We have seen: $\frac{\partial \rho}{\partial t} = -\{\rho, H\} = -\sum_{j\alpha}\left(\frac{\partial \rho}{\partial q_{j\alpha}}\frac{\partial H}{\partial p_{j\alpha}} - \frac{\partial \rho}{\partial p_{j\alpha}}\frac{\partial H}{\partial q_{j}}\right)$

$\rho(p^{3N}, q^{3N})$ is the probability that the system is found in the state p^{3N}, q^{3N}

What about quantum mechanics?

States accessible to the system $|\Psi_j\rangle$
Probabilities p_j; $\sum_j p_j = 1$

Operator $\hat{A}$: $\langle \hat{A} \rangle = \sum_j p_j \langle \Psi_j | \hat{A} | \Psi_j \rangle$

We encode all information about the system in the density $\frac{\text{matrix}}{\text{operator}}$ $\hat{\rho}$

$$\hat{\rho} = \sum_j p_j |\Psi_j\rangle\langle\Psi_j|$$

Then: $\langle \hat{A} \rangle = \mathrm{Tr}(\hat{\rho}\hat{A}) = \sum_n \langle \chi_n | \hat{\rho}\hat{A} | \chi_n \rangle$

$\{|\chi_n\rangle\}$ is an orthonormal basis

$\rightarrow \langle \chi_n | \chi_m \rangle = \delta_{nm}$

$\underline{\text{Proof}}$ ① $\sum_n |\chi_n\rangle\langle\chi_n| = \mathbb{1}$.

Consider $|\Psi\rangle = \sum_m c_m |\chi_m\rangle$

$$\sum_n |\chi_n\rangle \underbrace{\langle\chi_n| \sum_m c_m |\chi_m\rangle}_{\delta_{nm}} = \sum_n c_n |\chi_n\rangle = |\Psi\rangle$$

$$Tr(\hat{\rho}\hat{A}) = \sum_n \langle\chi_n| \underbrace{\sum_j p_j |\Psi_j\rangle\langle\Psi_j|}_{\hat{\rho}} \hat{A} |\chi_n\rangle$$

$$= \sum_j p_j \underbrace{\sum_n \langle\Psi_j| \hat{A} |\chi_n\rangle\langle\chi_n|}_{\mathbb{1}} \Psi_j\rangle$$

$$= \sum_j p_j \langle\Psi_j|\hat{A}|\Psi_j\rangle \quad \underline{\text{qed}}$$

$\hat{\rho}$ contains all the information that we may want to know about the system.

$\Rightarrow$ $\hat{\rho}$ is sufficient for calculating outcomes of experiments

Time evolution:

$$\frac{\partial\hat{\rho}}{\partial t} = \sum_j p_j \left[\frac{\partial}{\partial t}\left(|\Psi_j\rangle\right)\langle\Psi_j| + |\Psi_j\rangle\frac{\partial}{\partial t}\left(\langle\Psi_j|\right)\right]$$

$$i\hbar\frac{\partial}{\partial t}|\Psi_j\rangle = \hat{H}|\Psi_j\rangle \;;\; -i\hbar\frac{\partial}{\partial t}\langle\Psi_j| = \langle\Psi_j|\hat{H}$$

$$\frac{\partial \hat{\rho}}{\partial t} = \sum_j p_j \frac{1}{i\hbar}\left[\hat{H}|\psi_j\rangle\langle\psi_j| - |\psi_j\rangle\langle\psi_j|\hat{H}\right] =$$

$$\frac{1}{i\hbar}\left(\hat{H}\hat{\rho} - \hat{\rho}\hat{H}\right) = \frac{-1}{i\hbar}\left[\hat{\rho}, \hat{H}\right].$$

$$\frac{\partial \rho_{cl}}{\partial t} = -\{\rho_{cl}, H_{cl}\}$$

$$\neq$$

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$p_0 = p_1 = 1/2$$

$$\hat{\rho} = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = \frac{1}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \end{pmatrix} =$$

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

Properties of $\hat{\rho}$: $\operatorname{Tr}\hat{\rho} = 1$.

For a pure state: $P_\psi = 0$

$$\hat{\rho} = |\psi\rangle\langle\psi|; \quad \hat{\rho}^2 = \hat{\rho}.$$