# Temperature and its uncertainty in nonequilibrium steady state plasmas

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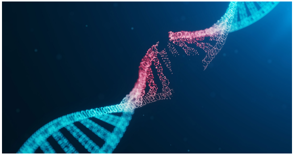

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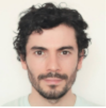

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# The *kappa* distribution of velocities

The (symmetrical) *kappa* distribution for the velocity $v$ of a particle in a plasma* can be written as

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

Here, $\kappa$ is the *spectral index* and $v_{\text{th}}$ is the so-called *thermal velocity*, such that

$$\frac{m v_{\text{th}}^2}{2} = k_B T \tag{1}$$

defines a temperature $T$.

The limit $\kappa \to \infty$ of the *kappa* distribution is the Maxwell-Boltzmann distribution,

$$\lim_{\kappa\to\infty} P(\boldsymbol{v}|\kappa, v_{\text{th}}) = \left(\sqrt{\frac{m}{2\pi k_B T}}\right)^3 \exp\left(-\frac{m\boldsymbol{v}^2}{2k_B T}\right). \tag{2}$$

*G. Livadiotis and D. J. McComas. Astrophys. J. **741**, 88 (2011).

# The *kappa* distribution as a $q$-canonical distribution

By defining the $q$-exponential function

$$\exp(x;q) := \Big[1+(1-q)x\Big]_{+}^{\frac{1}{1-q}} \tag{3}$$

such that $\exp(x;1) = \exp(x)$, we can write the *kappa* distribution as

$$P(\boldsymbol{v}|\kappa, v_{\text{th}}) = \frac{1}{\eta_\kappa(v_{\text{th}})} \exp\left(-\frac{m\boldsymbol{v}^2}{2k_B T_0}; q\right), \tag{4}$$

provided that we set $q = 1 + \dfrac{1}{\kappa+1}$ and $k_B T_0 = \left(\dfrac{\kappa - \frac{3}{2}}{\kappa+1}\right)\dfrac{m v_{\text{th}}^2}{2}$.

In the limit $\kappa \to \infty$ we see that $q \to 1$ and $T_0 \to T$.

# The *kappa* distribution from Tsallis entropy

Maximizing the non-extensive (Tsallis) entropy*

$$\mathcal{S}_q[p] := \frac{1}{q-1}\left(1 - \int d\boldsymbol{v} p(\boldsymbol{v})^q\right) \tag{5}$$

subject to the constraints on the *escort expectation*

$$\int d\boldsymbol{v}\; p(\boldsymbol{v})^q \left(\frac{m\boldsymbol{v}^2}{2}\right) = \bar{k} \tag{6}$$

and normalization,

$$\int d\boldsymbol{v} p(\boldsymbol{v}) = 1, \tag{7}$$

we can recover the *kappa* distribution as

$$p(\boldsymbol{v}) \propto \left[1 + (q-1)\frac{m\boldsymbol{v}^2}{2k_B T_0}\right]^{\frac{1}{1-q}} = \exp\left(-\frac{m\boldsymbol{v}^2}{2k_B T_0}; q\right). \tag{8}$$

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*C. Tsallis. *Introduction to Nonextensive Statistical Mechanics: Approaching a Complex World* . Springer, 2009.

# Temperature of steady states

Recall the Liouville equation for a nonequilibrium, Hamiltonian system,

$$\frac{\partial P(\mathbf{\Gamma}|t)}{\partial t} + \Big\{P(\mathbf{\Gamma}|t), \mathcal{H}(\mathbf{\Gamma})\Big\} = 0. \tag{9}$$

A particular family of time-independent solutions are

$$P(\mathbf{\Gamma}|S) = \rho\big(\mathcal{H}(\mathbf{\Gamma}); S\big), \tag{10}$$

where $\rho(E; S)$ is the *ensemble function* with parameters $S$.

For these *steady states* we will define* the *fundamental inverse temperature*

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

such that $\beta_S := \big\langle \beta_F \big\rangle_S$ is the inverse temperature of the ensemble.

> Just as $\beta$ is a parameter of the canonical ensemble $P(\mathbf{\Gamma}|\beta)$,
> $\beta_F$ is a feature of the steady state ensemble $P(\mathbf{\Gamma}|S)$.

*S. Davis, G. Gutiérrez. Physica A **533**, 122031 (2019).

