Unique additive information measures – Boltzmann-Gibbs-Shannon, Fisher and beyond

Peter Ván
BME, Department of Chemical Physics
Thermodynamic Research Group
Hungary

1. Introduction – the observation of Jaynes
2. Weakly nonlocal additive information measures
3. Power law tails
   - Microcanonical and canonical equilibrium distributions
4. Dynamics – quantum mechanics
5. Conclusions

Entropy in local statistical physics

(information theoretical, predictive, bayesian)

(Jaynes, 1957):

The measure of information is unique under general physical conditions.

(Shannon, 1948; Rényi, 1963)

- Extensivity (mean, density)
- Additivity

$$s(f_1 f_2) = s(f_1) + s(f_2)$$

(unique solution)

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

Entropy in weakly nonlocal statistical physics

(estimation theoretical, Fisher based)

(Fisher, …., Frieden, Plastino, Hall, Reginatto, Garbaczewski, …):

- Extensivity

- Additivity

$$s(f_1 f_2, D(f_1 f_2)) = \tilde{s}(f_1, Df_1) + \tilde{s}(f_2, Df_2)$$

- Isotropy

$$s(f, Df) = \hat{s}(f, (Df)^2)$$

$\Rightarrow$ (unique solution)

$$\widehat{s}(f,(Df)^2) = -k\ln f - k_1\frac{(Df)^2}{f^2}$$

Boltzmann-Gibbs-Shannon

Fisher

$$\widehat{s}(f,(Df)^2) = -k\ln f - k_1\frac{(Df)^2}{f^2}$$

– What about higher order derivatives?

Dimension dependence

–What is the physics behind the second term?

Equilibrium distributions with power law tails

–What could be the value of k_1?

Dynamics - quantum systems

Second order weakly nonlocal information measures

- Extensivity
- Additivity

$$s(f_1 f_2, D(f_1 f_2), D^2(f_1 f_2)) =$$
$$\tilde{s}(f_1, Df_1, D^2 f) + \tilde{s}(f_2, Df_2, D^2 f_2)$$

- Isotropy in 3D

$$s_3(f, Df, D^2 f) = \hat{s}_3(f,\ (Df)^2,\ Df \cdot D^2 f \cdot Df,\ Df \cdot (D^2 f)^2 \cdot Df,$$
$$Tr(D^2 f),\ Tr(D^2 f)^2,\ Tr(D^2 f)^3)$$

(unique solution)

$$
\begin{aligned}
s_3(f, Df, D^2 f) = \\
& -k \ln f - k_1 \frac{(Df)^2}{f^2} - (k_2 + k_5)\frac{(Df)^4}{f^4} + (k_3 + k_6)\frac{(Df)^6}{f^6} \\
& -k_2 \frac{1}{f^3} Df \cdot D^2 f \cdot Df + (2k_3 + 3k_6)\frac{(Df)^2}{f^5} Df \cdot D^2 f \cdot Df \\
& -k_3 \frac{1}{f^4} Df \cdot (D^2 f)^2 \cdot Df - k_4 \frac{1}{f} Tr(D^2 f) - k_5 \frac{1}{f^2} Tr(D^2 f)^2 \\
& -k_6 \frac{1}{f^3} Tr(D^2 f)^3)
\end{aligned}
$$

Depends on the dimension of the phase space.

