A superstatistical measure of distance from canonical equilibrium

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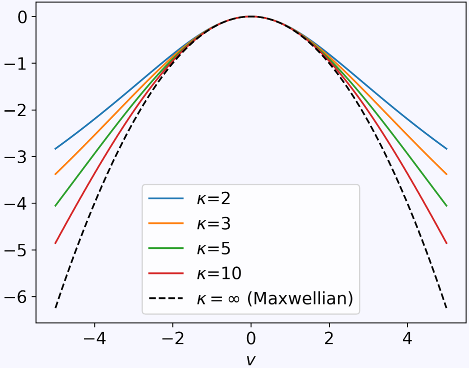
Outline of the Talk

- Non-canonical ensembles and superstatistics
- An impossibility theorem within superstatistics
- A superstatistical distance from equilibrium
- Example: particles with kappa-distributed velocities
- Concluding remarks

The kappa distribution as a non-canonical distribution

The kappa distribution for the velocity v of a particle can be written as

$$P(\boldsymbol{v}|\kappa, v_{\text{th}}) = \frac{1}{\eta(\kappa, v_{\text{th}})}\left[1 + \frac{1}{\kappa - \frac{3}{2}}\frac{\boldsymbol{v}^2}{v_{\text{th}}^2}\right]^{-(\kappa+1)}, \qquad \kappa \geq \frac{3}{2}$$



It reduces to the Maxwell-Boltzmann distribution when $\kappa \to \infty$.

How to explain non-canonical distributions?

$$P(v|\kappa, v_{\text{th}}) = \frac{1}{\eta(\kappa, v_{\text{th}})}\left[1 + \frac{1}{\kappa - \frac{3}{2}}\frac{\boldsymbol{v}^2}{v_{\text{th}}^2}\right]^{-(\kappa+1)} \qquad \neq \qquad \frac{\exp\left(-\beta\frac{m\boldsymbol{v}^2}{2}\right)}{Z(\beta)}$$

There are several proposals aimed at recovering non-canonical distributions. Among them,

- Maximization of a generalized entropy functional (e.g. Tsallis)
- Mechanisms of deformation of the distributions (e.g. Kaniadakis)
- Superstatistics

Superstatistics only slightly modifies standard statistical mechanics, being fully compatible with (Bayesian) probability theory

Superstatistics (C. Beck, E. G. D. Cohen, 2003)

In superstatistics, the inverse temperature $\beta := 1/(k_B T)$ is promoted from a constant to an unknown ("random") quantity with joint probability density

$$P(\boldsymbol{\Gamma}, \beta|\boldsymbol{\lambda}) = P(\boldsymbol{\Gamma}|\beta, \boldsymbol{\lambda})P(\beta|\boldsymbol{\lambda}) = P(\beta|\boldsymbol{\lambda}) \left[\frac{\exp\big(-\beta\mathcal{H}(\boldsymbol{\Gamma})\big)}{Z(\beta)}\right]. \tag{1}$$

The probability (density) of observing a microstate $\boldsymbol{\Gamma}$ is given by the marginalization rule as

$$P(\boldsymbol{\Gamma}|\boldsymbol{\lambda}) = \int_0^\infty d\beta P(\beta|\boldsymbol{\lambda}) \left[\frac{\exp\big(-\beta\mathcal{H}(\boldsymbol{\Gamma})\big)}{Z(\beta)}\right]. \tag{2}$$

Superstatistical ensembles are then superpositions of canonical ensembles at different values of β. The canonical ensemble is a particular case, as

$$P(\beta|\beta_0) = \delta(\beta - \beta_0) \quad \Longrightarrow \quad P(\boldsymbol{\Gamma}|\beta_0) = \frac{\exp\big(-\beta_0\mathcal{H}(\boldsymbol{\Gamma})\big)}{Z(\beta_0)}$$

