4. Pure States and density matrices

remember:

→ projection operator: $\hat{P}_\psi = |\psi\rangle\langle\psi|$

defining property: $\hat{P}_\psi^2 = \hat{P}_\psi$

→ trace: $\mathrm{Tr}(\hat{O}) = \sum_n \langle n|\hat{O}|n\rangle$ ↖ complete basis

↳ for operator products

$$\mathrm{Tr}(\hat{A}\hat{B}\hat{C}) = \mathrm{Tr}(\hat{B}\hat{C}\hat{A}) = \mathrm{Tr}(\hat{C}\hat{A}\hat{B})$$

Proof: $\sum_{nml} A_{nm} B_{ml} C_{ln}$

→ trace is basis independent

$$\mathrm{Tr}(\hat{\tilde{O}}) = \mathrm{Tr}(\hat{U}^\dagger \hat{O} \hat{U}) = \mathrm{Tr}(\underbrace{\hat{U}\hat{U}^\dagger}_{=\mathbb{1}} \hat{O})$$

$$\rightarrow \langle\hat{O}\rangle_\psi = \langle\psi|\hat{O}|\psi\rangle = \sum_n \langle\psi|\hat{O}|n\rangle\langle n|\psi\rangle$$

$$= \sum_n \langle n|\psi\rangle\langle\psi|\hat{O}|n\rangle$$

$$= \mathrm{Tr}(\underbrace{|\psi\rangle\langle\psi|}_{\hat{P}_\psi}\hat{O})$$

Define: $\hat{\rho} = |\psi\rangle\langle\psi|$ (pure states)

$$\langle \hat{O} \rangle_\psi = \mathrm{Tr}(\hat{\rho}\hat{O})$$

Generalization to mixed states

$$\hat{\rho} = \sum_{k=1}^{N} p_k \overbrace{|\psi_k\rangle\langle\psi_k|}^{\text{projector}}, \quad p_k \in \mathbb{R}, \quad \sum_{k=1}^{N} p_k = 1$$

weight of each pure state

→ we not require that $\langle\psi_k|\psi_{k'}\rangle = 0$ for $k \neq k'$

Example:

generic two-state system: $|\uparrow\rangle, |\downarrow\rangle$

pure state: $|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle$

$$\hat{\rho} = |\psi\rangle\langle\psi| = |\alpha|^2 |\uparrow\rangle\langle\uparrow| + \beta\alpha^* |\downarrow\rangle\langle\uparrow| + \alpha\beta^* |\uparrow\rangle\langle\downarrow| + |\beta|^2 |\downarrow\rangle\langle\downarrow|$$

$$\hat{\rho} \hat{=} \begin{pmatrix} \rho_{\uparrow\uparrow} & \rho_{\uparrow\downarrow} \\ \rho_{\downarrow\uparrow} & \rho_{\downarrow\downarrow} \end{pmatrix} = \begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \beta\alpha^* & |\beta|^2 \end{pmatrix}$$

coherences (p-set)

populations

Is a given state pure?

1) If $\hat{\rho} = |\psi\rangle\langle\psi| \Rightarrow \hat{\rho}^2 = \hat{\rho}$

i.e. if $\hat{\rho}^2 = \hat{\rho}$: pure $\rightarrow$ otherwise mixed

2) Check von Neumann entropy

natural logarithm

$$S(\hat{\rho}) = -k_B \mathrm{Tr}(\hat{\rho} \ln \hat{\rho}) ,$$ evaluate in eigenbasis

$$= -k_B \sum_k \lambda_k \ln \lambda_k \qquad \hat{\rho} \hat{=} \begin{pmatrix} \lambda_1 & & & \\ & \ddots & & \\ & & \lambda_k & \\ & & & \ddots \end{pmatrix}$$

If $S(\hat{\rho}) = 0 \Leftrightarrow$ pure state

If $S(\hat{\rho}) > 0 \Leftrightarrow$ mixed state

assume

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

$\hat{\rho}\,\underline{|\varphi\rangle} = \lambda\,\underline{|\varphi\rangle}$

$|\varphi\rangle = |\underline{\psi}\rangle \rightarrow \lambda = 1$

$\lambda = 0$

Properties of density operators

1) $\mathrm{Tr}(\hat{\rho}) = 1$ (normalization)