# Some examples of fundamental temperature

**Canonical ensemble:**

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

**$q$-canonical (Tsallis) ensemble:**

$$\rho(E;q,\beta) = \frac{1}{Z_q(\beta_0)}\Big[1+(q-1)\beta_0 E\Big]_+^{\frac{1}{1-q}} \quad \Longleftrightarrow \quad \beta_F(E;q,\beta_0) = \frac{\beta_0}{1+(q-1)\beta_0 E}$$

**Gaussian ensemble:**

$$\rho(E;A,E_0) = \frac{1}{\eta_A(E_0)}\exp\Big(-A(E-E_0)^2\Big) \quad \Longleftrightarrow \quad \beta_F(E;A,E_0) = 2A(E-E_0)$$

# Equivalence between temperatures

Defining the *microcanonical inverse temperature* $\beta_\Omega$ as

$$\beta_\Omega(E) := \frac{\partial}{\partial E}\ln\Omega(E) = \frac{1}{k_B}\left(\frac{\partial S_E}{\partial E}\right) \tag{11}$$

with $\Omega(E) := \int d\mathbf{\Gamma}\delta(\mathcal{H}(\mathbf{\Gamma}) - E)$ the density of states, we can show that

$$\beta_S = \big\langle \beta_F \big\rangle_S = \big\langle \beta_\Omega \big\rangle_S. \tag{12}$$

Moreover, because in the microcanonical ensemble we have

$$\big\langle \beta_R \big\rangle_E = \beta_\Omega(E) \tag{13}$$

with $\beta_R$ the Rugh-Rickayzen* "dynamical temperature",

$$\beta_R(\mathbf{\Gamma}) := \nabla\cdot\left(\frac{\boldsymbol{\omega}}{\boldsymbol{\omega}\cdot\nabla\mathcal{H}}\right), \tag{14}$$

for a differentiable field $\boldsymbol{\omega}(\mathbf{\Gamma})$, it follows by taking expectation of Eq. 13 that

$$\beta_S = \big\langle \beta_F \big\rangle_S = \big\langle \beta_R \big\rangle_S. \tag{15}$$

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*H. H. Rugh. Phys. Rev. Lett. **78**, 772 (1997) ; G. Rickayzen, J. G. Powles. J. Chem. Phys. **114**, 4333 (2001).

# Superstatistics

Superstatistics* is a framework where the inverse temperature is promoted to a random variable.

The joint distribution of $\beta$ with the microstates $\mathbf{\Gamma}$ is

$$P(\mathbf{\Gamma}, \beta|S) = P(\mathbf{\Gamma}|\beta)P(\beta|S) = \left[\frac{\exp\big(-\beta\mathcal{H}(\mathbf{\Gamma})\big)}{Z(\beta)}\right]P(\beta|S). \tag{16}$$

Marginalization of $\beta$ gives the *superstatistical ensemble*

$$P(\mathbf{\Gamma}|S) = \int_0^\infty d\beta P(\beta|S)\left[\frac{\exp(-\beta\mathcal{H}(\mathbf{\Gamma}))}{Z(\beta)}\right] = \rho(\mathcal{H}(\mathbf{\Gamma}); S) \tag{17}$$

which can be understood as a "deformation" of the canonical ensemble.

The ensemble function is given by

$$\rho(E; S) = \int_0^\infty d\beta\, f(\beta)\exp(-\beta E) \;\text{ where }\; f(\beta) := \frac{P(\beta|S)}{Z(\beta)}$$

i.e. is the Laplace transform of $f(\beta)$.

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*C. Beck and E. G. D. Cohen. Physica A **322**, 267 (2003).

# Superstatistics and the *kappa* distribution

The *kappa* distribution can be obtained from superstatistics using a gamma distribution of inverse temperatures,

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

where $\beta_S = \big\langle \beta \big\rangle_{u,\beta_S}$ and $u := \dfrac{\big\langle (\delta\beta)^2 \big\rangle_{u,\beta_S}}{(\beta_S)^2}$ is the relative variance of $\beta$.

The original parameters $\kappa$ and $v_{\text{th}}$ are

$$\kappa = \frac{1}{u} + \frac{1}{2}, \qquad \frac{m v_{\text{th}}^2}{2} = \frac{1}{(1-u)\beta_S}, \tag{18}$$

and we see that $u \to 0$ is equivalent to $\kappa \to \infty$ (Maxwell-Boltzmann). In fact,

$$\lim_{u\to 0} P(\beta|u,\beta_S) = \delta(\beta-\beta_S), \tag{19}$$

then superstatistics reduces to the canonical ensemble.

