# *Thermodynamics from relative entropy*

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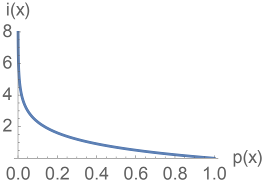
# *Entropy and information*

[Claude Shannon (1948), also Ludwig Boltzmann, Willard Gibbs (∼1875)]

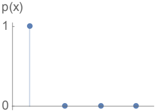
- consider a random variable $x$ with probability distribution $p(x)$
- information content or "surprise" associated with outcome $x$

$$i(x) = -\ln p(x)$$

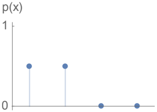



- entropy is expectation value of information content

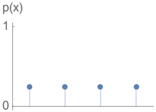
$$S(p) = \langle i(x) \rangle = -\sum_x p(x) \ln p(x)$$




$S = 0$




$S = \ln(2)$




$S = 2\ln(2)$

## *Thermodynamics*

[..., Antoine Laurent de Lavoisier, Nicolas Léonard Sadi Carnot, Hermann von Helmholtz, Rudolf Clausius, Ludwig Boltzmann, James Clerk Maxwell, Max Planck, Walter Nernst, Willard Gibbs, ...]

- micro canonical ensemble: maximum entropy $S$ for given conserved quantities $E, N$ in given volume $V$
- starting point for development of thermodynamics ...

$$S(E, N, V), \qquad dS = \frac{1}{T}dE - \frac{\mu}{T}dN + \frac{p}{T}dV$$

- ... grand canonical ensemble with density operator ...

$$\rho = \frac{1}{Z}e^{-\frac{1}{T}(H-\mu N)}$$

- ... Einsteins probability for classical thermal fluctuations ...

$$dW \sim e^{S(\xi)}d\xi$$

## *Fluid dynamics*

- uses thermodynamics *locally*

$$T(x), \qquad \mu(x), \qquad u^\mu(x), ...$$

- evolution from conservation laws

$$\nabla_\mu T^{\mu\nu}(x) = 0, \qquad \nabla_\mu N^\mu(x) = 0.$$

- local dissipation = local entropy production

$$\nabla_\mu s^\mu(x) = \partial_t s(x) + \vec{\nabla} \cdot \vec{s}(x) > 0$$

- in Navier-Stokes approximation with shear viscosity $\eta$, bulk viscosity $\zeta$

$$\nabla_\mu s^\mu = \frac{1}{T} \left[ 2\eta \sigma_{\mu\nu} \sigma^{\mu\nu} + \zeta (\nabla_\rho u^\rho)^2 \right]$$

- how to understand this in quantum field theory?

# *Entropy in quantum theory*

[John von Neumann (1932)]

$$S = -\mathrm{Tr}\{\rho \ln \rho\}$$

- based on the quantum density operator $\rho$
- for pure states $\rho = |\psi\rangle\langle\psi|$ one has $S = 0$
- for diagonal mixed states $\rho = \sum_j p_j |j\rangle\langle j|$

$$S = -\sum_j p_j \ln p_j > 0$$

- unitary time evolution conserves entropy

$$-\mathrm{Tr}\{(U\rho U^\dagger)\ln(U\rho U^\dagger)\} = -\mathrm{Tr}\{\rho \ln \rho\} \qquad \to \qquad S = \text{const.}$$

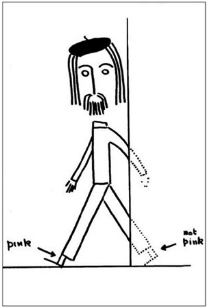
- quantum information is globally conserved

# *Quantum entanglement*

- *Can quantum-mechanical description of physical reality be considered complete?* [Albert Einstein, Boris Podolsky, Nathan Rosen (1935), David Bohm (1951)]