Example: recovering Tsallis distributions

Let us assume a gamma distribution of inverse temperatures,

$$P(\beta|\boldsymbol{\lambda}) = \frac{1}{u\beta_S\Gamma(1/u)}\exp\left(-\frac{\beta}{u\beta_S}\right)\left(\frac{\beta}{u\beta_S}\right)^{\frac{1}{u}-1} = P(\beta|u,\beta_S) \qquad (3)$$

where

$$\beta_S = \big\langle \beta \big\rangle_{u,\beta_S} \quad , \quad u = \frac{\big\langle (\delta\beta)^2 \big\rangle_{u,\beta_S}}{\big\langle \beta \big\rangle^2_{u,\beta_S}} \quad \text{and} \quad u = 0 \iff \text{canonical}$$

For a system with constant specific heat, that is, $E = \alpha k_B T$, we have

$$Z(\beta) = Z_0\,\beta^{-(\alpha+1)}$$

and we can replace $Z(\beta)$, obtaining

$$P(\boldsymbol{\Gamma}|\boldsymbol{\lambda}) = \int_0^\infty d\beta\, P(\beta|\boldsymbol{\lambda})\,\frac{\exp\big(-\beta\mathcal{H}(\boldsymbol{\Gamma})\big)}{Z(\beta)} = \frac{\Big(1 + u\beta_S\,\mathcal{H}(\boldsymbol{\Gamma})\Big)^{\frac{1}{1-q}}}{Z_u(\beta_S)}$$

where

$$Z_u(\beta_S) = \frac{\Gamma(\alpha+1)\Gamma(1/u)}{\Gamma(\alpha+1+1/u)}(u\beta_S)^{-(\alpha+1)}, \qquad q = 1 + \frac{u}{1+u(\alpha+1)}$$

Inverse temperature in general steady states

Superstatistical ensembles belong to the larger family of steady state ensembles, where

$$P(\boldsymbol{\Gamma}|\boldsymbol{\lambda}) = \rho\big(\mathcal{H}(\boldsymbol{\Gamma}); \boldsymbol{\lambda}\big), \tag{4}$$

with ρ the *ensemble function*. In superstatistics, this is a Laplace transform,

$$\rho(E; \boldsymbol{\lambda}) = \int_0^\infty d\beta f(\beta; \boldsymbol{\lambda}) \exp(-\beta E), \qquad f(\beta; \boldsymbol{\lambda}) := \frac{P(\beta|\boldsymbol{\lambda})}{Z(\beta)} \tag{5}$$

For a general steady state we define the *fundamental inverse temperature*,

$$\boxed{\beta_F(E; \boldsymbol{\lambda}) := -\frac{\partial}{\partial E} \ln \rho(E; \boldsymbol{\lambda})}$$

Notice that $\beta_F(E; \boldsymbol{\lambda})$ is a constant if and only if the ensemble is canonical. That is,

$$\rho(E; \beta_0) = \frac{\exp(-\beta_0 E)}{Z(\beta)} \quad \Longleftrightarrow \quad -\frac{\partial}{\partial E} \ln \rho(E; \beta_0) = \beta_0$$

Inverse temperature in Tsallis ensembles

From the microstate distribution

$$P(\boldsymbol{\Gamma}|u,\beta_S) = \frac{1}{Z_u(\beta_S)}\Big(1+u\beta_S\,\mathcal{H}(\boldsymbol{\Gamma})\Big)^{-(\frac{1}{u}+\alpha+1)} \tag{6}$$

we determine the fundamental inverse temperature as

$$\beta_F(E;u,\beta_S) = \beta_S\cdot\frac{1+u(\alpha+1)}{1+u\beta_S E} = \frac{\beta_0}{1+(q-1)\beta_0 E} \tag{7}$$

with $\beta_0 = \beta_S\big(1+u(\alpha+1)\big)$. The expected value of β_F is given by

$$\big\langle \beta_F\big\rangle_{u,\beta_S} = \frac{1}{Z_u(\beta_S)}\int_0^\infty d\boldsymbol{\Gamma}\,\big(1+u\beta_S\mathcal{H}(\boldsymbol{\Gamma})\big)^{-(\frac{1}{u}+\alpha+1)}\beta_F\big(\mathcal{H}(\boldsymbol{\Gamma});u,\beta_S\big) = \beta_S. \tag{8}$$

in agreement with the superstatistical mean inverse temperature.

