Information geometry and generating functionals for quantum field theory

Stefan Floerchinger (Friedrich-Schiller-Universität Jena)

Functional Methods in Strongly Correlated Systems, September 2023
Darmstädter Haus, Hirschegg

FRIEDRICH-SCHILLER-
UNIVERSITÄT
JENA

The ideas of information geometry

[Ronald A. Fisher, Calyampudi R. Rao, Shun'ich Amari, Nikolai N. Chentsov, ...]

- studies spaces of probability distributions $p(x,\xi)$ with parameters ξ^α
- Fisher information metric (symmetric, positive semi-definite)

$$G_{\alpha\beta}(\xi) = \int dx\, p(x,\xi) \left(\frac{\partial}{\partial \xi^\alpha} \ln p(x,\xi)\right) \left(\frac{\partial}{\partial \xi^\beta} \ln p(x,\xi)\right)$$

- unique Riemannian metric that is invariant under sufficient statistics [Chentsov 1972]
- higher geometric structure: pair of dual connections, non-metricity etc. [Amari, Chentsov, ...]
- extension to quantum states $\rho(\xi)$
- geometric structure follows from a *divergence* or *relative entropy*

$$D(p\|q) = \int dx\; p(x) \ln(p(x)/q(x))$$

Sufficient statistics and Chentsov's theorem

- start from random variable x with probability distribution $p(x, \xi)$ where ξ^α are parameters
- consider map to new random variable $x \to y = f(x)$ with probability distribution $q(y, \xi)$
- information about ξ^α could get lost in the map
- new random variable y is called *sufficient statistic* for ξ when no information about ξ is lost:

$$p(x, \xi) = p(x|y, \xi) q(y, \xi) = r(x) q(y, \xi) \qquad \text{factorizes}$$

or

$$p(x|y, \xi) = \frac{p(x, \xi)}{q(y, \xi)} = r(x) \qquad \text{independent of} \quad \xi^\alpha$$

- Chentsov's invariance property: for sufficient statistic

$$\begin{aligned} G_{\alpha\beta}(\xi) &= \int dx\, p(x, \xi) \left(\frac{\partial}{\partial \xi^\alpha} \ln p(x, \xi) \right) \left(\frac{\partial}{\partial \xi^\beta} \ln p(x, \xi) \right) \\ &= \int dy\, q(y, \xi) \left(\frac{\partial}{\partial \xi^\alpha} \ln q(y, \xi) \right) \left(\frac{\partial}{\partial \xi^\beta} \ln q(y, \xi) \right) \end{aligned}$$

Square roots of probabilities

- Fisher information metric

$$G_{\alpha\beta}(\xi) = \int dx\, p(x,\xi) \left(\frac{\partial}{\partial \xi^\alpha} \ln p(x,\xi) \right) \left(\frac{\partial}{\partial \xi^\beta} \ln p(x,\xi) \right)$$
$$= 4 \int dx \left(\frac{\partial}{\partial \xi^\alpha} \sqrt{p(x,\xi)} \right) \left(\frac{\partial}{\partial \xi^\beta} \sqrt{p(x,\xi)} \right)$$

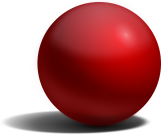
- for discrete random variable, take coordinates

$$p_j = \xi_j^2, \qquad j = 1, \ldots, N.$$

- normalization implies

$$\xi_1^2 + \ldots + \xi_N^2 = 1$$

- Fisher information metric is just induced Euclidean metric on the sphere!



