The information entropy of quantum mechanical states

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Motivation

How do I teach statistical mechanics...

(1) Thermal equilibrium $\rightsquigarrow$ canonical state

$$p_r \;=\; \frac{1}{Z}\mathrm{e}^{-\beta E_r}$$

(2) Deriving expression for $đQ$.

(3) Looking for an integration factor...

$$T \;=\; 1/\beta$$

(4) Defining entropy function

$$đQ \;=\; T d\mathcal{S}$$

(5) Writing the derived expression as

$$\mathcal{S} = -\sum_r p_r \ln(p_r)$$

Information theory point of view

Shannon:

$$\mathcal{S} = -\sum_r P_r \ln(P_r)$$

What is the lable r ?

r labels the possible outputs.

It is the energy in the themodynamic application.

Central observation:

One has to define the measurement setup.

How this is done?

classically - partitioning of phase space into cells.

quantum mechanically - choice of basis.

Classical definition of entropy

Classical state
(given partitioning $\mathcal{A}$ of phase space):

$$\rho \longrightarrow (P_1, P_2, P_3, ..., P_N)$$

Shannon formula:

$$S[\rho|\mathcal{A}] \; = \; -\sum_a P_a \ln(P_a)$$

Classical pure state:

$$S = 0$$

Classical mixture of n states:

$$S = \ln(n)$$

Maximally mixed state:

$$S = \ln(N)$$

Note: Chaos $\rightsquigarrow$ growth of entropy with time until ergodization. This assumes a partitioning $\mathcal{A}$ that does not commute with $\mathcal{H}$.

Quantal definition of entropy

Quantum mechanical state:

$\rho \rightarrow$ probability matrix $(N \times N)$

Assume basis $\mathcal{A}$ for measurement.

Maximally mixed state:

$$S[\rho|\mathcal{A}] = \ln(N)$$

General state:

$$S[\rho|\mathcal{A}] = -\sum_a P_a \ln(P_a)$$

where $P_a = \langle a|\rho|a\rangle$

Minimum entropy $\rightsquigarrow$ von Neumann

$$S_{\mathrm{H}}[\rho] = -\sum_r p_r \ln(p_r) = -\mathrm{trace}(\rho \ln(\rho))$$

Quantal definition of absolute entropy

$$S[\rho] \;=\; \overline{S[\rho|\mathcal{A}]} \;=\; S_0(N) + F(p_1, p_2, ...)$$

Reasoning:

$$S_{\text{total}} = S[\mathcal{A}] + \sum_{\mathcal{A}} P(\mathcal{A}) S[\rho|\mathcal{A}]$$

$S_0(N)$ is the minimum uncertainty entropy

(related to the entropic uncertainty of Deutsch).

Excess statistical entropy:

$$S_{\text{F}}[\rho] = S[\rho] - S_0(N) = F(p_1, p_2, ...)$$

It is a measure for lack of purity.

Derivation - part one

$$f(s) = -s\ln(s)$$

$$\begin{aligned} S &= \overline{\sum_a f\left(\sum_r p_r |\langle r|a\rangle|^2\right)}^{\,A} \\ &= \overline{\sum_s f\left(\sum_r p_r |\langle r|U|s\rangle|^2\right)}^{\,U} \\ &= \overline{N f\left(\sum_r p_r |\langle r|\Psi\rangle|^2\right)}^{\,\Psi} \\ &= \overline{N f\left(\sum_r p_r (x_r^2 + y_r^2)\right)}^{\,\text{sphere}} \\ &= N \int_0^\infty f(s)\; P(s) ds \end{aligned}$$

$$s = \sum_r p_r |\Psi_r|^2 = \sum_{r=1}^{N} p_r (x_r^2 + y_r^2)$$

We have to find $P(s)$, and do the integral...

Derivation - part 2

$$P(s) = \left\langle \delta(s - \sum_r p_r(x_r^2 + y_r^2)) \right\rangle_{\text{sphere}}$$

$$\begin{aligned}
&= (N-1)! \int_0^\infty ds_1..ds_N \ \delta(1-\sum_r s_r)\delta(s-\sum_r p_r s_r) \\
&= (N-1)! \int_0^\infty .. \int \frac{d\omega d\nu}{(2\pi)^2} \mathrm{e}^{(1-\sum_r s_r)(i\nu+0)+i(s-\sum_r p_r s_r)\omega} \\
&= (N-1)! \int \frac{d\omega d\nu}{(2\pi)^2} \mathrm{e}^{i\nu+i\omega s} \prod_r \frac{1}{i\omega p_r + i\nu + 0} \\
&= \int \frac{d\omega}{2\pi} \frac{(N-1)!}{(i\omega)^{N-1}} \sum_r \mathrm{e}^{i\omega(s-p_r)} \prod_{r'(\neq r)} \frac{1}{p_{r'} - p_r} \\
&= (N-1) \sum_{(p_r > s)} \left[\prod_{r'(\neq r)} \frac{1}{p_r - p_{r'}} \right] (p_r - s)^{N-2}
\end{aligned}$$