2) $\hat{\rho}^\dagger = \hat{\rho}$ (hermitian)

3) $\hat{\rho} \geq 0$ (pos. semi-definite, i.e. all $\lambda_i \geq 0$)

4) $\hat{\rho}^2 = \hat{\rho} \Leftrightarrow$ pure state

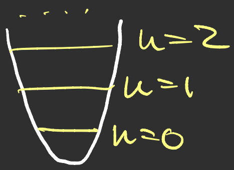
$\hat{\rho}^2 \neq \hat{\rho} \Leftrightarrow$ mixed

$\hat{\rho}$ in number representation

$$\hat{\rho} = \mathbb{1}\,\hat{\rho}\,\mathbb{1} = \sum_n |n\rangle \underbrace{\langle n|\hat{\rho} \sum_m |m\rangle}_{=\rho_{nm}} \langle m| = \sum_{nm} \rho_{nm} |n\rangle\langle m|$$

Thermal photon gas

Consider an EM cavity at thermal equilibrium



$$T \rightarrow \beta = \frac{1}{k_B T}$$

$$p_n = \frac{e^{-\beta E_n}}{Z}, \quad E_n = \hbar\omega\left(n + \tfrac{1}{2}\right)$$

$$Z = \sum_n e^{-\beta E_n} \quad \text{(partition function)}$$

$$\hat{\rho}_{th} = \sum_n p_n |n\rangle\langle n|$$

$$(\hat{\rho}_{therm})_{nm} = \frac{e^{-\beta E_n}}{Z}\,\delta_{nm}$$

Gas statistics

* mean photon number : $\langle \hat{n} \rangle = \bar{n} = \mathrm{Tr}(\hat{n}\,\hat{\rho}_{therm})$

$$= \sum_n n \cdot p_n = \sum_n n \frac{e^{-\beta E_n}}{Z}$$

$$= \frac{e^{-\beta \frac{\hbar\omega}{2}}}{Z} \sum_{n=0}^{\infty} n \cdot e^{-\underbrace{\beta\hbar\omega}_{=\alpha} n}$$

$$Z = \frac{e^{-\beta\frac{\hbar\omega}{2}}}{1-e^{-\beta\hbar\omega}} \qquad = \frac{e^{-\beta\frac{\hbar\omega}{2}}}{Z}\left(-\frac{\partial}{\partial\alpha}\underbrace{\sum_{n=0}^{\infty}\left(e^{-\alpha}\right)^n}_{\frac{1}{1-e^{-\alpha}}}\right)$$

$$= \frac{e^{-\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}}$$

$$\boxed{\bar{n} = \frac{1}{e^{\beta\hbar\omega}-1}}$$

* Visible light : $\hbar\omega \sim 1\,eV$, RT: $k_B T \sim 25\,meV$

$$\Rightarrow \bar{n} = e^{-40} \ll 1$$

* $\lambda = 10-100\,\mu m$, $\bar{n} \approx 1$

* microwaves, $\bar{n} \gg 1$

Variance:

$$\langle \hat{n}^2 \rangle = \mathrm{Tr}\left(\hat{n}^2 \rho_{th}\right) = \bar{n} + 2\bar{n}^2$$

$$\Delta n = \underbrace{\sqrt{\bar{n}^2 + \bar{n}}}_{\bar{n}\left(1+\frac{1}{\bar{n}}\right)^{1/2} \approx \bar{n}\left(1+\frac{1}{2}\frac{1}{\bar{n}}\right)} \xrightarrow{\bar{n} \gg 1} \Delta n \approx \bar{n} + \tfrac{1}{2}$$

For $\bar{n} \gg 1 \Rightarrow \dfrac{\Delta n}{\bar{n}} \to 1$ (very noisy)

$\to 1/\sqrt{\bar{n}}$ (for coherent states)

How to prepare mixed states?

1) Let two system A and B interact

2) Trace out one system to find reduced density matrix of the other.