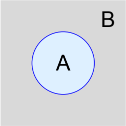
$$\psi = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_A|\downarrow\rangle_B - |\downarrow\rangle_A|\uparrow\rangle_B\right)$$
$$= \frac{1}{\sqrt{2}}\left(|\rightarrow\rangle_A|\leftarrow\rangle_B - |\leftarrow\rangle_A|\rightarrow\rangle_B\right)$$

- *Bertlemann's socks and the nature of reality* [John Stewart Bell (1980)]



# *Entropy and entanglement*

- consider a split of a quantum system into two $A + B$




- reduced density operator for system $A$

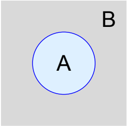
$$\rho_A = \mathrm{Tr}_B\{\rho\}$$

- entropy associated with subsystem A

$$S_A = -\mathrm{Tr}_A\{\rho_A \ln \rho_A\}$$

- pure product state $\rho = \rho_A \otimes \rho_B$ leads to $S_A = 0$
- pure entangled state $\rho \neq \rho_A \otimes \rho_B$ leads to $S_A > 0$
- $S_A$ is called entanglement entropy

# *Entanglement entropy in relativistic quantum field theory*




- entanglement entropy of region $A$ is a local notion of entropy

$$S_A = -\mathrm{tr}_A \{\rho_A \ln \rho_A\} \qquad \rho_A = \mathrm{tr}_B \{\rho\}$$

- for relativistic quantum field theories it is infinite

$$S_A = \frac{\mathrm{const}}{\epsilon^{d-2}} \int_{\partial A} d^{d-2}\sigma\sqrt{h} \, + \text{ subleading divergences } + \text{ finite}$$

- UV divergence proportional to entangling surface
- relativistic quantum fields are very strongly entangled already in vacuum
- Theorem [Helmut Reeh & Siegfried Schlieder (1961)]: local operators in region $A$ can create all (non-local) particle states

# *Entanglement entropy in non-relativistic quantum field theory*

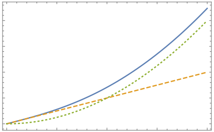
[Natalia Sanchez-Kuntz & Stefan Floerchinger, in preparation]

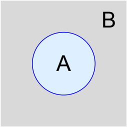
- non-relativistic quantum field theory for Bose gas

$$S = \int dt d^{d-1}x \left\{ \varphi^* \left[ i\partial_t + \frac{\vec{\nabla}^2}{2m} + \mu \right] \varphi - \frac{\lambda}{2} \varphi^{*2} \varphi^2 \right\}$$

- Bogoliubov dispersion relation

$$\omega = \sqrt{\frac{\vec{p}^2}{2M} \left( \frac{\vec{p}^2}{2M} + 2\lambda\rho \right)} \approx \begin{cases} c_s |\vec{p}| & \text{for} \quad p \ll \sqrt{2M\lambda\rho} \quad \text{(phonons)} \\ \frac{\vec{p}^2}{2M} & \text{for} \quad p \gg \sqrt{2M\lambda\rho} \quad \text{(particles)} \end{cases}$$






- entanglement entropy $S_A$ vanishes for $\rho = 0$ and $\omega = \frac{\vec{p}^2}{2M}$
- for large region $A$ like in relativistic theory
- inverse healing length $\sqrt{2M\lambda\rho}$ acts as UV regulator

# *Relative entropy*

- classical relative entropy or Kullback-Leibler divergence

$$S(p\|q) = \sum_j p_j \ln(p_j/q_j)$$

- not symmetric distance measure, but a *divergence*

$$S(p\|q) \geq 0 \qquad \text{and} \qquad S(p\|q) = 0 \quad \Leftrightarrow \quad p = q$$

