Superstatistical Monte Carlo simulation of kappa distributed particles using Gibbs sampling

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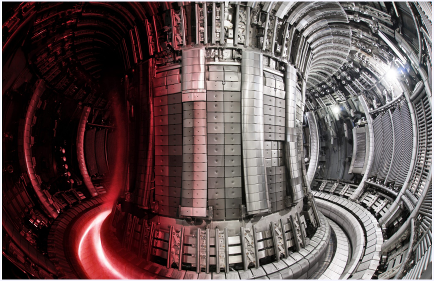
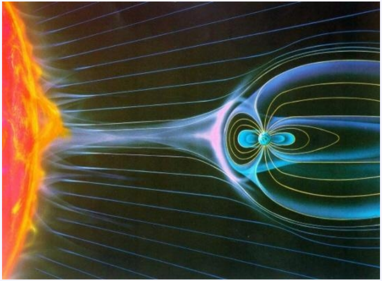
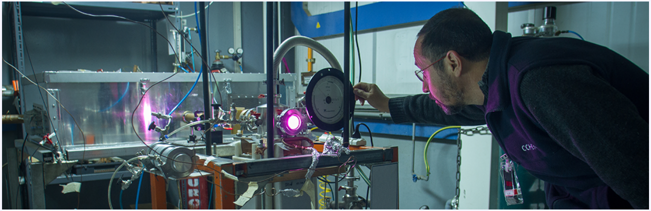
Motivation: Non-equilibrium Plasmas



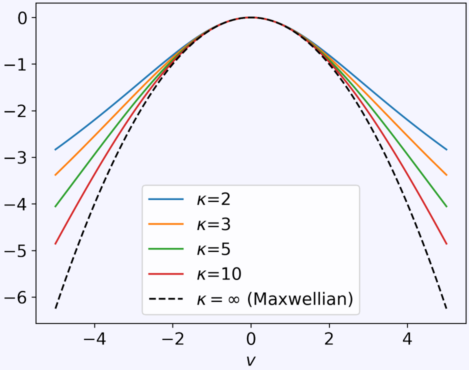




Velocity distributions in plasmas

$$P(\boldsymbol{v}|T) = \left(\frac{m}{2\pi k_B T}\right)^{\frac{3}{2}} \exp\left(-\frac{m\boldsymbol{v}^2}{2k_B T}\right)$$

(Maxwell-Boltzmann)



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

(Kappa)

Origin of the Maxwellian distribution

$$\mathbf{\Gamma} := (\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N, \boldsymbol{p}_1, \ldots, \boldsymbol{p}_N)$$

$$\mathcal{H}(\mathbf{\Gamma}) = \sum_{i=1}^{N} \frac{\boldsymbol{p}_i^2}{2m_i} + \Phi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N)$$

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

Gibbs Entropy

$$\mathcal{S} = -k_B \int d\mathbf{\Gamma}\, p(\mathbf{\Gamma}) \ln p(\mathbf{\Gamma})$$

$\downarrow$

Constraints

$$\langle \mathcal{H} \rangle = \int d\mathbf{\Gamma}\, p(\mathbf{\Gamma}) \mathcal{H}(\mathbf{\Gamma}) = E_0$$

$\downarrow$

Canonical Distribution

$$p(\mathbf{\Gamma}; \beta) = \frac{1}{Z(\beta)} \exp\big(-\beta \mathcal{H}(\mathbf{\Gamma})\big)$$

Non-extensive (Tsallis) statistics

It predicts power laws instead of exponentials:

$$P(\boldsymbol{\Gamma}|\beta) = \frac{\exp\big(-\beta\mathcal{H}(\boldsymbol{\Gamma})\big)}{Z(\beta)} \qquad \rightarrow \qquad P(\boldsymbol{\Gamma}|\beta_0, q) = \frac{1}{Z_q(\beta)}\Big[1 + (q-1)\beta_0\mathcal{H}(\boldsymbol{\Gamma})\Big]^{\frac{1}{1-q}}$$

In order to do this:

