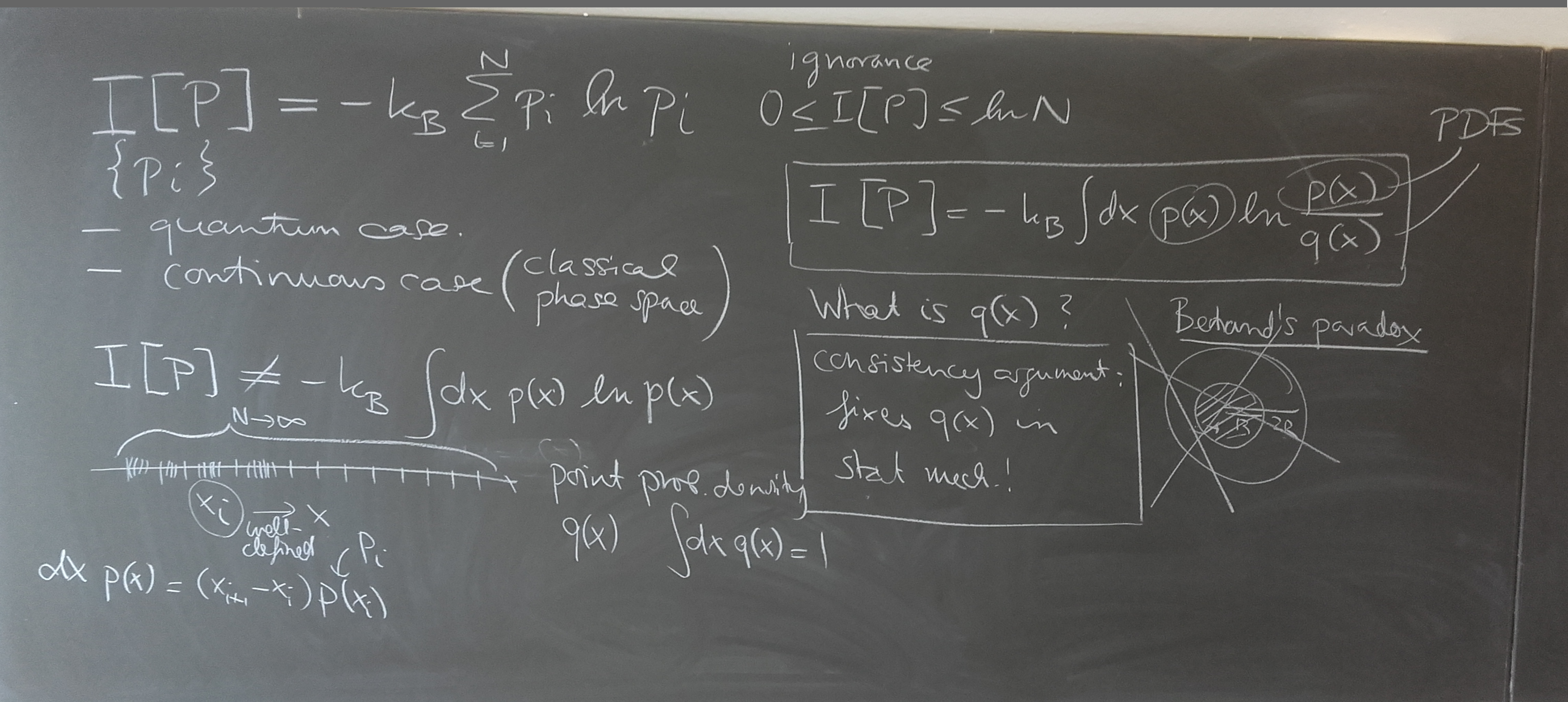
# Jaynes's principle and statistical mechanics

Ulrich Schollwöck, Bayes Forum, 11.1.2019



data $D \longrightarrow P = \arg\max\limits_{Q|D} I[Q]$

exact data $\mathring{D}$

means as data $\overline{D}$

$\mathcal{G} \stackrel{!}{=} \langle g \rangle = \sum P_\nu g_\nu$

$\overline{g}$ : time average

$P_\nu = \frac{1}{Z(\beta)} e^{-\beta g_\nu} \quad Z(\beta) = \sum\limits_\nu e^{-\beta g_\nu}$

