Now that we have defined the entropy as a function of the density operator, which in itself is defined in terms of microstates and the corresponding probability of finding them, we pose the following question:

Given that we have a set of constraints how can we determine the probability law that describes the Density operator?

Answer 1: If no information is available the distribution is uniform $P_m = 1/M \quad \forall m$ and $S[P] = -k \ln M$

Answer 2: If all is known

$$P_m \begin{cases} 1 & m = i \\ 0 & m \neq i \end{cases}$$ for a given microstate $|\Psi_i\rangle$

$$S[P] = 0$$

Answer 3: Assume we know for certain, for example, that the energy lies in the interval $[E, E+\Delta E]$

$\hookrightarrow \Delta E$ is small in the macroscopic scale but includes a large number of microstates

$\Rightarrow$ The probability is pretty much constant within ΔE

$$P_m = \frac{1}{M} \qquad M = \rho(E)\Delta E$$

$$D = \sum_r |r\rangle \frac{1}{M} \langle r|$$

$H|r\rangle = E|r\rangle$

states that satisfy the energy criteria

$$S[P] = -k \ln M$$

Microcanonical ensemble

Answer 4: We know operage quantities

$$A_i \equiv \langle \hat{A}_i \rangle = \mathrm{Tr}\, D A_i$$

Postulate of maximum statistical entropy

Given a set of macrorcopic constraints the Density operator that represents the macroscopic system in equilibrium is the one that gives the maximum entropy.

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(a) $\langle E \rangle = \mathrm{Tr}\, DH$ $\Rightarrow$ canonical ensemble

(b) $\langle E \rangle = \mathrm{Tr}\, DH$

$\langle N \rangle = \mathrm{Tr}\, D\hat{N}$ $\Rightarrow$ gran canonical ensemble

average number of particles

Let's find the extrema using Lagrange multipliers

$$\frac{1}{k}\tilde{S}[D] = -\mathrm{Tr}\, \overset{①}{D \ln D} + \sum_i \lambda_i \left(\mathrm{Tr}\, \overset{②}{D\hat{A}_i} - \langle A_i \rangle\right) - \lambda_0 \left(\overset{③}{\mathrm{Tr}\, D} - 1\right)$$

let's use $d(\mathrm{Tr}\, f(\hat{A})) = \mathrm{Tr}(f'(\hat{A})\, d\hat{A})$

① $f(\hat{D}) = D \ln D$ $\qquad f'(\hat{D}) = \ln D + \mathbb{I}$

② $f(\hat{D}) = \hat{D}\hat{A}_i$ $\qquad f'(\hat{D}) = \hat{A}_i$

③ $f(\hat{D}) = \hat{D}$ $\qquad f'(D) = \mathbb{I}$

$$\frac{1}{k} dS = -\mathrm{Tr}\left[(\ln D + \mathbb{I})\, dD\right] + \sum_i \lambda_i \,\mathrm{Tr}\, A_i dD - \lambda_0 \mathrm{Tr}\, dD$$

$$= -\mathrm{Tr}\left[dD\left[\ln D + \hat{\mathbb{I}} - \sum_i \lambda A_i + \lambda_0\right]\right] = 0 \leftarrow \text{extrema}$$

$$\ln D + \hat{\mathbb{I}} - \sum_i \lambda_i A_i + \lambda_0 = 0$$

$$\ln D = -(1+\lambda_0) + \sum_i \lambda_i \hat{A}_i$$

$$D = e^{-(1+\lambda_0)} \exp \sum_i \lambda_i \hat{A}_i$$

normalization constant

$$\underbrace{D_B = \frac{1}{Z} \exp\left(\sum_i \lambda_i \hat{A}_i\right)}_{\text{Boltzmann distribution}}$$

$$S_B = S_{st}[D_B] = -k_B \operatorname{Tr} D_B \ln D_B$$

$$S_B = -k \operatorname{Tr}\left[\frac{1}{Z} \exp\left(\sum_i \lambda_i \hat{A}_i\right) \left\{-\ln Z + \sum_i \lambda_i A_i\right\}\right]$$

$$= +k \ln Z \underbrace{\operatorname{Tr}\left[\frac{1}{Z} \exp\left(\sum_i \lambda_i \hat{A}_i\right)\right]}_{1} - k \underbrace{\operatorname{Tr}\left[\frac{\sum_i \lambda_i \hat{A}_i}{Z} \exp \sum_i \lambda_i \hat{A}_i\right]}_{\substack{\operatorname{Tr} \hat{B}\hat{D} = \langle \hat{B} \rangle \\ \hat{B} = \sum_i \lambda_i \hat{A}_i}}$$

$$= k \ln Z - k \left\langle \sum_i \lambda_i \hat{A}_i \right\rangle = k \ln Z - k \sum_i \lambda_i \langle \hat{A}_i \rangle$$