# Fundamental temperature in superstatistics

$$P(\mathbf{\Gamma},\beta|S) = \exp\big(-\beta\mathcal{H}(\mathbf{\Gamma})\big)f(\beta) \quad\Longrightarrow\quad P(E,\beta|S) = \exp(-\beta E)f(\beta)\Omega(E)$$

Because $P(E|S) = \big\langle\delta(\mathcal{H}-E)\big\rangle_S = \rho(E;S)\Omega(E)$ we can write

$$P(\beta|E,S) = \frac{P(E,\beta|S)}{P(E|S)} = \frac{\exp(-\beta E)f(\beta)\cancel{\Omega(E)}}{\rho(E;S)\cancel{\Omega(E)}}. \tag{20}$$

Using $\rho(E;S) = \int_0^\infty d\beta f(\beta)\exp(-\beta E)$ it follows that

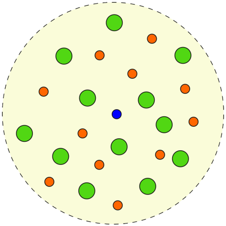
$$\beta_F(E) = -\frac{1}{\rho(E|S)}\frac{\partial\rho(E|S)}{\partial E} = \int_0^\infty d\beta\,\underbrace{\left[\frac{f(\beta)\exp(-\beta E)}{\rho(E;S)}\right]}_{=P(\beta|E,S)}\cdot\beta, \tag{21}$$

that is, $\beta_F(E;S) = \big\langle\beta\big\rangle_{E,S}$

Taking expectation of $\beta_F(E;S) = \big\langle\beta\big\rangle_{E,S}$, we have $\beta_S = \big\langle\beta\big\rangle_S$ so, in fact,

$$\beta_S = \big\langle\beta_F\big\rangle_S = \big\langle\beta_\Omega\big\rangle_S = \big\langle\beta_R\big\rangle_S = \big\langle\beta\big\rangle_S. \tag{22}$$

# A simple condition leads to *kappa*



$$P(v_1|S) = \int dv_2 \ldots dv_n \; p_n\big(\mathcal{E}(v_1, \ldots, v_n)\big)$$

$$\mathcal{E}(v_1, \ldots, v_n) = \underbrace{\frac{m_1 v_1^2}{2}}_{=k_1} + \underbrace{\sum_{i=2}^{n} \frac{m_i v_i^2}{2}}_{=K}$$

$$P(v_1|S) = p_1(k_1)$$

A **necessary and sufficient condition*** to have a *kappa* distribution is

$$k^* := \underset{k_1}{\text{argmax}}\, P(k_1|K, S) = \gamma_n + \alpha_n K$$

i.e. the most probable kinetic energy of the test particle **increases linearly** with the kinetic energy of the environment.

The complex character of the plasma is then encoded in the statement: “any given particle is correlated with its environment”

*S. Davis, G. Avaria, B. Bora, J. Jain, J. Moreno, C. Pavez, L. Soto. arXiv:**2304.3792** (2023).

# A sketch of the proof (1)

Recalling $P(v_1, \ldots, v_n|S) = p_n\big(\sum_{i=1}^{n} m_i v_i^2/2\big)$ we have the joint distribution

$$P(k_1, K|S) = p_n(k_1 + K)\Omega_1(k_1)\Omega_{n-1}(K) \qquad \text{with} \;\; \Omega_m(E) \propto E^{\frac{3m}{2}-1}$$

From this we obtain the conditional distribution of $k_1$ given $K$,

$$P(k_1|K, S) = \frac{p_n(k_1 + K)\Omega_1(k_1)}{p_{n-1}(K)}. \tag{23}$$

The condition that $k^*$ is an extremum of $k_1$ given $K$ leads to

$$\left[\frac{\partial}{\partial k_1} \ln P(k_1|K, S)\right]_{k_1=k^*} = -\beta_F^{(n)}(k^* + K) + \frac{1}{2k^*} = 0, \tag{24}$$

and after replacing $k^* = \gamma_n + \alpha_n K$ we solve for the fundamental temperature

$$\boxed{\beta_F^{(n)}(E) = \frac{\alpha_n + 1}{2\big(\gamma_n + \alpha_n E\big)}}$$

that is, we already see that $p_n(k_1 + K)$ corresponds to a $q$-canonical ensemble.