$\mathcal{G} \stackrel{!}{=} \langle g \rangle = -\frac{\partial}{\partial \beta} \ln Z(\beta)$

$\mathcal{G} = \mathcal{G}(\beta)$

$\stackrel{inv}{\Longrightarrow} \beta = \beta(\mathcal{G})$

$\underline{\ln Z \text{ convex}}$

$-\frac{\partial \mathcal{G}}{\partial \beta} = \frac{\partial^2}{\partial \beta^2} \ln Z(\beta) = \langle g^2 \rangle - \langle g \rangle^2 > 0$

discussion: $\boxed{\mathcal{G} \rightarrow \beta}$ $\boxed{\beta \longrightarrow \mathcal{G}}$

$$\boxed{I_{max}(\mathcal{G}) = \ln Z(\beta) - \beta \underbrace{\frac{\partial}{\partial \beta}(\ln Z(\beta))}_{-\mathcal{G}}}$$

Legendre-Trafo $I_{max}[\mathcal{G}]$ $\boxed{\text{concave}}$

$\Updownarrow$

$\ln Z(\beta)$ convex

## Stat. Phys:

data $D$ — macrodata fixing a TD equilibrium state | macro state

proposition: $\underline{X} \in$ Phasespace / $|\psi\rangle \in$ Hilbert space | micro state.

a priori th: cl./q. mech.

$\boxed{\text{Post. I}}$ $\rho_{eq}(D) = \underset{\rho | D}{\arg\max}\, I[\rho]$

$\mathcal{O} = \langle O \rangle = \mathrm{tr}\, \rho_{eq} O$ prediction

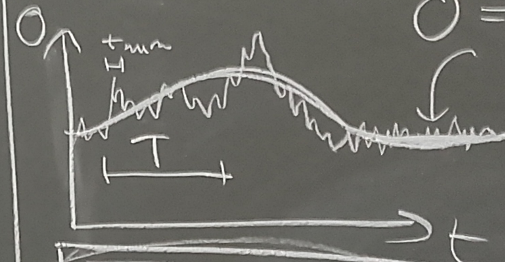
$\langle O^2 \rangle - \langle O \rangle^2 = ?$

predictivity

$\Delta O / |\langle O \rangle|$

$\underline{\rho_{eq}}$ is not distr. of microstates.

$$\bar{O} = \frac{1}{T} \int_0^T dt\, O(t)$$




$\boxed{\bar{O} = \langle O \rangle}$ problem! $T \to \infty$

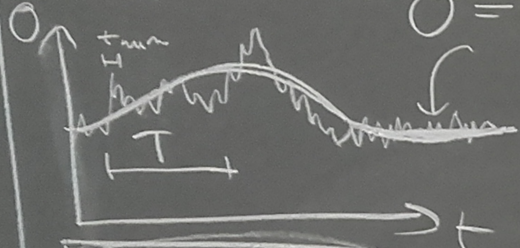
time-average = ensemble average

What is $S$?

$S_{\varphi}[\rho] = I[\rho]$

$\underline{\rho_{eq}}$ is not distr. of microstates.

$$\overline{O} = \frac{1}{T}\int_0^T dt\, O(t)$$




$$\boxed{\overline{O} = \langle O \rangle}$$

problem! $T \to \infty$

time-average = ensemble average

What is S?

$$S_{SP}[\rho] = I[\rho]$$

$$S_{SP}(D) = \underset{S_{SP}}{I}[\rho_{eq}(D)] = \max_{\rho \in D} S_{SP}[\rho]$$

extremal principle

$S_{SP}(D)$ looks mathematically like $S_{TD}$.

We can show that $S_{SP} = S_{TD}$ via laws of thermodynamics

hypothesis) $S_{TD}(D) \overset{\text{TD large}}{=} S_{SP}(D)$.