Boltzmann entropy

But is this a maximum?

$$\mathrm{Tr}\,\hat{X}\ln\hat{Y} - \mathrm{Tr}\,\hat{X}\ln\hat{X} \leq \mathrm{Tr}\,\hat{Y} - \mathrm{Tr}\,\hat{X}$$

$\hat{Y} \equiv D_B$

$\hat{X} \equiv D$ → some trial density matrix that satisfies $\langle\hat{A}_i\rangle = \mathrm{Tr}[\hat{A}_i D]$

$$\mathrm{Tr}\,D\ln D_B - \mathrm{Tr}\,D\ln D \leq 0 = \underbrace{\mathrm{Tr}\,D_B}_{1} - \underbrace{\mathrm{Tr}\,D}_{1}$$

$$-\mathrm{Tr}\,D\ln D \leq -\mathrm{Tr}\,D\ln D_B = -\mathrm{Tr}\left[D\left\{-\ln Z + \sum_i \lambda_i \hat{A}_i\right\}\right]$$

$$= +\ln Z\,\underbrace{\mathrm{Tr}\,D}_{1} - \underbrace{\mathrm{Tr}\,D\sum_i \lambda_i\hat{A}_i}_{\sum_i \lambda_i \mathrm{Tr}\,D\hat{A}_i = \sum_i \lambda_i\langle\hat{A}_i\rangle}$$

$$\Rightarrow \underbrace{-k\,\mathrm{Tr}\,D\ln D}_{S[D]} \leq \underbrace{k\ln Z - k\sum_i \lambda_i\langle\hat{A}_i\rangle}_{S_B[D_B]}$$

$$S[D] \leq S_B$$

↑ maximum entropy

[where the equality will only occur if $D = D_B$]

Furthermore

$$\langle \hat{A}_i \rangle = \mathrm{Tr}[\hat{A}_i D] = \mathrm{Tr}\left[\hat{A}_i \frac{1}{Z} e^{\sum_j \lambda_j \hat{A}_j}\right] = \frac{1}{Z}\mathrm{Tr}\left[\frac{\partial}{\partial \lambda_i} e^{\sum_j \lambda_j \hat{A}_j}\right]$$

$$= \frac{1}{Z}\frac{\partial}{\partial \lambda_i}\Big\{\underbrace{\mathrm{Tr}\Big[\exp\Big(\sum_j \lambda_j \hat{A}_j\Big)\Big]}_{Z}\Big\} = \frac{1}{Z}\frac{\partial Z}{\partial \lambda_i} = \frac{\partial \ln Z}{\partial \lambda_i}$$

As we will see $\ln Z$ is the quantity we want to calculate!

From the partition function it is actually possible to obtain the average of the different operators

differentiating with respect to the lagrange multiplyers...

$$\frac{1}{Z}\frac{\partial}{\partial\lambda_j} \mathrm{Tr} \exp \sum_i \lambda_i \hat{A}_i = \frac{1}{Z} \mathrm{Tr}\left[\hat{A}_j \exp\left(\sum_i \lambda_i A_i\right)\right]$$

true because we using the trace

$$= \mathrm{Tr}\left[A_j \underbrace{\frac{1}{Z}\exp\left(\sum_i \lambda_i A_i\right)}_{D_3}\right] = \langle \hat{A}_j \rangle$$

$$\langle \hat{A}_j \rangle = \frac{1}{Z}\frac{\partial Z}{\partial \lambda_j} = \frac{\partial}{\partial \lambda_j} \ln Z[\lambda_j]$$

$$\Rightarrow \quad \frac{1}{k} S_B = \ln Z - \sum_i \lambda_i \frac{\partial \ln Z}{\partial \lambda_i}$$ Legendre transform !!!