- quantum relative entropy of two density matrices (also a *divergence*)

$$S(\rho\|\sigma) = \mathsf{Tr}\,\{\rho\,(\ln\rho - \ln\sigma)\}$$

- signals how well state $\rho$ can be distinguished from a model $\sigma$

## *Significance of Kullback-Leibler divergence*

Uncertainty deficit

- true distribution $p_j$ and model distribution $q_j$
- *uncertainty deficit* is expected surprise $\langle -\ln q_j \rangle = -\sum_j p_j \ln q_j$ minus real information content $-\sum_j p_j \ln p_j$

$$S(p\|q) = -\sum_j p_j \ln q_j - \left( -\sum_j p_j \ln p_j \right)$$

Asymptotic frequencies

- true distribution $q_j$ and frequency after $N$ drawings $p_j = \frac{N(x_j)}{N}$
- probability to find frequencies $p_j$ for large $N$ goes like

$$e^{-NS(p\|q)}$$

- probability for fluctuation around expectation value $\langle p_j \rangle = q_j$ tends to zero for large $N$ and when divergence $S(p\|q)$ is large

## *Advantages of relative entropy*

Continuum limit $\quad p_j \to f(x)dx \qquad q_j \to g(x)dx$

- not well defined for entropy

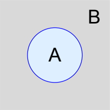
$$S = -\sum p_j \ln p_j \overset{\lightning}{\to} -\int dx f(x) \left[\ln f(x) + \ln dx\right]$$

- relative entropy remains well defined

$$S(p\|q) \to S(f\|g) = \int dx\, f(x) \ln(f(x)/g(x))$$

Local quantum field theory

- entanglement entropy $S(\rho_A)$ for spatial region divergent in relativistic QFT
- relative entanglement entropy $S(\rho_A\|\sigma_A)$ well defined
- rigorous definition in terms of Tomita–Takesaki theory of modular automorphisms on von-Neumann algebras [Huzihiro Araki (1976)]



## *Monotonicity of relative entropy*

[Göran Lindblad (1975)]

- monotonicity of relative entropy

$$S(\mathcal{N}(\rho)|\mathcal{N}(\sigma)) \leq S(\rho|\sigma)$$

with $\mathcal{N}$ completely positive, trace-preserving map

- $\mathcal{N}$ unitary time evolution

$$S(\mathcal{N}(\rho)|\mathcal{N}(\sigma)) = S(\rho|\sigma)$$

- $\mathcal{N}$ open system evolution with generation of entanglement to environment

$$S(\mathcal{N}(\rho)|\mathcal{N}(\sigma)) < S(\rho|\sigma)$$

- basis for many proofs in quantum information theory
- leads naturally to second-law type relations

# *Thermodynamics from relative entropy*

[Stefan Floerchinger & Tobias Haas, arXiv:2004.13533 (2020)]

- relative entropy has very nice properties
- but can thermodynamics be derived from it ?
- can *entropy* be replaced by *relative entropy* ?

# *Principle of maximum entropy*

[Edwin Thompson Jaynes (1963)]

- take macroscopic state characteristics as fixed, e. g.

  energy $E$, particle number $N$, momentum $\vec{p}$,

- principle of maximum entropy: among all possible microstates $\sigma$ (or distributions $q$) the one with *maximum entropy* $S$ is preferred

$$S(\sigma_{\text{thermal}}) = \text{max}$$

- why? assume $S(\sigma) < \text{max}$, than $\sigma$ would contain additional information not determined by macroscopic variables, which is not available
- maximum entropy $=$ minimal information

## *Principle of minimum expected relative entropy*

[Stefan Floerchinger & Tobias Haas, arXiv:2004.13533 (2020)]

- take macroscopic state characteristics as fixed, e. g.

  energy $E$, particle number $N$, momentum $\vec{p}$,

- principle of minimum expected relative entropy: preferred is the model $\sigma$ from which allowed states $\rho$ are least distinguishable on average

$$\langle S(\rho\|\sigma_{\text{thermal}})\rangle = \int D\rho\, S(\rho\|\sigma_{\text{thermal}}) = \text{min}$$

- similarly for classical probability distributions

$$\langle S(p\|q)\rangle = \int Dp\, S(p\|q) = \text{min}$$

- need to define *measures* $Dp$ and $D\rho$ on spaces of probability distributions $p$ and density matrices $\rho$, respectively