<u>MaxEnt calculations – the interaction of the two terms</u>

(1D ideal gas)

$$extr. = -\int f\left(k_1 \frac{(Df)^2}{f^2} - k\ln f\right)dp$$

$$-\beta\left(\int f\frac{p^2}{2m}dx - E\right) - \alpha\left(\int f dx - 1\right)$$

$$R := \sqrt{f}$$

$$R'' - \frac{k}{2k_1}R\ln R - \frac{\beta}{8mk_1}p^2 R - \frac{\alpha + k}{4k_1}R = 0$$

$$J_s = R'\delta R$$

$$R'' - \frac{k}{2k_1} R \ln R - \frac{\beta}{8mk_1} p^2 R - \frac{\alpha + k}{4k_1} R = 0$$

$$R'(0) = 0$$ symmetry

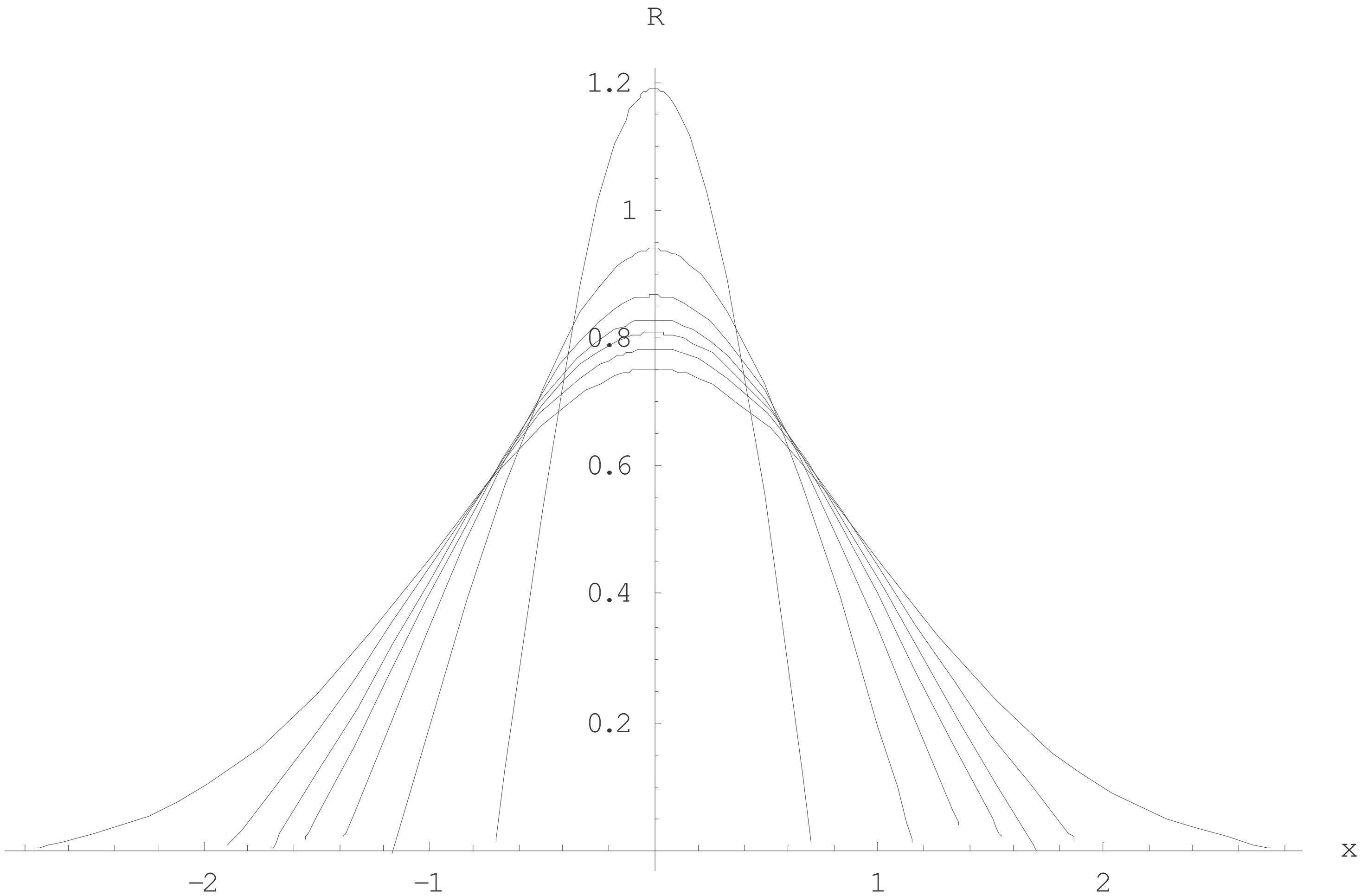
$$R(0) = C \quad \Rightarrow \quad \alpha$$