$\frac{1}{k} S_B$ Legendre transform of $\ln Z$

In differential form

average quantity

$$d \ln Z = \sum_i A_i \, d\lambda_i$$

$$dS_B = -k \sum_i \lambda_i \, dA_i$$

Fluctuation Response Theorem

Prologue

$$e^A e^B \neq e^A e^B \quad \text{unless } [A,B]$$

$$\exp A \exp B = \exp\left[A+B+\frac{1}{2}[A,B]+\frac{1}{12}\left([A,[A,B]]+[B[B,A]]\right)+\dots\right]$$

Let me define

$$K(x) = e^{x(A+B)}e^{-xA}$$

$$\frac{dK(x)}{dx} = \underbrace{e^{x(A+B)}(A+B)e^{-xA}}_{\text{commutes}} - e^{x(A+B)}\underbrace{Ae^{-xA}}_{\text{commutes}}$$

$$= e^{x(A+B)}Ae^{-xA} + e^{x(A+B)}Be^{-xA} - e^{x(A+B)}Ae^{-xA} = e^{x(A+B)}Be^{-xA}$$

$$\int_0^1 \frac{dK(x)}{dx}dx = \int_0^1 dx\, e^{x(A+B)}Be^{-xA}$$

$$K(1) - K(0) = \int_0^1 dx\, e^{x(A+B)}Be^{-xA}$$

$$K(0) = \hat{\mathbb{I}}$$

$$K(1) = e^{A+B}e^{-A}$$

$$e^{A+B}e^{-A} = \mathbb{I} + \int_0^1 dx\, e^{x(A+B)}Be^{-xA} \qquad \times e^{A}$$

does not depend on x

$$e^{A+B} = e^{A} + \int_0^1 dx\, e^{x(A+B)}Be^{(1-x)A}$$

taking $B \to \lambda B$ with $\lambda \to 0$

$$\exp \hat{A} \exp \lambda \hat{B} = \exp \underbrace{\left\{ \hat{A} + \lambda \hat{B} + \frac{1}{2}[\hat{A}, \lambda \hat{B}] + \frac{1}{12}\left([\hat{A},[\hat{A},\lambda\hat{B}]] + [\lambda\hat{B},[\lambda\hat{B},\hat{A}]]\right) + \dots \right\}}_{\mathbb{C} = A + \lambda D(\lambda)}$$

Keeping terms only to order λ

$$\exp A \exp \lambda B = \exp A(\mathbb{I} + \lambda \hat{B}) = \sum_{n=0}^{\infty} \frac{\mathbb{C}^n}{n!}$$

$$\Rightarrow \quad e^{\hat{A}+\lambda\hat{B}} = e^{\hat{A}} + \lambda \int_0^1 dx \, \underbrace{e^{x(\hat{A}+\lambda\hat{B})}}_{\sum_{n=0}^{\infty} \frac{x^n (A+\lambda B)^n}{n!}} \hat{B} e^{(1-x)\hat{A}}$$

Note: The only term that is not order λ or greater is e^{xA}

If it is order λ or greater the integral will be order λ^2 or greater

$$= e^{\hat{A}} + \lambda \int_0^1 dx \, e^{x\hat{A}} B e^{(1-x)\hat{A}}$$

Note: $\mathrm{Tr}[A, \lambda B] = 0$ $\quad \mathrm{Tr}[\lambda AB - \lambda BA] = \mathrm{Tr}[\lambda AB] - \underbrace{\mathrm{Tr}[\lambda BA]}_{\text{cyclical}}$

$= \mathrm{Tr}[\lambda AB]$

$$\mathrm{Tr}\left[e^{\hat{A}+\lambda\hat{B}}\right] = \mathrm{Tr}\left[e^{\hat{A}} e^{\lambda\hat{B}}\right] \sim \mathrm{Tr}\left[e^{\hat{A}}(1+\lambda\hat{B})\right]$$

$$\mathrm{Tr}\left[e^{\hat{A}+\lambda\hat{B}}\right] \sim \mathrm{Tr}\left[e^{\hat{A}} + \lambda e^{\hat{A}} B\right] = \mathrm{Tr}\left[e^{\hat{A}} + \lambda \int_0^1 dx \, e^{x\hat{A}} \hat{B} e^{(1-x)\hat{A}}\right]$$