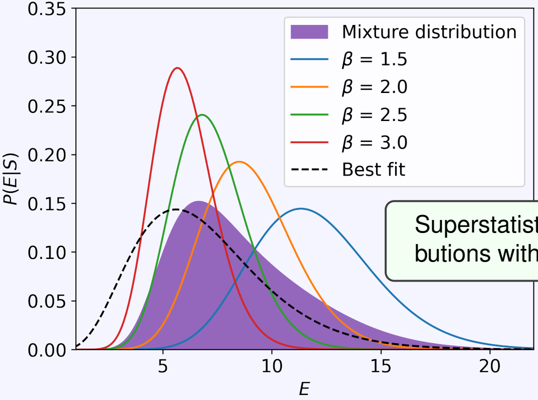
- It replaces the Gibbs entropy by the so-called "q-entropy" (Tsallis entropy),

$$\mathcal{S} := -\int d\boldsymbol{\Gamma}\, p(\boldsymbol{\Gamma}) \ln p(\Gamma) \qquad \rightarrow \qquad \mathcal{S}_q := \frac{1}{q-1}\left(1 - \int d\boldsymbol{\Gamma}\, p(\boldsymbol{\Gamma})^q\right)$$

- It replaces the expectation operation by a new "q-expectation" (*escort* distribution),

$$\big\langle A\big\rangle_p = \int d\boldsymbol{\Gamma}\, p(\boldsymbol{\Gamma}) A(\boldsymbol{\Gamma}) \qquad \rightarrow \qquad \big\langle\big\langle A\big\rangle\big\rangle = \frac{\int d\boldsymbol{\Gamma}\, p(\boldsymbol{\Gamma})^q A(\boldsymbol{\Gamma})}{\int d\boldsymbol{\Gamma}\, p(\boldsymbol{\Gamma})^q}$$

Superstatistics



Superstatistics explains non-canonical distributions without modifying the Gibbs entropy.

It does this by postulating models that are mixtures of canonical equilibria:

$$\exp\big(-\beta\mathcal{H}(\boldsymbol{\Gamma})\big) \quad \longrightarrow \quad \int_0^\infty d\beta\, f(\beta) \exp\big(-\beta\mathcal{H}(\boldsymbol{\Gamma})\big)$$

C. Beck, E. G. D. Cohen, Physica A **322**, 267-275 (2003).

Superstatistics: an explanation based on probability

The main idea:

A new (dynamical?) variable β is added to the microstate $\mathbf{\Gamma}$, such that

$$\mathbf{\Gamma} \quad \rightarrow \quad (\mathbf{\Gamma}, \beta)$$

That is, we replace the microstate distribution $P(\mathbf{\Gamma}|\boldsymbol{\lambda})$ by the joint distribution $P(\mathbf{\Gamma}, \beta|\boldsymbol{\lambda})$.

Here $\boldsymbol{\lambda}$ represents the particular set of parameters of the superstatistical model to be considered.

$$P(\mathbf{\Gamma}, \beta|\boldsymbol{\lambda}) = P(\mathbf{\Gamma}|\beta) \times P(\beta|\boldsymbol{\lambda}) = \frac{\exp\big(-\beta\mathcal{H}(\mathbf{\Gamma})\big)}{Z(\beta)} \times P(\beta|\boldsymbol{\lambda}) \tag{1}$$

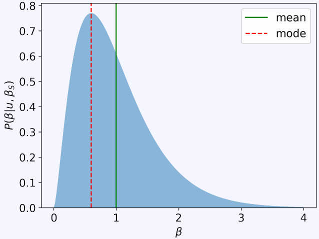
$$P(\mathbf{\Gamma}|\boldsymbol{\lambda}) = \int_0^\infty d\beta\, P(\mathbf{\Gamma}, \beta|\boldsymbol{\lambda}) = \int_0^\infty d\beta\, P(\beta|\boldsymbol{\lambda}) \left[\frac{\exp\big(-\beta\mathcal{H}(\mathbf{\Gamma})\big)}{Z(\beta)}\right] \tag{2}$$

Temperatures associated to the kappa distribution

Superstatistical velocity distributions are of the form

$$P(\boldsymbol{v}|\boldsymbol{\lambda}) = \int_0^\infty d\beta\, P(\beta|\boldsymbol{\lambda}) \left[\left(\frac{m\beta}{2\pi}\right)^{\frac{3}{2}} \exp\left(-\beta\frac{m\boldsymbol{v}^2}{2}\right)\right],$$

thus they are *deformations* of the Maxwellian distribution.