# A sketch of the proof (2)

The fundamental inverse temperature $b_F$ of the test particle is

$$b_F(k_1; S) = \left\langle \beta_F^{(n)} \right\rangle_{k_1,S} = \left\langle \frac{\alpha_n + 1}{2\big(\gamma_n + \alpha_n(k_1 + K)\big)} \right\rangle_{k_1,S} = \frac{\alpha_1 + 1}{2\big(\gamma_1 + \alpha_1 k_1\big)} \tag{25}$$

which is equal to $\beta_F^{(1)}$ and by integration leads to the *kappa* distribution

$$p_1(k_1) \propto \left[1 + \left(\frac{\alpha_1}{\gamma_1}\right) k_1\right]^{-\frac{1}{2}\left(1+\frac{1}{\alpha_1}\right)} \quad \text{with} \quad \kappa = \frac{1}{2\alpha_1} - \frac{1}{2}, \quad \frac{m v_{\text{th}}^2}{2} = \frac{2\gamma_1}{1 - 4\alpha_1}.$$

This agrees with the result from superstatistics using $P(\beta|u, \beta_S)$,

$$\begin{aligned} p_1(k_1) &= \left(\sqrt{\frac{m}{2\pi}}\right)^3 \int_0^\infty d\beta \left[\frac{\beta^{\frac{3}{2}} \exp(-\beta k_1)}{u\beta_S\, \Gamma(1/u)}\right] \exp\left(-\frac{\beta}{u\beta_S}\right) \left(\frac{\beta}{u\beta_S}\right)^{\frac{1}{u}-1} \\ &= \left(\sqrt{\frac{m u \beta_S}{2\pi}}\right)^3 \left[1 + u\beta_S k_1\right]^{-\left(\frac{1}{u}+\frac{3}{2}\right)} \end{aligned} \tag{26}$$

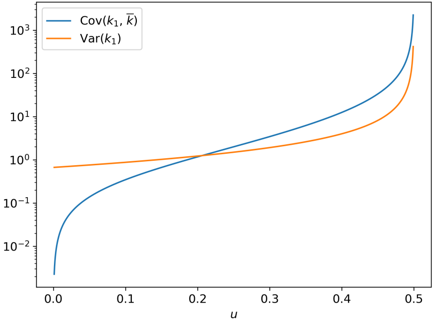
# Equipartition, uncertainty and correlation

The mean and variance of $k_1$ in the *kappa* distribution in terms of $(u, \beta_S)$ are

$$\big\langle k_1 \big\rangle_{u,\beta_S} = \frac{3}{2} \cdot \frac{k_B T_S}{1-u} \qquad \text{and} \qquad \big\langle (\delta k_1)^2 \big\rangle_{u,\beta_S} = \big\langle k_1 \big\rangle^2_{u,\beta_S} \cdot \frac{2+u}{3(1-2u)}$$

where $k_B T_S := 1/\beta_S$. It follows that $u < 1/2$, and then $\kappa > 5/2$.

With $u = 0$ we recover the well-known result for the relative variance of $k_1$ in the Maxwell-Boltzmann distribution, namely $2/3$.




$$\big\langle \delta k_1 \delta \bar{k} \big\rangle_{u,\beta_S} = \big\langle k_1 \big\rangle^2_{u,\beta_S} \cdot \frac{u}{1-2u} \geq 0$$

$$\text{where} \;\; \bar{k} := \lim_{n\to\infty} \frac{1}{n-1} \sum_{i=2}^{n} \frac{m_i v_i^2}{2}.$$

# A further connection between $\beta_F$ and $\beta$

Earlier results on the single-particle velocity distributions in collisionless plasmas[1] gave the *superstatistical approximation*

$$P(\beta|S) \approx \int_0^\infty dK P(K|S)\delta\big(\beta - \beta_F^{(n)}(K)\big) \tag{27}$$

for $k_1 \ll K$. Defining the fundamental inverse temperature of the environment

$$\mathcal{B}_F(K) := \beta_F^{(n-1)}(K) \tag{28}$$

and using Eq. 27 we arrive at

$$\boxed{P(\beta|S) = \lim_{n\to\infty} P(\mathcal{B}_F = \beta|S)}$$

In the thermodynamic limit we see that

$$\lim_{n\to\infty} \mathcal{B}_F(K) = \frac{3}{2\bar{k}} \quad \text{where} \quad \bar{k} = \lim_{n\to\infty} \frac{K}{n-1},$$

in complete agreement with a recent result[2] connecting $\beta$ in superstatistics and the equipartition temperature.

[1] S. Davis, G. Avaria, B. Bora, J. Jain, J. Moreno, C. Pavez, L. Soto. Phys. Rev. E **100**, 023205 (2019).
[2] E. Gravanis, E. Akylas, G. Livadiotis. EPL **130**, 30005 (2020).

# The inverse temperature covariance $\mathcal{U}$

For the *kappa* distribution, and, in general for superstatistics, we have

$$\mathcal{U} := u(\beta_S)^2 = \big\langle(\delta\beta)^2\big\rangle_S \geq 0. \tag{29}$$

However, it can be shown* that for an arbitrary steady state,

$$\mathcal{U} = \big\langle(\delta\beta_\Omega)^2\big\rangle_S + \big\langle{\beta_\Omega}'\big\rangle_S = \big\langle(\delta\beta_F)^2\big\rangle_S - \big\langle{\beta_F}'\big\rangle_S. \tag{30}$$

In the case of ${\beta_\Omega}' < 0$ and ${\beta_F}' > 0$, $\mathcal{U}$ could *in principle* be negative
$\Longrightarrow$ Cannot be described by superstatistics (!)