$$\Rightarrow \cancel{\mathrm{Tr}\left[e^{\hat{A}}\right]} + \cancel{\lambda}\mathrm{Tr}\left[e^{\hat{A}}\hat{B}\right] \sim \cancel{\mathrm{Tr}\left[e^{\hat{A}}\right]} + \cancel{\lambda}\mathrm{Tr}\left[\int_0^1 dx \, e^{x\hat{A}} \hat{B} e^{(1-x)\hat{A}}\right]$$

$$\Rightarrow \mathrm{Tr}\left[e^{\hat{A}}\hat{B}\right] = \mathrm{Tr}\left[\int_0^1 dx\, e^{x\hat{A}}\hat{B}e^{(1-x)\hat{A}}\right] \quad \text{I}$$

—//—

Let's take $\hat{A} \equiv \hat{A}(\lambda)$

$$\frac{d}{d\lambda}e^{\hat{A}(\lambda)} = \frac{d}{d\lambda}\left(\sum_{n=0}^{\infty}\frac{A(\lambda)^n}{n!}\right)$$

$$\frac{d\hat{A}(\lambda)^n}{d\lambda} = \sum_{m=0}^{n-1}\hat{A}(\lambda)^m\frac{d\hat{A}(\lambda)}{d\lambda}\hat{A}^{n-1-m}$$

Because $\hat{A}(\lambda)$ and $\frac{d\hat{A}(\lambda)}{d\lambda}$ do not necessarily commute

$$= \sum_{n=0}^{\infty}\frac{1}{n!}\sum_{m=0}^{n-1}\hat{A}(\lambda)^m\frac{d\hat{A}(\lambda)}{d\lambda}A(\lambda)^{n-m-1}$$

the first term $(n=0)$ is zero

$$= \sum_{n=1}^{\infty}\frac{1}{n!}\sum_{m=0}^{n-1}\hat{A}(\lambda)^m\frac{d\hat{A}}{d\lambda}A(\lambda)^{n-m-1}$$

$n'+1=n$

$$= \sum_{n=0}^{\infty}\frac{1}{(n+1)!}\sum_{m=0}^{n}A(\lambda)^m\frac{dA(\lambda)}{d\lambda}A(\lambda)^{n-m}$$

$$\Theta(n-m) = \begin{cases}1 & n \geq m\\ 0 & n < m\end{cases}$$

$$= \sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{\Theta(n-m)}{(n+1)!}A(\lambda)^m\frac{dA(\lambda)}{d\lambda}A(\lambda)^{n-m}$$

$$= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{\Theta(n-m)}{(n+1)!}A(\lambda)^m\frac{dA(\lambda)}{d\lambda}A(\lambda)^{n-m}$$

$p=n-m$

$-m \leq p \leq \infty$

$p \geq 0$

$$= \sum_{m=0}^{\infty}\sum_{p=-m}^{\infty}\frac{\Theta(p)}{(p+m+1)!}A(\lambda)^m\frac{dA(\lambda)}{d\lambda}A(\lambda)^p$$

$$= \sum_{m=0}^{\infty} \sum_{p=0}^{\infty} \frac{p!\, m!}{(p+m+1)!} \frac{A(\lambda)^m}{m!} \frac{dA(\lambda)}{d\lambda} \frac{A(\lambda)^p}{p!}$$

Beta function

$$B(x,y) = \int_0^1 t^{x-1}(1-t)^{y-1}\,dt = \frac{(x-1)!\,(y-1)!}{(x+y-1)!}$$

$$x - 1 = m$$
$$y - 1 = p$$

$$\int_0^1 t^m (1-t)^p\,dt = \frac{m!\,p!}{(p+m+1)!}$$

$$= \sum_{m=0}^{\infty} \sum_{p=0}^{\infty} \int_0^1 dx\; x^m (1-x)^p \frac{A(\lambda)^m}{m!} \frac{dA(\lambda)}{d\lambda} \frac{A(\lambda)^p}{p!}$$

$$= \int_0^1 dx \sum_{m=0}^{\infty} \frac{[x A(\lambda)]^m}{m!} \frac{dA(\lambda)}{d\lambda} \sum_{p=0}^{\infty} \frac{[(1-x)A(\lambda)]^p}{p!}$$

$$\Rightarrow \quad \frac{d e^{A(\lambda)}}{d\lambda} = \int_0^1 dx\; e^{xA(\lambda)} \frac{dA(\lambda)}{d\lambda} e^{(1-x)A(\lambda)} \qquad \text{II}$$