In general, it can be proved that, for any superstatistical ensemble,

$$\big\langle \beta_F\big\rangle_{\boldsymbol{\lambda}} = \big\langle \beta\big\rangle_{\boldsymbol{\lambda}}. \tag{9}$$

Inverse temperature in superstatistics

Recall the ensemble function of superstatistics,

$$\rho(E;\boldsymbol{\lambda}) = \int_0^\infty d\beta f(\beta;\boldsymbol{\lambda})\exp(-\beta E), \qquad f(\beta;\boldsymbol{\lambda}) := \frac{P(\beta|\boldsymbol{\lambda})}{Z(\beta)} \tag{10}$$

After some calculation, it can be shown that the conditional distribution

$$P(\beta|\boldsymbol{\Gamma},\boldsymbol{\lambda}) = \frac{P(\beta,\boldsymbol{\Gamma}|\boldsymbol{\lambda})}{P(\boldsymbol{\Gamma}|\boldsymbol{\lambda})} = \frac{f(\beta;\boldsymbol{\lambda})\exp\big(-\beta\mathcal{H}(\boldsymbol{\Gamma})\big)}{\rho\big(\mathcal{H}(\boldsymbol{\Gamma});\boldsymbol{\lambda}\big)} \tag{11}$$

has mean given by

$$\big\langle \beta \big\rangle_{\boldsymbol{\Gamma},\boldsymbol{\lambda}} = \beta_F(\mathcal{H}(\boldsymbol{\Gamma});\boldsymbol{\lambda}), \tag{12}$$

and variance

$$\big\langle (\delta\beta)^2 \big\rangle_{\boldsymbol{\Gamma},\boldsymbol{\lambda}} = -{\beta_F}'(\mathcal{H}(\boldsymbol{\Gamma});\boldsymbol{\lambda}). \tag{13}$$

The equality in (12) suggests a close connection between β and $\beta_F(\mathcal{H};\boldsymbol{\lambda})$, the latter being **an observable in phase space**.

An impossibility theorem within superstatistics

The equality

$$\langle \beta \rangle_{\mathbf{\Gamma},\boldsymbol{\lambda}} = \beta_F(\mathcal{H}(\mathbf{\Gamma});\boldsymbol{\lambda})$$

strongly suggests that β may be interchangeable with $\beta_F(\mathcal{H};\boldsymbol{\lambda})$. However, the following theorem holds.

Theorem (*): there is no function $B(\mathbf{\Gamma})$ such that

$$\big\langle G(\beta) \big\rangle_{\mathbf{\Gamma},\boldsymbol{\lambda}} = G\big(B(\mathbf{\Gamma})\big) \tag{14}$$

for any function G and a superstatistical, non-canonical steady state $\boldsymbol{\lambda}$.

In contrast, for the canonical ensemble (14) automatically holds, as

$$\big\langle G(\beta) \big\rangle_{\mathbf{\Gamma},\beta_0} = G(\beta_0) \tag{15}$$

for any function G, so $B(\mathbf{\Gamma}) = \beta_0$ is a constant function.

* S. Davis, G. Gutiérrez. Physica A **505**, 864-870 (2018).

A simplified proof of the theorem

Recall that

$$\langle \beta \rangle_{\mathbf{\Gamma},\boldsymbol{\lambda}} = \beta_F(\mathcal{H}(\mathbf{\Gamma}); \boldsymbol{\lambda}), \tag{16a}$$

$$\big\langle (\delta\beta)^2 \big\rangle_{\mathbf{\Gamma},\boldsymbol{\lambda}} = -{\beta_F}'(\mathcal{H}(\mathbf{\Gamma}); \boldsymbol{\lambda}). \tag{16b}$$

Let us assume that $B(\mathbf{\Gamma})$ exists such that $\langle G(\beta) \rangle_{\mathbf{\Gamma},\boldsymbol{\lambda}} = G(B(\mathbf{\Gamma}))$ for all $G(\bullet)$.