## *Measure on space of probability distributions*

- consider set of normalized probability distributions $p$ in agreement with macroscopic constraints
- manifold with local coordinates $\xi = \{\xi^1, \ldots, \xi^m\}$
- integration in terms of coordinates

$$\int Dp = \int d\xi^1 \cdots d\xi^m \, \mu(\xi^1, \ldots, \xi^m)$$

- want this to be invariant under coordinate changes $\xi \to \xi'(\xi)$
- possible choice is *Jeffreys prior* as integral measure [Harold Jeffreys (1946)]

$$\mu(\xi) = \text{const} \times \sqrt{\text{det } g_{\alpha\beta}(\xi)}$$

- uses Riemannian metric $g_{\alpha\beta}(\xi)$ on space of probability distributions: *Fisher information metric* [Ronald Aylmer Fisher (1925)]

$$g_{\alpha\beta}(\xi) = \sum_j \frac{\partial p_j(\xi)}{\partial \xi^\alpha} \frac{\partial \ln p_j(\xi)}{\partial \xi^\beta}$$

## *Permutation invariance*

- can now integrate functions of $p$

$$\int Dp\, f(p) = \int d^m\xi\, \mu(\xi)\, f(p(\xi))$$

- consider maps $\{p_1, \ldots p_{\mathcal{N}}\} \to \{p_{\Pi(1)}, \ldots p_{\Pi(\mathcal{N})}\}$ where $j \to \Pi(j)$ is a permutation, abbreviated $p \to \Pi(p)$
- want to show $Dp = D\Pi(p)$ such that

$$\int Dp\, f(p) = \int Dp\, f(\Pi(p))$$

- convenient to choose coordinates

$$p_j = \begin{cases} (\xi^j)^2 & \text{for } j = 1, \ldots, \mathcal{N}-1, \\ 1 - (\xi^1)^2 - \ldots - (\xi^{\mathcal{N}-1})^2 & \text{for } j = \mathcal{N}. \end{cases}$$

wich allows to write

$$\int Dp = \frac{1}{\Omega_{\mathcal{N}}} \int_{-1}^{1} d\xi^1 \cdots d\xi^{\mathcal{N}} \delta \left( 1 - \sqrt{\sum_{\alpha=1}^{\mathcal{N}} (\xi^\alpha)^2} \right) = \int D\Pi(p)$$

## *Minimizing expected relative entropy*

- consider now the functional

$$B(q,\lambda) = \int Dp \left[ S(p\|q) + \lambda \left( \sum_i q_i - 1 \right) \right]$$

- variation with respect to $q_j$

$$0 \overset{!}{=} \delta B = \sum_j \int Dp \left[ -\frac{p_j}{q_j} + \lambda \right] \delta q_j$$

leads by permutation invariance to the uniform distribution

$$q_j = \langle p_j \rangle = \frac{1}{\mathcal{N}}$$

- microcanonical distribution has minimum expected relative entropy!
- least distinguishable within the set of allowed distributions

# *Measure on space of density matrices*

- measure on space of density matrices $D\rho$ can be defined similarly in terms of coordinates $\xi$ but using now *quantum Fisher information metric*

$$g_{\alpha\beta}(\xi) = \mathsf{Tr}\left\{ \frac{\partial \rho(\xi)}{\partial \xi^\alpha} \frac{\partial \ln \rho(\xi)}{\partial \xi^\beta} \right\}$$

- definition uses symmetric logarithmic derivative such that

$$\frac{1}{2}\rho(d\ln\rho) + \frac{1}{2}(d\ln\rho)\rho = d\rho$$

- appears also as limit of relative entropy for states that approach each other

$$S(\rho(\xi + d\xi) \| \rho(\xi)) = \frac{1}{2} g_{\alpha\beta}(\xi) d\xi^\alpha d\xi^\beta + \dots$$