If we assume that $P(\beta|\boldsymbol{\lambda})$ is a gamma distribution,

$$\boxed{P(\beta|u, \beta_S) = \frac{1}{u\beta_S\Gamma(1/u)} \exp\left(-\frac{\beta}{u\beta_S}\right)\left(\frac{\beta}{u\beta_S}\right)^{\frac{1}{u}-1}} \qquad 0 \leq u < 1$$

we obtain the kappa distribution in the form

$$\boxed{P(\boldsymbol{v}|u, \beta_S) = \left(\frac{mu\beta_S}{2\pi}\right)^{\frac{3}{2}} \frac{\Gamma\left(\frac{3}{2}+\frac{1}{u}\right)}{\Gamma\left(\frac{1}{u}\right)} \left[1 + u\beta_S\frac{m\boldsymbol{v}^2}{2}\right]^{-\left(\frac{1}{u}+\frac{3}{2}\right)}}$$

S. Davis, G. Avaria, B. Bora, J. Jain, J. Moreno, C. Pavez, L. Soto. Phys. Rev. E **108**, 065207 (2023).

Invariant parameterization of the kappa distribution

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

The original parameters (κ, v_{th}) of the kappa distribution are obtained as

$$\kappa = \frac{1}{u} + \frac{1}{2} \qquad\qquad \frac{mv_{\text{th}}^2}{2} = \frac{1}{(1-u)\beta_S}$$

and we see that $u \to 0$ is equivalent to $\kappa \to \infty$ (Maxwellian).

The parameters u and β_S can be defined for any superstatistical model, as

$$\beta_S := \big\langle \beta \big\rangle_{\boldsymbol{\lambda}} \qquad\qquad u := \frac{\big\langle (\delta\beta)^2 \big\rangle_{\boldsymbol{\lambda}}}{(\beta_S)^2} \tag{3}$$

and are, in fact, **independent of the number of particles**.

N-particle kappa distribution

The single-particle kappa distribution

$$P(\boldsymbol{v}|u,\beta_S) = \left(\frac{mu\beta_S}{2\pi}\right)^{\frac{3}{2}} \frac{\Gamma\left(\frac{3}{2}+\frac{1}{u}\right)}{\Gamma\left(\frac{1}{u}\right)} \left[1 + u\beta_S \frac{m\boldsymbol{v}^2}{2}\right]^{-\left(\frac{1}{u}+\frac{3}{2}\right)} \tag{4}$$

is generalized for the case of N particles as

$$P(\boldsymbol{v}_1,\ldots,\boldsymbol{v}_N|u,\beta_S) = \left(\frac{\tilde{m}u\beta_S}{2\pi}\right)^{\frac{3N}{2}} \frac{\Gamma\left(\frac{3N}{2}+\frac{1}{u}\right)}{\Gamma\left(\frac{1}{u}\right)} \left[1 + u\beta_S K(\boldsymbol{V})\right]^{-\left(\frac{1}{u}+\frac{3N}{2}\right)} \tag{5}$$

with $\kappa_N := \dfrac{1}{u} + \dfrac{3N}{2} - 1$ the N-particle kappa index and where

$$K(\boldsymbol{V}) := \sum_{i=1}^{N} \frac{m_i \boldsymbol{v}_i^2}{2} \tag{6}$$

is the total kinetic energy of the system. From (5) we can see that

$$\boxed{P(\boldsymbol{v}_1,\ldots,\boldsymbol{v}_N|u,\beta_S) \neq \prod_{i=1}^{N} P(\boldsymbol{v}_i|u,\beta_S)}$$

except for $u=0$, therefore any pair of velocities $\boldsymbol{v}_i$, $\boldsymbol{v}_j$ ($i \neq j$) are **correlated**.