Because

$$\beta_\Omega{}'(E) = -\frac{\beta_\Omega(E)^2}{C_E} < 0, \tag{31}$$

a positive specific heat $C_E$ is required. Can we find *an actual example*?

*S. Davis. Physica A **608**, 128249 (2022).

# Systems with negative $\mathcal{U}$

For $\mathcal{H}(\mathbf{\Gamma}_1, \mathbf{\Gamma}_2) = \mathcal{H}_1(\mathbf{\Gamma}_1) + \mathcal{H}_2(\mathbf{\Gamma}_2)$ it can also be shown[1] that

$$\mathcal{U} = \Big\langle \delta b_\Omega(\mathcal{H}_1)\delta \mathcal{B}_\Omega(\mathcal{H}_2)\Big\rangle_S \tag{32}$$

$\mathcal{U} < 0 \Longrightarrow$ temperatures of target and environment are *anticorrelated*.

This can ocurr for an isolated system, i.e. when

$$\mathcal{H}_1(\mathbf{\Gamma}_1) + \mathcal{H}_2(\mathbf{\Gamma}_2) = E_0$$

if $b_\Omega$ and $\mathcal{B}_\Omega$ are both monotonically decreasing functions, that is, when both subsystems have $C_E > 0$.

- We have recently[2] illustrated this for an isolated Ising chain.
- Another example: Gaussian ensemble with constant $C_E$.
- Yet another: $q$-canonical (Tsallis) ensemble for $q < 1$ and constant $C_E$.

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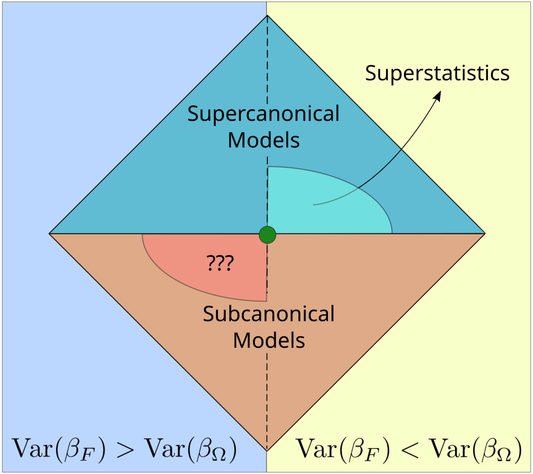
[1] S. Davis. Physica A **608**, 128249 (2022).

[2] C. Farías, S. Davis. Eur. Phys. J. B **96**, 39 (2023).

# A classification of nonequilibrium steady states




| | Sign of $\mathcal{U}$ | Signature | Ordering of variances | Sign of $C_E$ |
|---|---|---|---|---|
| Supercanonical A | $\mathcal{U} > 0$ | $(+,+)$ | $\mathrm{Var}(\beta_F) > \mathrm{Var}(\beta_\Omega)$ | $C_E < 0$ |
| Supercanonical B | $\mathcal{U} \geq 0$ | $(-,-)$ | $\mathrm{Var}(\beta_\Omega) > \mathrm{Var}(\beta_F)$ | $C_E > 0$ |
| Subcanonical A | $\mathcal{U} \leq 0$ | $(-,+)$ | $\mathrm{Var}(\beta_F) > \mathrm{Var}(\beta_\Omega)$ | $C_E > 0$ |
| Subcanonical B | $\mathcal{U} \leq 0$ | $(-,+)$ | $\mathrm{Var}(\beta_\Omega) > \mathrm{Var}(\beta_F)$ | $C_E > 0$ |

# In summary...

- The temperature of a steady state can be described by the fundamental ($\beta_F$) as well as the microcanonical ($\beta_\Omega$) inverse temperatures.
- In superstatistics, $\beta_F(E)$ is the conditional mean of $\beta$ given $E$ and, in fact, $\beta_F$ determines the superstatistical ensemble (**a theorem coming soon**).
- The *kappa* distribution follows from a simple condition on the most probable kinetic energy of a particle given that of its environment.
- There is a whole space of steady state models outside superstatistics: subcanonical models where $\mathcal{U} < 0$, as well as supercanonical models where $\mathcal{U} > 0$ but Var$(\beta_F) >$ Var$(\beta_\Omega)$.

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