There is no analitic solution in general

There is no partition function formalism

Numerical normalization

One free parameter: J_s



$$\Lambda = \frac{\alpha + k}{4k_1} = (1, 1.1, 1.2, 1.3, 1.5, 2, 5), \quad \frac{k}{2k_1} = 1, \quad \frac{\beta}{8mk_1} = 1$$

Quantum systems – the meaning of k_1

$f = \rho$ probability distribution

$$\widehat{s}(\rho, (\nabla\rho)^2) = k_1 \frac{(\nabla\rho)^2}{\rho^2} + \cancel{k \ln \rho}$$

Fisher

Boltzmann-Gibbs-Shannon

- Mass-scale invariance (particle interpretation)

$$s(\lambda\rho, \lambda\nabla\rho) = s(\rho, \nabla\rho)$$

- $\boxed{k_1 = \hbar^2}$

Why quantum?

A

$$R'' - \frac{k}{2k_1} R \ln R - \frac{\beta}{8mk_1} p^2 R - \frac{\alpha + k}{4k_1} R = 0$$

$$-\frac{\hbar^2}{2m}\varphi'' + \frac{D}{2} x^2 \varphi + E\varphi = 0$$

Time independent Schrödinger equation

B

Probability conservation
Momentum conservation
+ Second Law (entropy inequality)

→ Equations of Korteweg fluids with a potential

$$\dot{\rho} + \rho \nabla \cdot \mathbf{v} = 0$$

$$\rho \dot{\mathbf{v}} + \nabla \cdot \mathbf{P}(\mathrm{C}) = \mathbf{0}$$

Schrödinger-Madelung fluid

(Fisher entropy)

$$s_{SchM}(\rho, \mathbf{v}, \nabla\rho) = -\frac{\nu_{SchM}}{2}\left(\frac{\nabla\rho}{2\rho}\right)^2 - \frac{(m\mathbf{v})^2}{2}$$

$$\mathbf{P}^{\mathrm{r}}_{\mathrm{SchM}} = -\frac{1}{8}\left(\Delta\rho\mathbf{I} + \nabla^2\rho - \frac{2\nabla\rho\otimes\nabla\rho}{\rho}\right)$$

$$\Psi = \sqrt{\rho}\, e^{-i\frac{\hbar}{m}\nabla\mathbf{v}}$$

Bernoulli equation

Schrödinger equation

Logarithmic and Fisher together?

Nonlinear Schrödinger eqaution of Bialynicki-Birula and Mycielski (1976)
(additivity is preserved):

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\Delta\Psi-b\ln\left|\Psi\right|^2+U\Psi$$

Stationary equation for the wave function:

$$-\frac{\hbar^2}{2m}\varphi''+k\varphi\ln\left|\varphi\right|+\frac{D}{2}x^2\varphi+E\varphi=0$$

Existence of non dispersive free solutions –
solutions with finite support - Gaussons

Conclusions

– Corrections to equilibrium (?) distributions

– Corrections to equations of motion

– Unique = universal

  • Independence on micro details
  • General principles in backround

Thermodynamics ⟷ Statistical physics

Information theory

Concavity properties:

$$\delta_f^2 f\ \hat{s}(f) = -k_1 \begin{pmatrix} \frac{k}{k_1}\frac{1}{f} + \frac{(Df)^2}{4f^3} & -\frac{Df}{4f^2} \\ -\frac{Df}{4f^2} & \frac{1}{4f} \end{pmatrix}$$

Positive definite

If k is zero (pure Fisher): positive semidefinite!