Relative entropy

- classical relative entropy or Kullback-Leibler divergence

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

- not symmetric distance measure, but a *divergence*

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

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

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

- signals how well state ρ can be distinguished from a model σ
- Gibbs inequality: $D(\rho\|\sigma) \geq 0$
- $D(\rho\|\sigma) = 0$ if and only if $\rho = \sigma$

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 $-\sum_j p_j \ln p_j$

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

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 (similar: Sanov theorem)

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

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

Advantages of relative entropy: continuum limit

- consider transition from discrete to continuous distributions

$$p_j \to f(x)\,dx \qquad\qquad q_j \to g(x)\,dx$$

- not well defined for entropy

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

- relative entropy remains well defined

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

Information geometry for Euclidean quantum fields

[S. Floerchinger, 2303.04081 and 2303.04082]

- consider classical statistical field theories
- or bosonic quantum fields with real action in Euclidean space
- work out what information geometry has to say
- derive flow equation for divergence functional

Probabilities for Euclidean fields: exponential family

- probability density for Euclidean field theory with respect to measure $D\chi$

$$p[\chi, J] = \exp\left(-I[\chi] + J^\alpha \phi_\alpha[\chi] - W[J]\right)$$

- uses abstract index notation

$$J^\alpha \phi_\alpha = \int_x \sum_n J_n(x)\phi_n(x)$$

- partition function

$$e^{W[J]} = \int D\chi \exp\left(-I[\chi] + J^\alpha \phi_\alpha[\chi]\right)$$

- sources J^α could also compromise coupling constants
- will be considered as coordinates on space of probability distributions
- known as exponential family in information geometry

Affine geometry for sources

- exponential family is closed with respect to affine transformations

$$J^{\alpha} \to J'^{\alpha} = M^{\alpha}_{\ \beta} J^{\beta} + c^{\alpha}$$

- affine transformations respect convexity of $W[J]$
- so-called e-geodesics

$$J^{\alpha}(t) = (1-t) J'^{\alpha} + t J''^{\alpha}$$

characterized by differential equation

$$\frac{d^2}{dt^2} J^{\alpha}(t) + (\Gamma_{\mathsf{E}})_{\beta\ \gamma}^{\ \alpha}[J] \left(\frac{d}{dt} J^{\beta}(t) \right) \left(\frac{d}{dt} J^{\gamma}(t) \right) = 0$$

where the connection vanishes in terms of source coordinates

$$(\Gamma_{\mathsf{E}})_{\beta\ \gamma}^{\ \alpha}[J] = 0$$

Fisher information metric

- Fisher information metric

$$G_{\alpha\beta}[J] = \int D\chi\, p[\chi,J]\, \frac{\delta}{\delta J^\alpha} \ln p[\chi,J]\, \frac{\delta}{\delta J^\beta} \ln p[\chi,J]$$
$$= -\int D\chi\, p[\chi,J]\, \frac{\delta^2}{\delta J^\alpha \delta J^\beta} \ln p[\chi,J]$$

- Fisher-Rao distance between nearby probability distributions

$$ds^2 = G_{\alpha\beta}[J]\, dJ^\alpha\, dJ^\beta$$

- for the exponential family

$$G_{\alpha\beta}[J] = \frac{\delta^2}{\delta J^\alpha \delta J^\beta} W[J] = \langle \phi_\alpha[\chi]\phi_\beta[\chi]\rangle - \langle \phi_\alpha[\chi]\rangle\langle \phi_\beta[\chi]\rangle$$

- equal to connected two-point correlation function !
- generalization of Zamolodchikov metric for conformal field theories

Expectation value coordinates

- can also use field expectation values as coordinates for $p[\chi, \Phi]$

$$\Phi_\alpha = \langle \phi_\alpha[\chi] \rangle = \frac{\delta}{\delta J^\alpha} W[J] = \int D\chi \, p[\chi, J] \, \phi_\alpha[\chi]$$

- best described in terms of quantum effective action

$$\Gamma[\Phi] = \sup_J \left(J^\alpha \Phi_\alpha - W[J] \right) = -\inf_J \left(-\int D\chi \, p[\chi, J] \, \ln p[\chi, J] \right)$$

- Fisher-Rao distance

$$ds^2 = G_{\alpha\beta}[J] \, \delta J^\alpha \delta J^\beta = G^{\alpha\beta}[\Phi] \, \delta\Phi_\alpha \delta\Phi_\beta = \delta J^\alpha \delta\Phi_\beta$$