## *Unitary transformations as isometries*

- consider unitary map

$$\rho(\xi) \to \rho'(\xi) = U\rho(\xi)U^\dagger = \rho(\xi')$$

- again normalized density matrix but at coordinate point $\xi'$
- induced map on coordinates $\xi \to \xi'(\xi)$ is an *isometry*

$$g_{\alpha\beta}(\xi)d\xi^\alpha d\xi^\beta = g_{\alpha\beta}(\xi')d\xi'^\alpha d\xi'^\beta$$

- can be used to show invariance of measure such that

$$\int D\rho\, f(\rho) = \int D\rho\, f(U\rho U^\dagger)$$

# *Minimizing expected relative entropy on density matrices*

- consider now the functional

$$B = \int D\rho \, S(\rho \| \sigma) = \int d^m \xi \, \mu(\xi) \, S(\rho(\xi) \| \sigma)$$

- minimization $0 \stackrel{!}{=} \delta B$ leads to microcanonical density matrix

$$\sigma_{\mathsf{m}} = \frac{1}{\mathcal{N}} \mathbb{1}$$

  on space allowed by macroscopic constraints
- anyway only possibility for unique minimum $\sigma_{\mathsf{m}} = U \sigma_{\mathsf{m}} U^{\dagger}$

## *Microcanonical ensemble*

- microcanonical ensemble

$$\sigma_{\mathrm{m}} = \frac{1}{Z_{\mathrm{m}}} \delta(H - E(\sigma_{\mathrm{m}}))\delta(N - N(\sigma_{\mathrm{m}}))$$

- relative entropy of arbitrary state $\rho$ to microcanonical state

$$S(\rho \| \sigma_{\mathrm{m}}) = \begin{cases} -S(\rho) + S(\sigma_{\mathrm{m}}) & \text{for } E(\rho) \equiv E(\sigma_{\mathrm{m}}) \\ & \text{and } N(\rho) \equiv N(\sigma_{\mathrm{m}}) \\ +\infty & \text{else} \end{cases}$$

- differential for $dE(\rho) \equiv dE(\sigma_{\mathrm{m}})$ and $dN(\rho) \equiv dN(\sigma_{\mathrm{m}})$

$$\begin{aligned} dS(\rho \| \sigma_{\mathrm{m}}) &= -\, dS(\rho) + dS(\sigma_{\mathrm{m}}) \\ &= -\, dS(\rho) + \beta\, dE(\rho) - \beta\mu\, dN(\rho) \end{aligned}$$

- gives an alternative definition of temperature

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

# *Canonical and grand-canonical ensemble*

- transition to canonical and grand-canonical ensembles follows the usual construction

$$\sigma_{\text{gc}} = \frac{1}{Z} e^{-\beta(H-\mu N)}$$

- relative entropy of arbitrary state $\rho$ to grand-canonical state $\sigma_{\text{gc}}$

$$\begin{aligned} S(\rho\|\sigma_{\text{gc}}) = &- S(\rho) + S(\sigma_{\text{gc}}) + \beta\,(E(\rho) - E(\sigma_{\text{gc}})) \\ &- \beta\mu\,(N(\rho) - N(\sigma_{\text{gc}})). \end{aligned}$$

- differential

$$\begin{aligned} dS(\rho\|\sigma_{\text{gc}}) = &- dS(\rho) + \beta\,dE(\rho) - \beta\mu\,dN(\rho) \\ &+ (E(\rho) - E(\sigma_{\text{gc}}))\,d\beta \\ &- (N(\rho) - N(\sigma_{\text{gc}}))\,d(\beta\mu), \end{aligned}$$

- choices for $\beta = 1/T$ and $\mu$ such that $E(\rho) = E(\sigma_{\text{gc}})$ and $N(\rho) = N(\sigma_{\text{gc}})$ extremize relative entropy $S(\rho\|\sigma_{\text{gc}})$