$$s(f_1 f_2) = s(f_1) + s(f_2)$$

$$\frac{\partial}{\partial f_1} s(f_1 f_2) = f_2 s'(f_1 f_2) = s'(f_1)$$

$$\frac{\partial}{\partial f_2} s(f_1 f_2) = f_1 s'(f_1 f_2) = s'(f_2)$$

$$s'(f_1 f_2) = \frac{s'(f_1)}{f_2} = \frac{s'(f_2)}{f_1}$$

$$f\, s'(f) = const. = -\kappa$$

$$s(f) = -\int \frac{\kappa}{f} df = -\kappa \ln f + C$$

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

One component weakly nonlocal fluid

$$\dot{\rho} + \rho \nabla \cdot \mathbf{v} = 0$$
$$\rho \dot{\mathbf{v}} + \nabla \cdot \mathbf{P}(C) = \mathbf{0}$$
$$\rho \dot{s}(C) + \nabla \cdot \mathbf{j}_s(C) \geq 0$$

$(\rho, \mathbf{v})$ basic state

$$C_{wnl} = (\rho, \nabla\rho, \nabla\nabla\rho, \mathbf{v}, \nabla\mathbf{v})$$

constitutive state

$$s(C), \mathbf{j_s}(C), \mathbf{P}(C)$$

constitutive functions

Liu procedure (Farkas's lemma):

$$s(\rho, \mathbf{v}, \nabla\rho) = s_e(\rho, \nabla\rho) - \frac{\mathbf{v}^2}{2} \qquad \mathbf{j}_s = -\mathbf{v} \cdot \mathbf{P} + \ldots$$

$$\sigma_s = -\Big(\underbrace{\mathbf{P} - \overbrace{\rho^2\left[\qquad\qquad -\partial_\rho s\right]\mathbf{I}\qquad\qquad}^{\mathbf{P}^r\ \text{reversible pressure}}}_{\mathbf{P}^v = \mathbf{P} - \mathbf{P}^r}\Big) : \nabla\mathbf{v} \geq 0$$

- Potential form: $\nabla \cdot \mathbf{P}^{\mathrm{r}} = \rho \nabla \mathrm{U}_{\mathrm{Q}}$

- $U_Q = -\partial_\rho(\rho s_e) + \nabla \cdot (\rho \partial_{\nabla\rho} s_e)$

Euler-Lagrange form

↓

Variational origin

Schrödinger-Madelung fluid

(Fisher entropy)

$$s_{SchM}(\rho, \mathbf{v}, \nabla\rho) = -\frac{\nu_{SchM}}{2}\left(\frac{\nabla\rho}{2\rho}\right)^2 - \frac{\mathbf{v}^2}{2}$$

$$\mathbf{P}^{r}_{\mathrm{SchM}} = -\frac{1}{8}\left(\Delta\rho\mathbf{I} + \nabla^2\rho - \frac{2\nabla\rho\otimes\nabla\rho}{\rho}\right)$$

⇨ Bernoulli equation

$\Psi = \sqrt{\rho}e^{-i\nabla\mathbf{v}}$

⇨ Schrödinger equation

Alternate fluid

$$s_{Alt}(\rho, \nabla\rho) = -\nu_{Alt}\frac{(\nabla\rho)^2}{\rho}$$

$$\mathbf{P}^r_{Alt} = -\frac{\nu_{Alt}}{4}\left(\rho(\Delta\rho\mathbf{I} + \nabla^2\rho) - \nabla\rho \circ \nabla\rho\right)$$

$$U_{Alt} = -\frac{\nu_{Alt}}{2}\Delta\rho$$

Korteweg fluids:

$$\mathbf{P}^r_{Kor} = \left(-p + \alpha\Delta\rho + \beta(\nabla\rho)^2\right)\mathbf{I} + \delta\nabla\rho \circ \nabla\rho + \gamma\nabla^2\rho$$