- Fisher metric in expectation value coordinates

$$G^{\alpha\beta}[\Phi] = -\int D\chi \, p[\chi, \Phi] \, \frac{\delta^2}{\delta\Phi_\alpha \delta\Phi_\beta} \ln p[\chi, \Phi] = \frac{\delta^2 \Gamma[\Phi]}{\delta\Phi_\alpha \delta\Phi_\beta}$$

- another affine structure, dual to the one for sources

$$\Phi_\alpha \to \Phi'_\alpha = N_\alpha{}^\beta \Phi_\beta + d_\alpha$$

- defines so-called m-connection

Divergence functional in source coordinates

- functional generalization of Kullback-Leibler divergence

$$D[J\|J'] = \int D\chi \, p[\chi, J] \ln \left(p[\chi, J]/p[\chi, J'] \right)$$

- compares two probability distributions in asymmetric way
- non-negative

$$D[J\|J'] \geq 0$$

- equals Fisher-Rao distance for close-by distributions

$$D[J\|J'] = \frac{1}{2} G_{\alpha\beta}[J] \delta J^\alpha \delta J^\beta + \ldots$$

- characterizes probabilities for large deviations (Sanovs theorem)
- can be written as Bregman divergence

$$D[J\|J'] = (J^\alpha - J'^\alpha) \frac{\delta W[J]}{\delta J^\alpha} - W[J] + W[J']$$

- functional derivatives w.r.t. second argument yield connected correlation functions !

Divergence functional in expectation value coordinates

- Divergence functional in terms of expectation values

$$D[\Phi\|\Phi'] = \int D\chi\, p[\chi,\Phi] \ln\left(p[\chi,\Phi]/p[\chi,\Phi']\right)$$
$$= \Gamma[\Phi] - \Gamma[\Phi'] - \frac{\delta\Gamma[\Phi']}{\delta\Phi'_\lambda}(\Phi_\lambda - \Phi'_\lambda)$$

- functional derivatives w.r.t. first argument yield one-particle irreducible correlation functions (for $n \geq 2$)

$$D^{(n,0)}[\Phi\|\Phi'] = \Gamma^{(n)}[\Phi],$$

- mixed representation generates connected and 1-P.I. correlation functions

$$D[\Phi\|J'] = \Gamma[\Phi] + W[J'] - J'^{\alpha}\Phi_\alpha$$

Functional integral representations

- divergence functional in source coordinates

$$e^{-D[J\|J']} = \frac{e^{W[J]-J^\alpha\Phi_\alpha}}{e^{W[J']-J'^\alpha\Phi_\alpha}} = \frac{\int D\chi \, \exp\left(-I[\chi] + J^\alpha(\phi_\alpha[\chi] - \Phi_\alpha)\right)}{\int D\tilde{\chi} \, \exp\left(-I[\tilde{\chi}] + J'^\alpha(\phi_\alpha[\tilde{\chi}] - \Phi_\alpha)\right)}$$

- well defined as ratio of functional integrals
- similar in expectation value coordinates

Information geometry from divergence functional

- Fisher metric from functional derivative of divergence

$$G_{\alpha\beta}[J] = -\frac{\delta^2}{\delta J^\alpha \delta J'^\beta} D[J \| J']\big|_{J=J'}$$

- transforms automatically as a metric under coordinate changes $J \to \Psi[J]$
- m-connection symbols

$$(\Gamma_{\mathsf{M}})_{\alpha\beta\gamma}[J] = -\frac{\delta^2}{\delta J^\alpha \delta J^\gamma} \frac{\delta}{\delta J'^\beta} D[J \| J']\big|_{J=J'}$$

- e-connection symbols

$$(\Gamma_{\mathsf{E}})_{\alpha\beta\gamma}[J] = -\frac{\delta}{\delta J^\beta} \frac{\delta^2}{\delta J'^\alpha \delta J'^\beta} D[J \| J']\big|_{J=J'}$$

- automatically transform like connections under $J \to \Psi[J]$
- m-covariant derivative for one-particle irreducible correlation functions
- e-covariant derivative for connected correlation functions
- there are other useful coordinate choices

