = \sum_i P_i \underbrace{\langle\psi_i|\hat{A}|\psi_i\rangle}_{\text{quantum avg}} = \mathrm{tr}\,\hat{\rho}\hat{A} = \mathrm{tr}\,\hat{A}\hat{\rho}$$

ensemble

Evolution of density matrix in the Schrödinger representation is given by

$$\hat{\rho}(t) = e^{-iHt} |\psi\rangle\langle\psi| e^{iHt}$$

$$\frac{d\hat{\rho}}{dt} = -i[\hat{H}, \hat{\rho}]$$

cfr evolution of operators in Heisenberg's represent

$$\hat{A}_H = e^{iHt} A e^{-iHt} \qquad \frac{dA_H}{dt} = i[\hat{H}, \hat{A}]$$

and evolution of classical probability distribution according Liouville's theorem

$$\frac{\partial\rho}{\partial t} = -\{\rho, H\} \qquad \frac{1}{i\hbar}[\,,\,] \rightarrow \{\,,\,\}$$

• Averages

$$\langle\psi|\hat{A}|\psi\rangle = \Sigma_{nm} \langle\psi|n\rangle\langle n|A|m\rangle\langle m|\psi\rangle$$

$$= \sum_{nm} \langle m|\psi\rangle\langle\psi|n\rangle\langle n|A|m\rangle$$

$$= \operatorname{tr} \hat{\rho}\hat{A} = \operatorname{tr} \hat{A}\hat{\rho}$$

• Eigenvalues

$$\hat{\rho}|\lambda\rangle = \lambda|\lambda\rangle \qquad \text{for normalized eigenvector}$$

$$\Sigma_i P_i |\psi_i\rangle\langle\psi_i|\lambda\rangle = \lambda|\lambda\rangle \qquad \lambda = \Sigma_i P_i \underbrace{\langle\lambda|\psi_i\rangle\langle\psi_i|\lambda\rangle}_{|\langle\lambda|\psi_i\rangle|^2} \geq 0$$

stationary distribution

$[\hat{\rho}, \hat{H}] = 0 \qquad \hat{\rho} = f(\hat{H})$

the eigenstate of energy are also eigenstates of $\hat{\rho}$

in the energy basis

$$\langle m | \rho_{stat} | n \rangle = \delta_{n,m} \langle n | \rho_{stat} | n \rangle$$

therefore in the energy basis a non stationary $\hat{\rho}(t)$ undergoes time evolution leading to

$$\langle n | \rho_{(t)} | m \rangle \longrightarrow \delta_{n,m} \, \rho_{stat}^{n,m}$$

1) tends to stationary diagonal elements (dissipation)

2) tends to loose off diagonal elements (decoherence)

in the energy basis

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

$$\langle n|\hat{\rho}(t)|m\rangle = e^{-iE_nt}\langle n|\hat{\rho}(0)|m\rangle\, e^{iE_mt}$$

$n = m$ $\quad \langle n|\hat{\rho}(t)|n\rangle = \langle n|\hat{\rho}(0)|n\rangle$

$n \neq m$ $\quad \langle n|\hat{\rho}(t)|m\rangle = e^{-i(E_n - E_m)t}\langle n|\hat{\rho}(0)|m\rangle$

for this reason ~~do~~ both dissipation and decoherence should appear as a result of large N limit for an isolated system i.e. all typical $\hat{\rho}(0)$ should be such that are diagonal and stationary

Interaction with a bath leads a non isolated system to both decoherence and dissipation

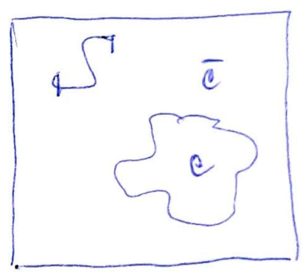
Reduced Density Matrix

if we want to reduce the degree of freedom of a given system i.e. we want to know averaged properties of only a part of the system (c) we integrate out the degree of freedom related to the part ($\bar{c}$) i.e. if

part of interest

$S = c + \bar{c}$ the remaining part

whole system



$$\rho^{(c)} = \mathrm{tr}_{(\bar{c})}\, \rho$$

reduced density matrix

is again a density matrix since

$$\mathrm{tr}\, \rho^{(c)} = \mathrm{tr}_{(c)}\, \rho^{(c)} = \mathrm{tr}_{(c)}\, \mathrm{tr}_{(\bar{c})}\, \rho = 1$$

and for any observable defined only on (c) $\hat{A}^{(c)}$

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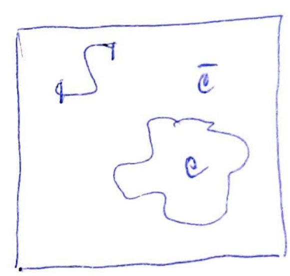

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Time average in QM

Consider an observable $\hat{A} = \hat{A}^{+}$

the Quantum Average ofter a state $|\psi\rangle$ is

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

a time-average colud he defined as

$$\overline{(A)}_T = \frac{1}{T} \int_0^T dt' \langle \psi, t' | \hat{A} | \psi, t' \rangle$$

ergodicity could be stated as

$$\boxed{\lim_{T \to \infty} \frac{1}{T} \int_0^T dt \langle \psi, t | \hat{A} | \psi, t \rangle = \mathrm{tr}\, \hat{\rho}_{stat} \hat{A}}$$