Using $G(\beta) = \delta(\beta - \beta_0)$ we clearly see that

$$P(\beta = \beta_0 | \mathbf{\Gamma}, \boldsymbol{\lambda}) = \delta\big(\beta_0 - B(\mathbf{\Gamma})\big)$$

so from (16a) and (16b) it follows that

$$\boxed{B(\mathbf{\Gamma}) = \beta_F(\mathcal{H}(\mathbf{\Gamma}); \boldsymbol{\lambda})} \quad \text{and} \quad \boxed{{\beta_F}'(\mathcal{H}(\mathbf{\Gamma}); \boldsymbol{\lambda}) = 0}$$

respectively. Then $\beta_F(\mathcal{H}(\mathbf{\Gamma}); \boldsymbol{\lambda})$ is a constant and the ensemble is canonical.

In non-canonical superstatistics, there is no $B(\mathbf{\Gamma})$ interchangeable with β.

Consequences of the theorem

Since

$$\big\langle (\delta\beta)^2 \big\rangle_{\boldsymbol{\Gamma},\boldsymbol{\lambda}} = -{\beta_F}'(\mathcal{H}(\boldsymbol{\Gamma}); \boldsymbol{\lambda}) \geq 0 \tag{17}$$

with equality only for the canonical ensemble, we have that

$$\boxed{\big\langle (\delta\beta)^2 \big\rangle_{\boldsymbol{\Gamma},\boldsymbol{\lambda}} > 0}$$

for a non-canonical superstatistical state.

There is an intrinsic uncertainty about the value of β, which does not vanish even when including perfect knowledge of $\boldsymbol{\Gamma}$.

Example: For Tsallis distributions with $q \geq 1$, we have

$$\big\langle (\delta\beta)^2 \big\rangle_{\boldsymbol{\Gamma},q,\beta_0} = (\beta_S)^2\,(q-1) \geq 0 \tag{18}$$

with equality only for $q = 1$ (canonical).

Information contained in the microstate about β

Let us define the mutual information between β and $\mathbf{\Gamma}$ as

$$\mathcal{D}(\boldsymbol{\lambda}) := \left\langle \ln\left[\frac{P(\mathbf{\Gamma},\beta|\boldsymbol{\lambda})}{P(\beta|\boldsymbol{\lambda})P(\mathbf{\Gamma}|\boldsymbol{\lambda})}\right]\right\rangle_{\boldsymbol{\lambda}} \geq 0$$

This mutual information can be rewritten as

$$\begin{aligned}\mathcal{D}(\boldsymbol{\lambda}) &= \int_0^\infty d\beta \int d\mathbf{\Gamma} P(\mathbf{\Gamma},\beta|\boldsymbol{\lambda}) \ln\left[\frac{P(\mathbf{\Gamma}|\beta)P(\beta|\boldsymbol{\lambda})}{P(\mathbf{\Gamma}|\boldsymbol{\lambda})P(\beta|\boldsymbol{\lambda})}\right] \\ &= -\int_0^\infty d\beta \int d\mathbf{\Gamma}\, P(\mathbf{\Gamma},\beta|\boldsymbol{\lambda}) \ln\left[\frac{P(\mathbf{\Gamma}|\boldsymbol{\lambda})}{P(\mathbf{\Gamma}|\beta)}\right] = \left\langle -\ln\left[\frac{P(\mathbf{\Gamma}|\boldsymbol{\lambda})}{P(\mathbf{\Gamma}|\beta)}\right]\right\rangle_{\boldsymbol{\lambda}}.\end{aligned} \tag{19}$$

Note that $\mathcal{D}$ is different from the expected value of the relative entropy

$$\mathcal{S}_{\mathbf{\Gamma}}(\beta_0 \to \boldsymbol{\lambda}) := \left\langle -\ln\left[\frac{P(\mathbf{\Gamma}|\boldsymbol{\lambda})}{P(\mathbf{\Gamma}|\beta_0)}\right]\right\rangle_{\boldsymbol{\lambda}} = -\int d\mathbf{\Gamma} P(\mathbf{\Gamma}|\boldsymbol{\lambda}) \ln\left[\frac{P(\mathbf{\Gamma}|\boldsymbol{\lambda})}{P(\mathbf{\Gamma}|\beta_0)}\right], \tag{20}$$

because

$$\Big\langle \mathcal{S}_{\mathbf{\Gamma}}(\beta \to \boldsymbol{\lambda})\Big\rangle_{\boldsymbol{\lambda}} = -\int_0^\infty d\beta \int d\mathbf{\Gamma}\, P(\beta|\boldsymbol{\lambda})P(\mathbf{\Gamma}|\boldsymbol{\lambda}) \ln\left[\frac{P(\mathbf{\Gamma}|\boldsymbol{\lambda})}{P(\mathbf{\Gamma}|\beta)}\right] \tag{21}$$