Gibbs sampling

Makes it possible to generate samples $\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$ of variables X, Y when their joint distribution $P(X, Y|\boldsymbol{\lambda})$ is unknown or difficult to use.

Instead of the joint distribution, we just need the conditional distributions $P(X|Y, \boldsymbol{\lambda})$ and $P(Y|X, \boldsymbol{\lambda})$.

Algorithm:

(1) Begin with a seed (x_0, y_0), initialize $t = 0$

(2) Generate x_{t+1} using the conditional distribution $P(X|Y = y_t, \boldsymbol{\lambda})$

(3) Generate y_{t+1} using the conditional distribution $P(Y|X = x_{t+1}, \boldsymbol{\lambda})$

(4) Save the sample (x_{t+1}, y_{t+1})

(5) Make $t = t + 1$ and go back to (2)

Please note that this method is rejection-free!

¿Can we use this idea to generate kappa velocities for N particles with the correct correlations?

Generation of kappa velocities for N particles

The challenge:

Generate samples of $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_N$ according to the N-particle kappa distribution

$$P(\boldsymbol{v}_1, \ldots, \boldsymbol{v}_N | u, \beta_S) = \left(\frac{\tilde{m} u \beta_S}{2\pi}\right)^{\frac{3N}{2}} \frac{\Gamma\left(\frac{3N}{2} + \frac{1}{u}\right)}{\Gamma\left(\frac{1}{u}\right)} \Big[1 + u\beta_S K(\boldsymbol{V})\Big]^{-\left(\frac{1}{u} + \frac{3N}{2}\right)}$$

Solution: Gibbs sampling using the Maxwellian (**Gaussian**) distributions

$$P(\boldsymbol{v}_1, \ldots, \boldsymbol{v}_N | \beta) = \prod_{i=1}^{N} P(\boldsymbol{v}_i | \beta), \qquad P(\boldsymbol{v}_i | \beta) = \left(\frac{m_i \beta}{2\pi}\right)^{\frac{3}{2}} \exp\left(-\beta \frac{m_i \boldsymbol{v}_i^2}{2}\right)$$

and the inverse temperature distribution (**gamma**) given all particle velocities,

$$P(\beta | \boldsymbol{v}_1, \ldots, \boldsymbol{v}_N, u, \beta_S) = \frac{1}{\beta_0 \, \Gamma\left(\frac{1}{u} + \frac{3N}{2}\right)} \exp\left(-\frac{\beta}{\beta_0}\right) \left(\frac{\beta}{\beta_0}\right)^{\frac{1}{u} + \frac{3N}{2} - 1}. \tag{7}$$

$$\text{where} \;\; \beta_0 := \frac{u\beta_S}{1 + u\beta_S K(\boldsymbol{V})}$$

Algorithm: Gibbs sampling for N kappa particles

(1) Initialize the value of inverse temperature: $\beta = \beta_S$

(2) For each $i = 1, 2, \ldots, N$:

Generate the new velocity $\boldsymbol{v}_i$ from the Maxwellian $P(\boldsymbol{v}_i|\beta)$

Save $\boldsymbol{v}_i$

(3) Calculate β_0 using the current kinetic energy $K(\boldsymbol{V}) = \sum_{i=1}^{N} \frac{m_i \boldsymbol{v}_i^2}{2}$

(4) Update β from the distribution $P(\beta|\boldsymbol{v}_1, \ldots, \boldsymbol{v}_N, u, \beta_S)$

(5) Go back to (2)

