Traditional QM problems: wave-functions $\psi(\vec{r},t)$ used to describe the evolution of the system

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi$$

Normally, we identify the complete orthonormal set of eigenfunctions $\{u_n(\vec{r},t)\}$ Such that $\hat{H}|u_n\rangle = E_n|u_n\rangle$ and solve for $\psi(\vec{r},t)$ as a linear combination of u_n

$$|\psi\rangle = \sum_n a_n(t)|u_n\rangle \qquad \langle u_m|\psi\rangle = \sum_n a_n \underbrace{\langle u_m|u_n\rangle}_{\delta_{mn}} = a_m$$

$$\langle\psi|\psi\rangle = \sum_n |a_n(t)|^2$$

At the same time, the wavefunction is not physically measurable entity; in reality we measure probability of being in a particular state $P_n = |a_n|^2$.

Also, we often need to find the expectation value of an operator: $\hat{Q}$

$$\langle Q\rangle = \langle\psi|\hat{Q}|\psi\rangle = \sum_{n,m} a_m^* a_n \underbrace{\langle u_m|\hat{Q}|u_n\rangle}_{Q_{mn}}$$

matrix element

Density matrix operator $\hat{\rho} = |\psi\rangle\langle\psi|$

$$\rho_{mn} = \langle u_m|\hat{\rho}|u_n\rangle = \langle u_m|\psi\rangle\langle\psi|u_n\rangle = a_m a_n^*$$

then $P_n = \rho_{nn}$

$$\langle Q\rangle = \sum_{n,m} \rho_{nm} Q_{nm} = \sum_n [\hat{\rho}\hat{Q}]_{nn} = Tr[\hat{\rho}\hat{Q}]$$

Just as we can follow the dynamics of the system using a wave function, we can do it using a density matrix

$$\frac{d}{dt}\hat{\rho} = \frac{d}{dt}|\psi\rangle\langle\psi| = \left[\frac{d}{dt}|\psi\rangle\right]\langle\psi| + |\psi\rangle\left[\frac{d}{dt}\langle\psi|\right]$$

$$= \frac{1}{i\hbar}\hat{H}|\psi\rangle\langle\psi| + \frac{1}{-i\hbar}|\psi\rangle\langle\psi|\hat{H} = \frac{1}{i\hbar}\left[\hat{H}\hat{\rho} - \hat{\rho}\hat{H}\right] =$$

$$i\hbar\frac{d}{dt}\hat{\rho} = \{\hat{H}, \hat{\rho}\}$$

Density matrix elements have no phase ambiguity

$$|\tilde{\psi}\rangle \to e^{i\varphi}|\psi\rangle$$

$$\hat{\rho} \to e^{i\varphi}|\psi\rangle\langle\psi|e^{-i\varphi} = |\psi\rangle\langle\psi| = \rho$$

$\rho^2 = \rho$ (idempotent operator)

$\rho_{nn} \geq 0$ since $\rho_{nn} = |a_n|^2$

For a pure state there is no difference b/w using $|\psi\rangle$ or $\hat{\rho}$ — why bother?

The state must be pure and continuously evolving to be described by the wave function.

Density matrix can handle mixed state

Statistical mixture

A system can be in the state $|\psi_i\rangle$ with a probability p_i $\left(\sum_i p_i = 1\right)$

This is different from a superposition

$$|\psi\rangle = \sqrt{p_1}\,|\psi_1\rangle + \sqrt{p_2}\,|\psi_2\rangle + \ldots$$

We are forced to use the statistical description when we lack full information about the evolution of the system.

How we can describe the state of the system now?

For example, if we need to find the expectation value of an operator, for each of the states $\langle Q\rangle_i = \langle\psi_i|\hat{Q}|\psi_i\rangle =$
$= \mathrm{Tr}\,(\hat{\rho}_i\hat{Q})$

and $\langle Q\rangle = \sum_i p_i \langle Q\rangle_i = \sum_i p_i \,\mathrm{Tr}\,(\hat{\rho}_i\hat{Q}) =$

$$= \mathrm{Tr}\left(\left[\sum_i p_i\hat{\rho}_i\right]\hat{Q}\right) = \mathrm{Tr}\,(\hat{\rho}\hat{Q})$$

where $\hat{\rho} = \sum_i p_i\,\hat{\rho}_i$ "average" of the density matrix operators over the ensemble

Similarly $i\hbar \dfrac{\partial\hat{\rho}}{\partial t} = [\hat{H}, \hat{\rho}]$

but $\hat{\rho}^2 < \hat{\rho}$ for non-pure state.