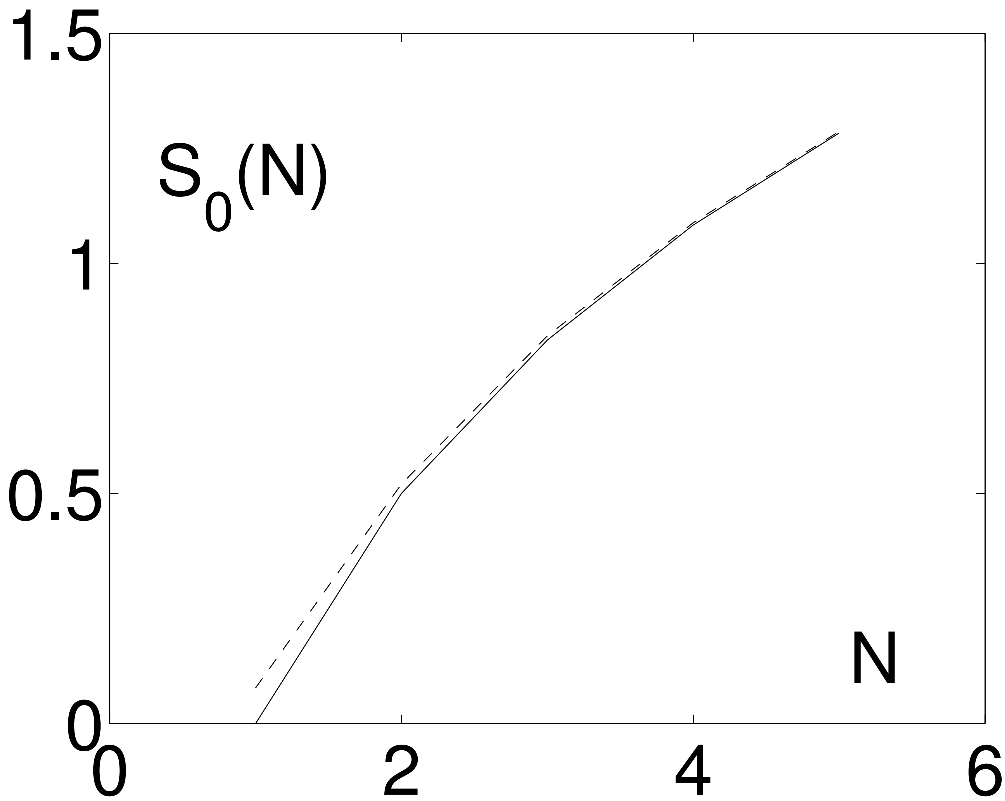
$$\int_0^p (p-s)^{N-2} s \ln(s) ds = \frac{p^N}{N(N-1)} \left[\ln(p) - \sum_{k=2}^{n} \frac{1}{k} \right]$$

Calculation for pure state

$$P(s) = (N-1)(1-s)^{N-2}$$

$$S_0(N) \; = \; \sum_{k=2}^{N} \frac{1}{k} \; \approx \; \ln(N) - (1-\gamma) + \frac{1}{2N}$$