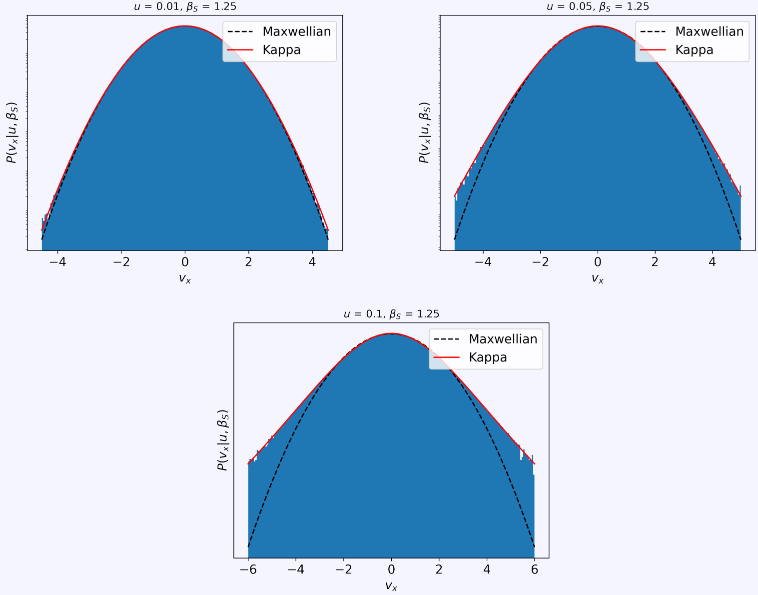
The Gibbs sampling ensures that β is distributed according to $P(\beta|u, \beta_S)$.

Note that β is an auxiliary variable which is obtained from

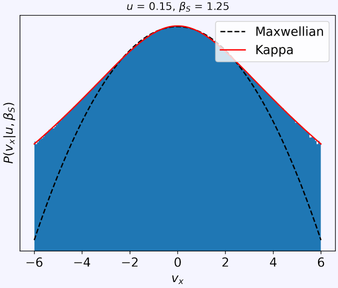
$$P(\beta|\boldsymbol{v}_1, \ldots, \boldsymbol{v}_N, u, \beta_S) = \frac{1}{\beta_0\,\Gamma\left(\frac{1}{u} + \frac{3N}{2}\right)} \exp\left(-\frac{\beta}{\beta_0}\right)\left(\frac{\beta}{\beta_0}\right)^{\frac{1}{u} + \frac{3N}{2} - 1}$$

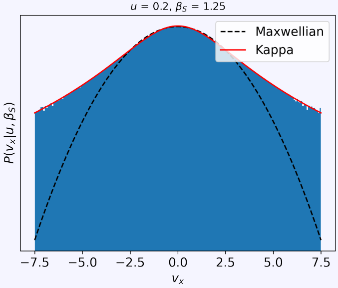
$$\text{where} \quad \beta_0 := \frac{u\beta_S}{1 + u\beta_S\,K(\boldsymbol{V})}$$

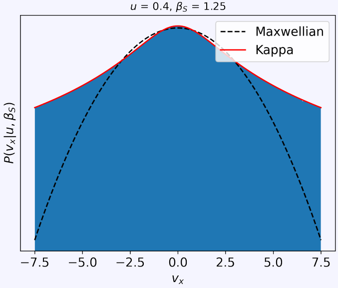
Kappa velocity distributions using Gibbs sampling



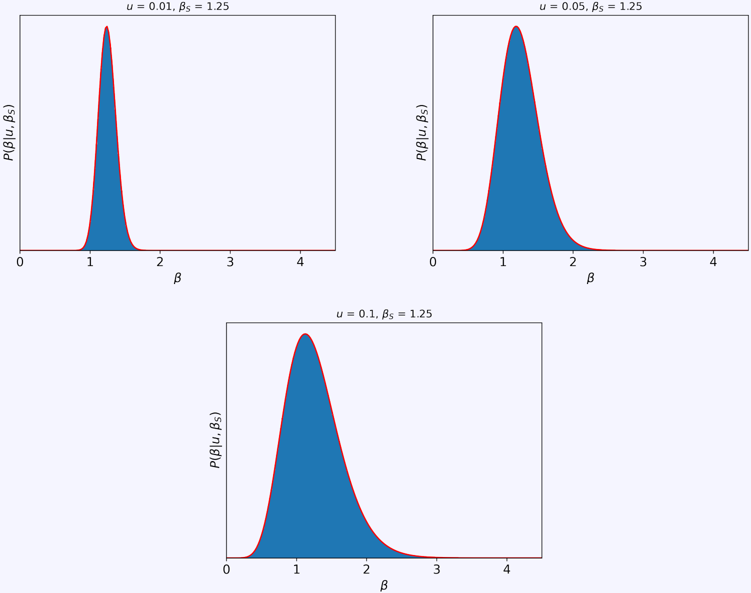
Kappa velocity distributions using Gibbs sampling