Regularized probability distribution

- introduce now quadratic regulator in probability density

$$p_k[\phi, J] = \exp\left(-S[\phi] - \frac{1}{2} R_k^{\alpha\beta} \phi_\alpha \phi_\beta + J^\alpha \phi_\alpha - W_k[J]\right),$$

- with modified partition function

$$e^{W_k[J]} = \int D\phi \exp\left(-S[\phi] - \frac{1}{2} R_k^{\alpha\beta} \phi_\alpha \phi_\beta + J^\alpha \phi_\alpha\right).$$

- regulator can be chosen to suppress fluctuations, e. g.

$$R_k^{\alpha\beta} = k^2 \delta^{\alpha\beta}$$

Divergence functionals with regulator

- divergence functional with regulator

$$\tilde{D}_k[J\|J'] = \int D\phi\, p_k[\phi, J] \ln(p_k[\phi, J]/p_k[\phi, J'])$$
$$= (J^\alpha - J'^\alpha) \frac{\delta W_k[J]}{\delta J^\alpha} - W_k[J] + W_k[J']$$

- flowing divergence in expectation value coordinates

$$D_k[\Phi\|\Phi'] = \tilde{D}_k[\Phi\|\Phi'] - \Delta D_k[\Phi\|\Phi']$$
$$= \Gamma_k[\Phi] - \Gamma_k[\Phi'] - \frac{\delta\Gamma_k[\Phi']}{\delta\Phi'_\lambda}(\Phi_\lambda - \Phi'_\lambda)$$

with regulator piece subtracted

$$\Delta D_k[\Phi\|\Phi'] = \frac{1}{2} R_k^{\alpha\beta}(\Phi_\alpha - \Phi'_\alpha)(\Phi_\beta - \Phi'_\beta)$$

Limit of large and small regulator

- for large k saddle point approximation becomes valid

$$\lim_{k\to\infty} D_k[\Phi\|\Phi'] = S[\Phi] - S[\Phi'] - \frac{\delta}{\delta\Phi'_\alpha} S[\Phi'](\Phi_\alpha - \Phi'_\alpha)$$

- for small k the full Kullback-Leibler divergence functional is recovered

$$\lim_{k\to 0} D_k[\Phi\|\Phi'] = D[\Phi\|\Phi']$$

General field coordinates

- geometric significance of divergence functional
- work with general field coordinates $\Phi \to \Psi[\Phi]$

$$D_k[\Psi \| \Psi'] = D_k[\Phi[\Psi] \| \Phi[\Psi']]$$

- define regulator matrix in general coordinates

$$R_k^{\alpha\beta}[\Psi] = -\frac{\delta}{\delta\Psi_\alpha}\frac{\delta}{\delta\Psi'_\beta}\Delta D_k[\Psi\|\Psi']\big|_{\Psi'=\Psi}$$

- regularized inverse propagator in general coordinates

$$\left(G_k^{-1}[\Psi]\right)^{\alpha\beta} = -\frac{\delta^2}{\delta\Psi_\alpha\delta\Psi'_\beta}\left(D_k[\Psi\|\Psi'] + \Delta D_k[\Psi\|\Psi']\right)\big|_{\Psi'=\Psi}$$

- need also m-covariant second functional derivative

$$\begin{aligned}(\tilde{D}_{k,\mathsf{M}}^{(0,2)}[\Psi\|\Psi'])^{\lambda\kappa} =& \frac{\delta^2}{\delta\Psi'_\lambda\delta\Psi'_\kappa}\left(D_k[\Psi\|\Psi'] + \Delta D_k[\Psi\|\Psi']\right) \\ & - \left(\Gamma_{\mathsf{M}}[\Psi']\right)^{\lambda}{}_{\rho}{}^{\kappa}\frac{\delta}{\delta\Psi'_\rho}\left(D_k[\Psi\|\Psi'] + \Delta D_k[\Psi\|\Psi']\right)\end{aligned}$$