## *Thermal fluctuations and relative entropy*

- "mesoscopic" quantities $\xi$ fluctuate in thermal equilibrium, for example energy in a subvolume
- traditional theory goes back to Einsteins work on critical opalescence [Albert Einstein (1910)]

$$dW \sim e^{S(\xi)} d\xi$$

- entropy can be replaced by relative entropy between state $\rho(\xi)$ (where $\xi$ is sharp) and thermal state $\sigma$ (where it $\xi$ is fluctuating)

$$dW = \frac{1}{Z} e^{-S(\rho(\xi)\|\sigma)} \sqrt{\det g_{\alpha\beta}(\xi)}\, d^m \xi$$

- resembles closely probability for fluctuations in frequencies $p_j = \frac{N(x_j)}{N}$

$$\sim e^{-NS(p\|q)}$$

# *Third law of thermodynamics*

[Walter Nernst (1905)]

- many equivalent formulations available already
- [Max Planck (1911)]: entropy $S$ approaches a constant for $T \to 0$ that is independent of other thermodynamic parameters

$$\lim_{T \to 0} S(\sigma) = S_0 = \text{const}$$

- new formulation with relative entropy: relative entropy $S(\rho_0 \| \sigma)$ between ground state $\rho_0$ and a thermodynamic model state $\sigma$ approaches zero for $T \to 0$

$$\lim_{T \to 0} S(\rho_0 \| \sigma) = 0$$

- second law can also be formulated with relative entropy

## *Local thermal equilibrium in a quantum field theory*

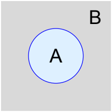
- consider non-equilibrium situation with
  - true density matrix $\rho$
  - local equilibrium approximation

$$\sigma = \frac{1}{Z} e^{-\int d\Sigma_\mu \{\beta_\nu(x) T^{\mu\nu} + \alpha(x) N^\mu\}}$$

- reduced density matrices $\rho_A = \mathrm{Tr}_B\{\rho\}$ and $\sigma_A = \mathrm{Tr}_B\{\sigma\}$
- $\sigma$ is very good model for $\rho$ in region $A$ when

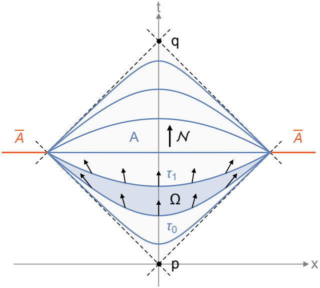
$$S_A = \mathrm{Tr}_A\{\rho_A(\ln \rho_A - \ln \sigma_A)\} \to 0$$

- does *not* imply that globally $\rho = \sigma$



# *Towards fluid dynamics in the context of quantum field theory*

[Neil Dowling, Stefan Floerchinger & Tobias Haas, in preparation]




- local description of quantum field theories in space-time regions bounded by two light cones [e. g. Rudolf Haag (1992), Huzihiro Araki (1992)]
- unitary evolution for isolated systems, CPTP map otherwise
- clarify the role of entanglement for local dissipation in fluids

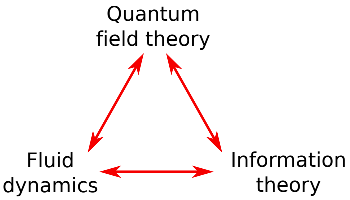
$$\nabla_\mu s^\mu(x) \geq 0$$

# *Conclusions & outlook*

- thermodynamics can be formulated in terms of relative entropy
- interesting new "functional integral" in spaces of probability distributions and density matrices
- connections to quantum information and information geometry
- entanglement properties of relativistic quantum fields rather interesting
- experimental tests with cold atoms?
- local form of second law & relativistic fluid dynamics
- functional integral representation for relative modular operators and for relative entropy

*Backup*

# *Quantum field dynamics*




- hypothesis

local dissipation = quantum entanglement generation

- quantum information is spread
- locally, quantum state approaches mixed state form
- full loss of *local* quantum information = *local* thermalization