In summary

The 2018 theorem means that, for a non-canonical superstatistical ensemble,

$$\big\langle (\delta\beta)^2 \big\rangle_{\mathbf{\Gamma},\boldsymbol{\lambda}} > 0.$$

There is non-zero uncertainty about β even when knowing $\mathbf{\Gamma}$.

The amount of information that $\mathbf{\Gamma}$ carries about β is given by

$$\mathcal{D}(\boldsymbol{\lambda}) := \left\langle \ln\left[\frac{P(\mathbf{\Gamma},\beta|\boldsymbol{\lambda})}{P(\beta|\boldsymbol{\lambda})P(\mathbf{\Gamma}|\boldsymbol{\lambda})}\right]\right\rangle_{\boldsymbol{\lambda}} = \left\langle -\ln\left[\frac{P(\mathbf{\Gamma}|\boldsymbol{\lambda})}{P(\mathbf{\Gamma}|\beta)}\right]\right\rangle_{\boldsymbol{\lambda}} \geq 0 \qquad (22)$$

and it is only zero if $\boldsymbol{\lambda}$ represents a canonical ensemble at some value of β.

Example: particles with kappa-distributed velocities

We generalize the Maxwell-Boltzmann distribution for a system of N particles,

$$P(\boldsymbol{V}|\beta) = \frac{\exp\big(-\beta K(\boldsymbol{V})\big)}{Z_N(\beta)} \tag{23}$$

with

$$K(\boldsymbol{V}) = \frac{1}{2}\sum_{i=1}^{N} m_i \boldsymbol{v}_i^2, \tag{24}$$

by using superstatistics under a gamma distribution of inverse temperatures,

$$P(\beta|u,\beta_S) = \frac{1}{u\beta_S\Gamma(1/u)}\exp\left(-\frac{\beta}{u\beta_S}\right)\left(\frac{\beta}{u\beta_S}\right)^{\frac{1}{u}-1}. \tag{25}$$

That is, (23) is replaced by

$$P(\boldsymbol{V}|u,\beta_S) = \int_0^\infty d\beta\, P(\beta|u,\beta_S)\left[\frac{\exp\big(-\beta K(\boldsymbol{V})\big)}{Z_N(\beta)}\right]. \tag{26}$$

Example: particles with kappa-distributed velocities

After integrating over β we have

$$P(\boldsymbol{V}|u, \beta_S) = \frac{C_N(u)}{Z_N(\beta_S)}\Big(1 + u\beta_S\, K(\boldsymbol{V})\Big)^{-\frac{1}{u}-\frac{3N}{2}}, \qquad 0 \leq u \leq \frac{1}{2} \tag{27}$$

where

$$C_N(u) := \frac{u^{\frac{3N}{2}}\,\Gamma\left(\frac{3N}{2}+\frac{1}{u}\right)}{\Gamma\left(\frac{1}{u}\right)}. \tag{28}$$

Introducing the auxiliary function

$$\phi(z) := z\,\Gamma'(z) \tag{29}$$

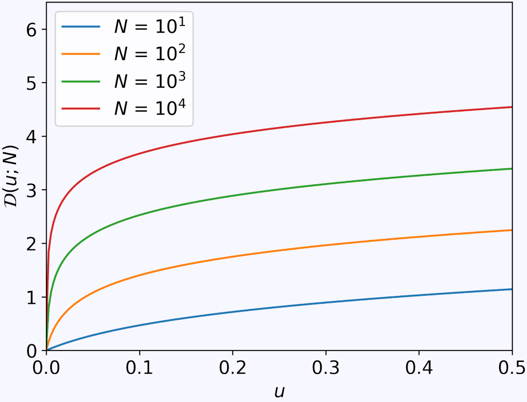
with $\Gamma'(z)$ the digamma function, and after lengthy calculations, we obtain

$$\mathcal{D}(u;N) = \ln\Gamma\left(\frac{1}{u}\right) - \ln\Gamma\left(\frac{3N}{2}+\frac{1}{u}\right) + \phi\left(\frac{3N}{2}+\frac{1}{u}\right) - \phi\left(\frac{1}{u}\right) - \frac{3N}{2}$$

Interestingly, $\mathcal{D}$ does not depend on temperature, only on u and N.