Flow equation for the divergence functional

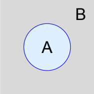
- exact flow equation in general field coordinates

$$\frac{\partial}{\partial k} D_k[\Psi \| \Psi'] = \frac{1}{2} \left(\frac{\partial}{\partial k} R_k^{\alpha\beta}[\psi] \right) (G_k[\Psi])_{\alpha\beta} - \frac{1}{2} \left(\frac{\partial}{\partial k} R_k^{\alpha\beta}[\psi'] \right) (G_k[\Psi'])_{\alpha\lambda} \, (\tilde{D}_{k,\mathsf{M}}^{(0,2)}[\Psi \| \Psi'])^{\lambda\kappa} \, (G_k[\Psi'])_{\kappa\beta}$$

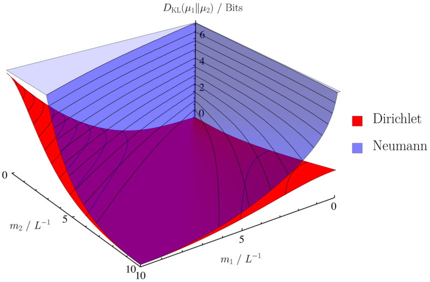
- close relative of Polchinskis and Wetterichs equations
- starting point for approximate solutions
- can be used to flow from large to small regulators
- flow vanishes when $\Psi = \Psi'$
- $D_k[\Psi \| \Psi']$ contains all geometric information
  - connected correlation functions: e-covariant derivatives
  - one-particle irreducible correlation functions: m-covariant derivatives

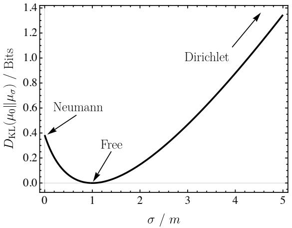
Bounded regions

[S. Floerchinger & M. Schröfl, *Relative Entropy and Mutual Information in Gaussian Statistical Field Theory*, 2307.15548]



- consider finite bounded region A
- boundary conditions: von Neumann, Dirichlet, Robin, periodic, free, etc.
- compare Gaussian theories with different masses or boundary conditions through relative entropy $D_{\mathsf{KL}}(\mu_1\|\mu_2)$
- for interval L in $d = 1$ dimension





Conclusions

- information geometry concepts can be applied to quantum and statistical field theories
- divergence functional encodes the information about geometry: metric, e-connection, m-connection etc.
- divergence functional is generating functional for connected and one-particle irreducible correlation functions
- connected and one-particle irreducible correlation functions correspond to two dual connections
- new exact flow equation for divergence functional
- general coordinates can be used

Backup

Advantages / disadvantages of divergence functional

- information theoretic meaning
- positivity $D[\Phi\|\Phi'] \geq 0$ instead of convexity for $\Gamma[\Phi]$
- geometric realization
  - connected correlation functions: e-connection
  - one-particle irreducible: m-connection
- general coordinate changes $\Phi \to \Psi[\Phi]$

$$D[\Psi\|\Psi'] = D[\Phi[\Psi]\|\Phi'[\Psi']]$$

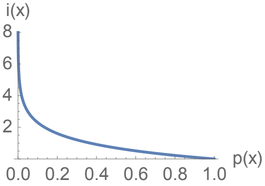
  preserve geometric structure
- equilibrium expectation value Φ_{eq} corresponding to $J = 0$ must be known in addition

Entropy and information

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

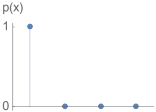
- consider a random variable x with probability distribution $p(x)$
- information content or "surprise" associated with outcome x

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

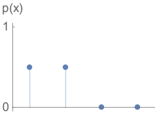


- entropy is expectation value of information content

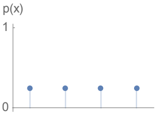
$$S(p) = \langle i(x) \rangle = -\sum_x p(x) \ln p(x)$$



$S = 0$



$S = \ln(2)$



$S = 2\ln(2)$

Entropy in quantum theory

[John von Neumann (1932)]