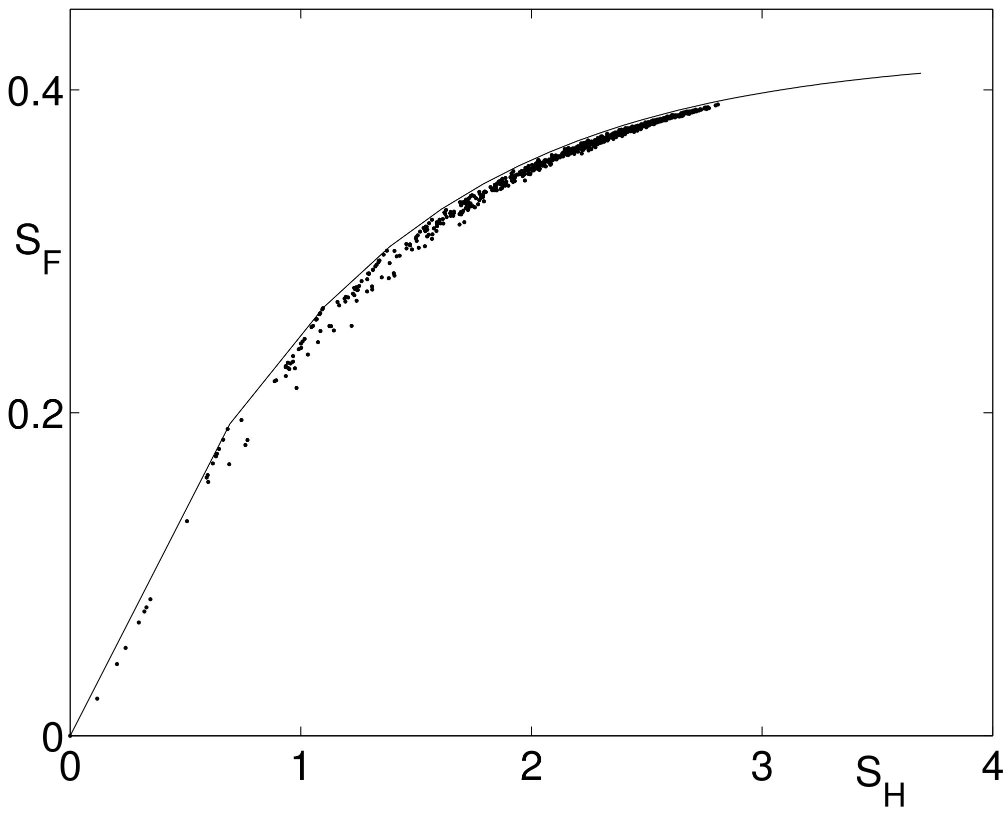
$$\rightsquigarrow \qquad S_{\mathrm{F}}[\rho] \; < \; 1-\gamma$$



Calculation for mixed state

$$P(s) = (N-1) \sum_{(p_r > s)} \left[\prod_{r'(\neq r)} \frac{1}{p_r - p_{r'}} \right] (p_r - s)^{N-2}$$

$$S_{\mathrm{F}}[\rho] = - \sum_{r} \left[\prod_{r'(\neq r)} \frac{p_r}{p_r - p_{r'}} \right] \, p_r \ln(p_r)$$



Special cases

For a mixture of two states we get:

$$S_{\mathrm{F}}[\rho] = -\frac{1}{p_1 - p_2}\left(p_1^2 \ln(p_1) - p_2^2 \ln(p_2)\right)$$

For a uniform mixture of n states we get:

$$S_{\mathrm{F}}[\rho] \quad = \quad \ln(n) - \sum_{k=2}^{n} \frac{1}{k}$$

Inequalities

Entropy of a subsystem:

$$S[\sigma] < S[\rho]$$

System composed of two independent subsystems:

$$S[\rho|\mathcal{A} \otimes \mathcal{B}] = S[\sigma_{\rm A}|\mathcal{A}] + S[\sigma_{\rm B}|\mathcal{B}]$$

Hence

$$S[\rho] \geq S[\sigma_{\rm A}] + S[\sigma_{\rm B}]$$

A particular case is:

$$S_0(NM) > S_0(N) + S_0(M)$$

On the other hand (generalization):

$$S_{\rm F}[\rho] \leq S_{\rm F}[\sigma_{\rm A}] + S_{\rm F}[\sigma_{\rm B}]$$

As in the case with von-Neumann:

$$S_{\rm H}[\rho] \leq S_{\rm H}[\sigma_{\rm A}] + S_{\rm H}[\sigma_{\rm B}]$$

Summary

We have found explicit expressions
for the minimum uncertainty entropy $S_0(N)$,
and for the excess statistical entropy $S_{\mathrm{F}}[\rho]$.

$S_{\mathrm{F}}[\rho]$ can be used as a measure for lack of purity of quantum mechanical states, and it is strongly correlated with the von-Neumann entropy $S_{\mathrm{H}}[\rho]$.

$S_{\mathrm{F}}[\rho]$ is bounded from above by $(1-\gamma)$.

The absolute information entropy $S[\rho]$, unlike the von-Neumann entropy, has properties that do make sense from information theory point of view.