$\boxed{\text{2nd law}}$

$$I[\varrho] = -k_B \int d\mu(\underline{X})\, \varrho(\underline{X}) \ln \frac{\varrho(\underline{X})}{\varrho_0(\underline{X})} \qquad \underline{X} = (\underline{q}, \underline{p})^{6N}$$

$$\varrho_0(\underline{X}) = \text{cst.}$$

$$I[\varrho] = -k_B \int d\mu(\underline{X})\, \varrho(\underline{X}) \ln \varrho(\underline{X})$$

Jacobi-det of can. trafos = 1 $\quad (\underline{q}, \underline{p}) \to (\underline{Q}, \underline{P})$

Ham eq:

$$\dot{p} = \{H, q\}$$

$$\dot{q} = \{H, p\}$$

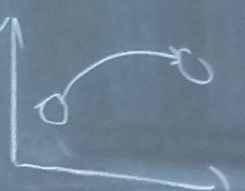
$K[\rho|\rho_0]$

If $I[\rho]$ is an information measure, then it must be t-indep under dynamics

$$\boxed{\frac{dI}{dt}=0}$$

$$\underline{V} = \left(\frac{\partial H}{\partial \underline{P}}, -\frac{\partial H}{\partial \underline{Q}}\right)$$

Liouville: $\boxed{\frac{\partial\rho}{\partial t}+\underline{V}\cdot\underline{\nabla}\rho=0}$



$\rho_0(\underline{X}, \cancel{t})$

norav

$\boxed{dq_1 \dots dp_N}$

$$0 \overset{!}{=} \frac{dI}{dt} = -\int \frac{d\underline{X}}{h^{3N}N!}\left(\frac{\partial\rho}{\partial t}\ln\frac{\rho}{\rho_0} + \cancel{\frac{\partial\rho}{\partial t}}\right)$$

$$= +\int dX\,(\underline{V}\cdot\underline{\nabla}\rho)\ln\frac{\rho}{\rho_0}$$

$$\underbrace{\frac{\partial}{\partial t}\int dX\,\rho}_{=0}$$

$$= -\int d\underline{X}\,\rho\,\underline{V}\cdot\underline{\nabla}\ln\frac{\rho}{\rho_0}$$

$$= -\int dX\left(\underline{V}\cdot\underline{\nabla}\rho - \rho\,\underline{V}\cdot\underline{\nabla}\ln\rho_0\right)$$

$$= \int dX\,\rho\,\underline{V}\cdot\underline{\nabla}\ln\rho_0$$

$$\frac{1}{X}$$

$$\Rightarrow \underline{V}\cdot\underline{\nabla}\ln\rho_0 = 0 \Rightarrow \underline{\nabla}\ln\rho_0 = 0$$

$\rho_0 = \text{const}$

$\bar{O} = \langle O \rangle = \mathrm{tr}\, \rho O \qquad \frac{1}{N}\sum_i x_i$

measure: $\langle \bar{O} \rangle = \cancel{\frac{1}{T}\int_0^T dt\, \langle O(t) \rangle} = \langle O \rangle$

$\bar{O} \stackrel{?}{=} \langle O \rangle$

$\boxed{\langle \bar{O} \rangle = \langle O \rangle}$

$\cancel{x}\ \langle O^2 \rangle - \langle O \rangle^2$

$\langle \bar{O}^2 \rangle - \langle \bar{O} \rangle^2$

$\bar{O} = \langle \bar{O} \rangle$

$\boxed{\bar{O} = \langle O \rangle}$

$\boxed{\mathcal{C} = \langle O(0)\, O(t) \rangle - \langle O \rangle^2}$

$(O(t) - \bar{O})(O(t') - \bar{O})$

$$\Delta^2 \bar{O} = \frac{1}{T^2}\iint_0^T dt_1\, dt_2 \left(\langle O(t_1) O(t_2) \rangle - \langle O(t_1) \rangle \langle O(t_2) \rangle\right)$$

$$= \frac{2}{T^2}\int_0^T d\tau\, (T - \tau)\, C(\tau)$$

$$\sim \frac{1}{T} \longrightarrow \Delta \bar{O} \sim \frac{1}{\sqrt{T}}$$

$\int_0^\infty C(\tau)\, d\tau < \infty$

$\int_0^\infty C(\tau)\, \tau\, d\tau < \infty$

$E(t)$

$\overline{\delta^2 O} = \frac{1}{T}\int dt\, (O(t) - \bar{O})^2$

$\langle \overline{\delta^2 O} \rangle = \Delta^2 O - \cancel{\Delta^2 \bar{O}}$