Following Snider
Journal of Mathematical Physics
5, 1580 (1964)

I

$$\mathrm{Tr}\left[e^{\hat{A}}\hat{B}\right] = \mathrm{Tr}\left[\int_0^1 dx\, e^{x\hat{A}}\hat{B}\, e^{(1-x)\hat{A}}\right]$$

$$\hat{B} \to \frac{d\hat{A}}{d\lambda}$$

$$\mathrm{Tr}\left[e^{\hat{A}}\frac{d\hat{A}}{d\lambda}\right] = \mathrm{Tr}\left[\int_0^1 dx\, e^{x\hat{A}}\frac{d\hat{A}}{d\lambda}\, e^{(1-x)\hat{A}}\right]$$

II

$$\mathrm{Tr}\left[\frac{de^{A(\lambda)}}{d\lambda}\right] = \mathrm{Tr}\left[\int_0^1 dx\, e^{x\hat{A}(\lambda)}\frac{d\hat{A}}{d\lambda}\, e^{(1-x)\hat{A}}\right]$$

$$\frac{d}{d\lambda}\left[\mathrm{Tr}\left[e^{A(\lambda)}\right]\right] = \mathrm{Tr}\left[e^{\hat{A}}\frac{d\hat{A}}{d\lambda}\right]$$

$$\frac{\partial\langle\hat{A}_i\rangle}{\partial\lambda_j} = \frac{d}{d\lambda_j}\left(\mathrm{Tr}[\hat{A}_i\mathcal{D}]\right) = \mathrm{Tr}\left[\cancelto{0}{\frac{d\hat{A}_i}{d\lambda_j}}\mathcal{D} + \hat{A}_i\frac{\partial\mathcal{D}}{\partial\lambda_j}\right]$$

$$\hat{A}_i\frac{\partial\mathcal{D}}{\partial\lambda_j} = \hat{A}_i\frac{\partial}{\partial\lambda_j}\left[\frac{1}{Z}\exp\left(\sum_k\lambda_k\hat{A}_k\right)\right] = \overset{①}{-\frac{\hat{A}_i\, e^{\sum_k\lambda_k\hat{A}_k}}{Z^2}\frac{\partial Z}{\partial\lambda_j}} + \overset{②}{\frac{\hat{A}_i}{Z}\frac{\partial}{\partial\lambda_j}e^{\sum_k\lambda_k\hat{A}_k}}$$

② $$\frac{\hat{A}_i}{Z}\frac{\partial}{\partial\lambda_j}e^{\sum_k\lambda_k\hat{A}_k} = \frac{\hat{A}_i}{Z}\int_0^1 dx\; e^{x\hat{A}(\lambda)}\frac{d}{d\lambda_j}\left(\sum_k\lambda_k\hat{A}_k\right)e^{(1-x)\hat{A}(\lambda)}$$

$$\hat{A}(\lambda) = \sum_k\lambda_k\hat{A}_k \qquad \frac{\partial\hat{A}(\lambda)}{\partial\lambda_j} = \hat{A}_j$$

$$= \hat{A}_i\int_0^1 dx\;\frac{e^{x\hat{A}(\lambda)}}{Z^x}\hat{A}_j\frac{e^{(1-x)\hat{A}(\lambda)}}{Z^{(1-x)}} = \hat{A}_i\int_0^1 dx\left(\frac{e^{\hat{A}(\lambda)}}{Z}\right)^x\hat{A}_j\left(\frac{e^{\hat{A}(\lambda)}}{Z}\right)^{(1-x)}$$

$$\mathcal{D} = \frac{e^{\sum_k\lambda_k\hat{A}_k}}{Z} = \frac{e^{A(\lambda)}}{Z}$$

$$= \int_0^1\hat{A}_i\mathcal{D}^x\hat{A}_j\mathcal{D}^{(1-x)}\,dx$$

①

$$-\hat{A}_i\frac{e^{\sum_k\lambda_k\hat{A}_k}}{Z^2}\frac{\partial Z}{\partial\lambda_j} = -\hat{A}_i\frac{\mathcal{D}}{Z}\frac{\partial Z}{\partial\lambda_j} = -\frac{\hat{A}_i\mathcal{D}}{Z}\mathrm{Tr}\frac{\partial e^{\sum_k\hat{A}_k\lambda_k}}{\partial\lambda_j}$$

