Quantum Liouville operator [tln47]

The density operator $\rho(t)$ is a positive definite Hermitian operator. Like its classical counterpart, the phase-space density $\rho(\mathbf{X}, t)$, it describes what we know about the state of the system.

Normalization: $\mathrm{Tr}[\rho(t)] = 1$. Expectation value: $\langle A(t)\rangle = \mathrm{Tr}[A\rho(t)]$.

Diagonal representation: $\rho(t) = \sum_i p_i |\pi_i(t)\rangle\langle\pi_i(t)|$.

p_i: probability of finding the system in the state $|\pi_i(t)\rangle$.

$$\Rightarrow \langle A(t)\rangle = \sum_i p_i \langle\pi_i(t)|A|\pi_i(t)\rangle = \sum_{nn'} \langle n|A|n'\rangle\langle n'|\rho(t)|n\rangle.$$

$\{|n\rangle\}$: orthonormal basis. $\langle n'|\rho(t)|n\rangle$: elements of the density matrix.

Schrödinger equation: $H|\pi_i(t)\rangle = i\hbar\frac{\partial}{\partial t}|\pi_i(t)\rangle$.

$$\Rightarrow i\hbar\frac{\partial\rho}{\partial t} = \sum_i p_i \left[H|\pi_i(t)\rangle\langle\pi_i(t)| - |\pi_i(t)\rangle\langle\pi_i(t)|H\right] = H\rho - \rho H = [H, \rho].$$

Liouville operator: $L \equiv \frac{1}{\hbar}[H,\ ]$.

Liouville equation: $i\frac{\partial\rho}{\partial t} = \frac{1}{\hbar}[H, \rho] = L\rho$.

Formal solution: $\rho(t) = e^{-iLt}\rho(0) = e^{-iHt/\hbar}\rho(0)e^{iHt/\hbar}$.

Time evolution carried by density operator or by dynamical variable:

$$\langle A(t)\rangle = \mathrm{Tr}[Ae^{-iHt/\hbar}\rho e^{iHt/\hbar}] = \mathrm{Tr}[e^{iHt/\hbar}Ae^{-iHt/\hbar}\rho].$$

von Neumann equation: $i\hbar\frac{\partial\rho}{\partial t} = [H, \rho] \ \Rightarrow\ \rho(t) = e^{-iHt/\hbar}\rho(0)e^{iHt/\hbar}$.

Heisenberg equation: $i\hbar\frac{\partial A}{\partial t} = -[H, A] \ \Rightarrow\ A(t) = e^{iHt/\hbar}A(0)e^{-iHt/\hbar}$.

Density matrix in energy representation $H|\lambda\rangle = E_\lambda|\lambda\rangle$:

$$\rho_{\lambda\lambda'}(t) = \sum_{\lambda\lambda'} \langle\lambda|\rho|\lambda'\rangle e^{-i(E_\lambda - E_{\lambda'})t/\hbar}.$$

Stationarity of density operator: $i\hbar\frac{\partial\rho}{\partial t} = 0 \ \Rightarrow\ [H, \rho] = 0$.

$\Rightarrow$ ρ is diagonal in the energy representation: $\rho = \sum_\lambda p_\lambda|\lambda\rangle\langle\lambda|$.