Distance increases with u and N

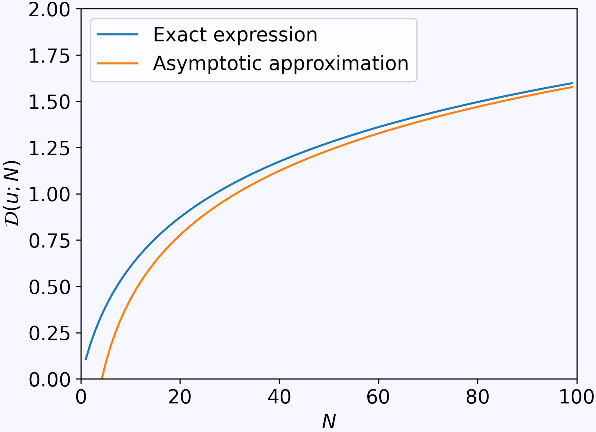
$$\mathcal{D}(u;N) = \ln\Gamma\left(\frac{1}{u}\right) - \ln\Gamma\left(\frac{3N}{2}+\frac{1}{u}\right) + \phi\left(\frac{3N}{2}+\frac{1}{u}\right) - \phi\left(\frac{1}{u}\right) - \frac{3N}{2}$$



Note that $\mathcal{D}(0;N) = 0$ for all N.

Asymptotic approximation

$$\mathcal{D}(u;N) \sim \frac{1}{2}\ln\,(3N) + \frac{1}{u} + \ln\Gamma(1/u) - \phi(1/u) - \ln 2 - \frac{1}{2}(1+\ln\pi)$$



Concluding Remarks

- We have presented in a new light an impossibility theorem which denies the existence of an observable inverse temperature $B(\mathbf{\Gamma})$ in non-canonical superstatistics
- The theorem is equivalent to the statement that there is a minimum, non-zero uncertainty on β given $\mathbf{\Gamma}$ unless the ensemble is canonical
- The mutual information $\mathcal{D}$ between β and $\mathbf{\Gamma}$ has the form of a superstatistical distance from equilibrium
- In the case of particles with kappa-distributed velocities, the use of κ as a measure of departure from equilibrium can be justified, as for fixed N, $\mathcal{D}$ is a function only of u
- A more general definition of distance from equilibrium outside superstatistics remains to be explored

Some references

- S. Davis, G. Gutiérrez. *Temperature is not an observable in superstatistics*. Phys. A **505**, 864-870 (2018).
- S. Davis, G. Gutiérrez. *Emergence of Tsallis statistics as a consequence of invariance*. Phys. A **533**, 122031 (2019).
- S. Davis. *On the possible distributions of temperature in nonequilibrium steady states*. J. Phys. A: Math. Theor. **53**, 045004 (2020).
- S. Davis. *Conditional maximum entropy and superstatistics*. J. Phys. A: Math. Theor. **53**, 445006 (2020).
- H. Umpierrez, S. Davis. *Fluctuation theorems in q-canonical ensembles*. Phys. A **563**, 125337 (2021).
- S. Davis. *Fluctuating temperature outside superstatistics: Thermodynamics of small systems*. Phys. A **589**, 126665 (2022).
- S. Davis. *A classification of nonequilibrium steady states based on temperature correlations*. Phys. A **608**, 128249 (2022).
- C. Farías, S. Davis. *Temperature distribution in finite systems: Application to the one-dimensional Ising chain*. Eur. Phys. J. B **96**, 39 (2023).
- S. Davis. *Superstatistics and the fundamental temperature of steady states*. AIP Conf. Proc. **2731**, 030006 (2023).

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