But from ②

$$\frac{1}{Z}\frac{\partial e^{\sum_k\lambda_k\hat{A}_k}}{\partial\lambda_k} = \int_0^1\mathcal{D}^x\hat{A}_j\mathcal{D}^{(1-x)}dx$$

$$\Rightarrow \quad -\hat{A}_i \mathcal{D}\, \mathrm{Tr}\left[\int_0^1 \mathcal{D}^x \hat{A}_j \mathcal{D}^{(1-x)} dx\right]$$

$$\frac{\partial \hat{A}_i}{\partial \lambda_j} = \mathrm{Tr}\left[-\hat{A}_i \mathcal{D}\, \underbrace{\mathrm{Tr}\int_0^1 \mathcal{D}^x \hat{A}_j \mathcal{D}^{(1-x)} dx}_{\text{number} \Rightarrow \text{can be taken out of the trace}}\right] + \mathrm{Tr}\left[\int_0^1 \hat{A}_i \mathcal{D}^x \hat{A}_j \mathcal{D}^{(1-x)} dx\right]$$

$$\frac{\partial \hat{A}_j}{\partial \lambda_j} = -\underbrace{\mathrm{Tr}\left[\hat{A}_i \mathcal{D}\right]}_{\langle \hat{A}_i \rangle} \mathrm{Tr}\left[\int_0^1 \mathcal{D}^x \hat{A}_j \mathcal{D}^{(1-x)} dx\right] + \mathrm{Tr}\left[\int_0^1 \hat{A}_i \mathcal{D}^x \hat{A}_j \mathcal{D}^{(1-x)} dx\right]$$

Note that

$$\mathrm{Tr}\left[\int_0^1 dx\, \mathcal{D}^x \mathcal{D}^{1-x}\right] = \int_0^1 \underbrace{\mathrm{Tr}\left[\mathcal{D}^x \mathcal{D}^{1-x}\right]}_{1} dx = \int_0^1 dx = 1$$

$$\Rightarrow \frac{\partial A_i}{\partial \lambda_j} = \int_0^1 \mathrm{Tr}\left[(\hat{A}_i - \langle A_i \rangle)\mathcal{D}^x \hat{A}_j \mathcal{D}^{(1-x)}\right] dx$$

Let's now calculate

$$\int_0^1 \mathrm{Tr}\left[(\hat{A}_i - \langle A_i \rangle)\mathcal{D}^x \langle \hat{A}_j \rangle \mathcal{D}^{1-x}\right] dx = \int_0^1 \mathrm{Tr}\left[(\hat{A}_i - \langle \hat{A}_i \rangle)\mathcal{D}\right] dx \langle \hat{A}_j \rangle$$

$$= \langle A_j \rangle \left\{ \underbrace{\int_0^1 \mathrm{Tr}\left[\hat{A}_i \mathcal{D}\right] dx}_{\langle \hat{A}_i \rangle} - \langle A_i \rangle \underbrace{\int_0^1 \mathrm{Tr}\left[\mathcal{D}\right] dx}_{1} \right\} = 0$$

so... without loss of generality we can add or subtract this term

$$C_{ij} = \frac{\partial A_i}{\partial \lambda_j} = \frac{\partial \ln Z}{\partial \lambda_i \partial \lambda_j} = \int_0^1 dx \, \mathrm{Tr}\left[\left(\hat{A}_i - \langle A_i \rangle \right) D^x \left(\hat{A}_j - \langle A_j \rangle \right) D^{1-x} \right.$$