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

- based on the quantum density operator ρ
- 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

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

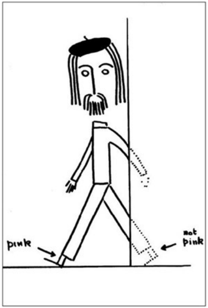
- quantum information is globally conserved

Quantum entanglement

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

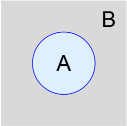
$$\psi = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle_A |\downarrow\rangle_B - |\downarrow\rangle_A |\uparrow\rangle_B \right)$$
$$= \frac{1}{\sqrt{2}} \left(|\rightarrow\rangle_A |\leftarrow\rangle_B - |\leftarrow\rangle_A |\rightarrow\rangle_B \right)$$

- *Bertlemann's socks and the nature of reality* [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

Classical statistics

- consider system of two random variables x and y
- joint probability $p(x, y)$, joint entropy

$$S = -\sum_{x,y} p(x, y) \ln p(x, y)$$

- reduced or marginal probability $p(x) = \sum_y p(x, y)$
- reduced or marginal entropy

$$S_x = -\sum_x p(x) \ln p(x)$$

- one can prove: **joint entropy is greater than** or equal to **reduced entropy**

$$S \geq S_x$$

- **globally pure** state $S = 0$ is also **locally pure** $S_x = 0$

Quantum statistics

- consider system with two subsystems A and B
- combined state ρ , combined or full entropy

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

- reduced density matrix $\rho_A = \mathsf{Tr}_B\{\rho\}$
- reduced or entanglement entropy

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

- for quantum systems **entanglement makes a difference**

$$S \ngeq S_A$$

- **coherent information** $I_{B\rangle A} = S_A - S$ can be **positive**!
- **globally pure** state $S = 0$ can be **locally mixed** $S_A > 0$

Entanglement entropy in non-relativistic quantum field theory

[Natalia Sanchez-Kuntz & Stefan Floerchinger, PRA 103, 043327 (2021)]

- non-relativistic quantum field theory for Bose gas

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

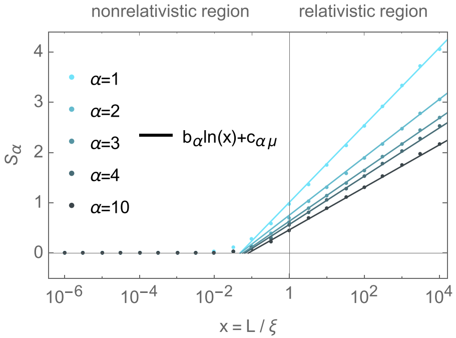
- Bogoliubov dispersion relation

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

- low momentum regime like theory of massless relativistic scalar particles
- high momentum regime non-relativistic
- what atre the entanglement properties?
- for $\rho = 0$ the entanglement entropy vanishes

Entanglement entropy in Bose-Einstein condensates

[Natalia Sanchez-Kuntz & Stefan Floerchinger, PRA 103, 043327 (2021)]



- one-dimensional Bose-Einstein condensate with subregion A of length L
- reduced density matrix $\rho_A = \text{Tr}_B\{\rho\}$
- Rényi entanglement entropy

$$S_\alpha = -\frac{1}{\alpha - 1} \ln \text{Tr}\{\rho_A^\alpha\}$$

- inverse healing length $1/\xi = \sqrt{2M\lambda\rho}$ acts like UV regulator
- at large $L \gg \xi$ we confirm CFT behaviour with $b_\alpha = c\frac{\alpha+1}{6\alpha}$

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

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 σ (or distributions q) the one with *maximum entropy* S is preferred

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

- why? assume $S(\sigma) < \text{max}$, than σ 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, PRE 102, 052117 (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 σ from which allowed states ρ 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 ρ, respectively

Measure on space of probability distributions

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

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

- 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)]

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

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

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

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 ξ 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 ξ'
- 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