Fluctuation response theorem

for arbitrary a_i

$$\sum_{ij} a_i a_j C_{ij} = \int_0^1 dx \; \mathrm{Tr}\Big[\underbrace{\sum_i c_i(\hat{A}_i - \langle A_i\rangle)}_{\hat{B}} \mathcal{D}^x \underbrace{\sum_j c_j(\hat{A}_j - \langle A_j\rangle)}_{\hat{B}} \mathcal{D}^{1-x}\Big]$$

$$\hat{B} = \sum_\ell c_\ell (\hat{A}_\ell - \langle \hat{A}_\ell \rangle)$$

a general matrix because the a_i are arbitrary

$$= \int_0^1 dx \; \mathrm{Tr}\left[\hat{B}\mathcal{D}^x \hat{B}\mathcal{D}^{1-x}\right]$$

I'll calculate the trace in the basis that diagonalizes $\mathcal{D}$

$$\mathcal{D} = \sum_m P_m |m\rangle\langle m|$$

$$\mathcal{D}^x |m\rangle = P_m^x |m\rangle$$

$$\mathcal{D}^{1-x} |m\rangle = P_m^{1-x}$$

$$= \int_0^1 dx \sum_m \langle m|\hat{B} \sum_{m'} P_{m'}^x |m'\rangle\langle m'| B \, P_m^{1-x} |m\rangle$$

$$= \int_0^1 dx \sum_{m\,m'} P_{m'}^x \underbrace{\langle m|\hat{B}|m'\rangle}_{B_{mm'}} \underbrace{\langle m'|B|m\rangle}_{B_{m'm}} P_m^{1-x} \geq 0$$

$|B_{mm'}|^2 \geq 0$ $\quad P_{m'}^x \geq 0$ $\quad P_m^{1-x} \geq 0$

Convex function of λ_i

Finally, let's calculate the time evolution of the statistical entropy

In principle

$$\frac{d}{dt}[\underbrace{-kD\ln D}_{f(D)}]$$

Expanding as a Taylor series

$$f(\hat{A}) = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(0)\,\hat{A}^n$$

but in general $\left[\frac{d\hat{A}}{dt}, \hat{A}\right] \neq 0$

so $$\frac{d\hat{A}^n}{dt} = \frac{d\hat{A}}{dt}\hat{A}^{n-1} + \hat{A}\frac{d\hat{A}}{dt}\hat{A}^{n-2} + \ldots + \hat{A}^{n-1}\frac{d\hat{A}}{dt} \neq n\hat{A}^{n-1}\frac{d\hat{A}}{dt}$$

in general

But

$$\mathrm{Tr}\, AB = \mathrm{Tr}\, BA$$

exercise $$\mathrm{Tr}\, ABC = \mathrm{Tr}\, CAB = \mathrm{Tr}\, BCA$$ → cyclical

$$\Rightarrow \mathrm{Tr}\left(\frac{d\hat{A}^n}{dt}\right) = n\,\mathrm{Tr}\left(\hat{A}^{n-1}\frac{d\hat{A}}{dt}\right)$$

$$\Rightarrow \mathrm{Tr}\left(\frac{d}{dt}f(A)\right) = \mathrm{Tr}\left[f'(A)\frac{dA}{dt}\right]$$

In differential form

$$d(\mathrm{Tr}\, f(A)) = \mathrm{Tr}\,(f'(A)\,dA)$$

In our case

$$S[D] = -k D \ln D$$

$$\frac{d(x \ln x)}{dx} = \ln x + \frac{x}{x} = \ln x + 1$$

$$S[D] = -k \,\mathrm{Tr}\left[(\ln D + D)\frac{dD}{dt}\right] = -k \,\mathrm{Tr}\left[\ln D \frac{dD}{dt}\right]$$

But $\mathrm{Tr} \frac{dD}{dt} = 0$

—//—

Using

$$i\hbar \frac{dD}{dt} = [H, D]$$

$$\frac{dS[D]}{dt} = -k \,\mathrm{Tr}\left[\ln D \frac{1}{i\hbar}[H, D]\right] = -\frac{k}{i\hbar} \mathrm{Tr}\left[\ln D (HD - DH)\right]$$

$$= -\frac{k}{i\hbar} \mathrm{Tr}\left[-H \ln D\, D + H D \ln D\right] = -\frac{k}{i\hbar} \mathrm{Tr}\left[H \underbrace{[D, \ln D]}_{\text{commute}}\right]$$

trace is cyclic

$$\frac{dS[D]}{dt} = 0$$

$S[D]$ is conserved !!!

Note: This is true even when $H = H(t)$
(we will return to this point later)