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

- relative entropy of arbitrary state ρ to microcanonical state

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

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

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

- 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 ρ to grand-canonical state σ_{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 μ 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 ξ 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 ξ is sharp) and thermal state σ (where it ξ 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 ρ_0 and a thermodynamic model state σ 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

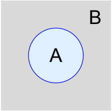
- consider non-equilibrium situation with
  - true density matrix ρ
  - local equilibrium approximation

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

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

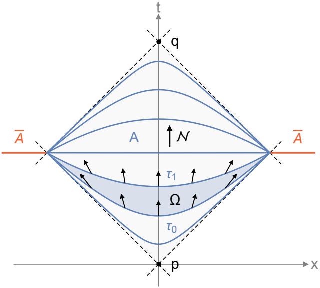
$$S_A = \text{Tr}_A\{\rho_A(\ln \rho_A - \ln \sigma_A)\} \to 0$$

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



Local form of second law for open systems 1

[Neil Dowling, Stefan Floerchinger & Tobias Haas, PRD 102, 105002 (2020)]



- 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, more generally CPTP map

$$\rho(\tau_0) \to \mathcal{N}(\rho(\tau_0)) = \rho(\tau_1)$$

Local form of second law for open systems 2

[Neil Dowling, Stefan Floerchinger & Tobias Haas, PRD 102, 105002 (2020)]

- compare to global equilibrium state

$$\sigma = \frac{1}{Z} \exp\left[- \int_{\Sigma(\tau)} d\Sigma_\mu \left\{ \beta_\nu T^{\mu\nu} + \alpha N^\mu \right\} \right]$$

with entropy current

$$s^\mu = -\beta_\nu T^{\mu\nu} - \alpha N^\mu + p\beta^\mu$$

- relative entropy

$$\begin{aligned} S(\rho\|\sigma) &= \mathrm{Tr}\left\{\rho\big(\ln(\rho) - \ln(\sigma)\big)\right\} \\ &= - S(\rho) + \ln(Z) + \mathrm{Tr}\Big\{\rho \int d\Sigma_\mu \big(\beta_\nu T^{\mu\nu} + \alpha N^\mu\big)\Big\} \\ &= - S(\rho) + \int d\Sigma_\mu \Big\{ - s^\mu(\sigma) + \beta_\nu \big[T^{\mu\nu}(\rho) - T^{\mu\nu}(\sigma)\big] + \alpha\big[N^\mu(\rho) - N^\mu(\sigma)\big]\Big\} \end{aligned}$$

- monotonicity of relative entropy

$$\Delta S(\rho\|\sigma) = S(\rho(\tau_1)\|\sigma(\tau_1)) - S(\rho(\tau_0)\|\sigma(\tau_0)) \leq 0$$

- allows to formulate local forms of the second law for fluids

Local form of second law for open systems 3

[Neil Dowling, Stefan Floerchinger & Tobias Haas, PRD 102, 105002 (2020)]

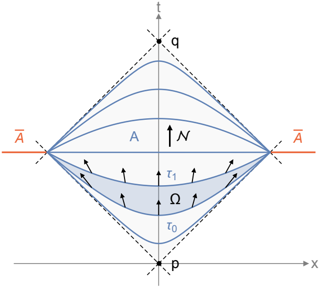
- assume now that one can write

$$\Delta S(\rho) = S(\rho(\tau_1)) - S(\rho(\tau_0)) = \int_\Omega d^d x \sqrt{g}\, \mathfrak{s}(\rho)(x)$$

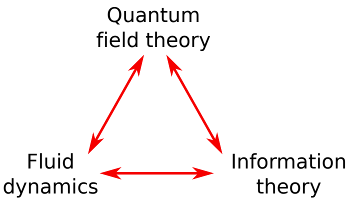
- find from monotonicity of relative entropy a local form of the second law

$$\mathfrak{s}(\rho) + \beta_\nu \nabla_\mu T^{\mu\nu}(\rho) + \alpha \nabla_\mu N^\mu(\rho) \geq 0$$

- next step: time evolution for isolated fluids



Quantum field dynamics



- new 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