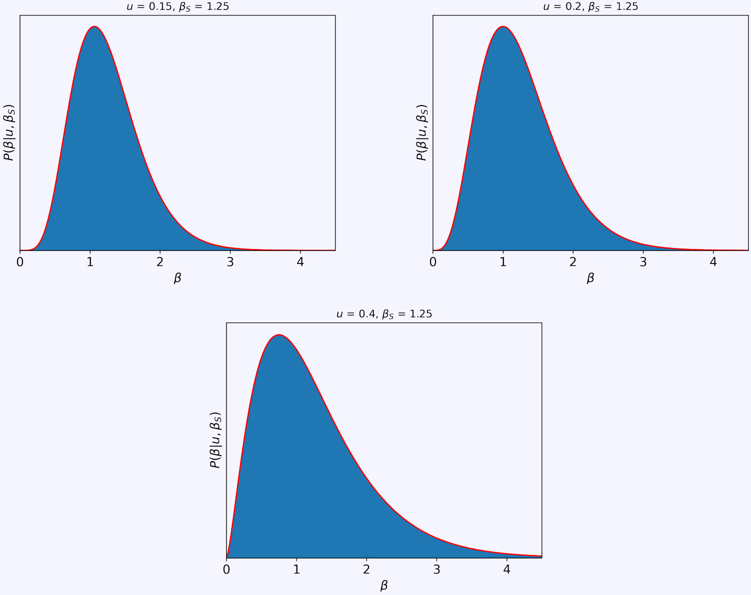




Inverse temperature distributions from Gibbs sampling

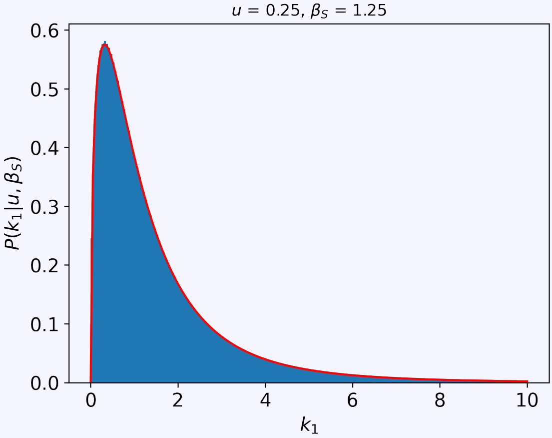


Inverse temperature distributions from Gibbs sampling



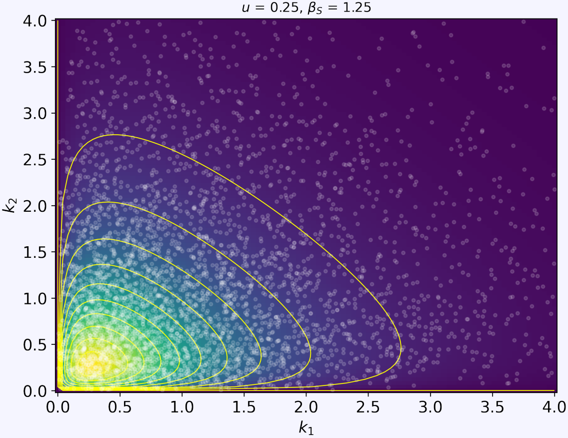
Single-particle energy distribution

$$P(k_1|u,\beta_S) = \frac{2}{\sqrt{\pi}}(u\beta_S)^{\frac{3}{2}}\frac{\Gamma\left(\frac{3}{2}+\frac{1}{u}\right)}{\Gamma\left(\frac{1}{u}\right)}\left[1+u\beta_S k_i\right]^{-\left(\frac{1}{u}+\frac{3}{2}\right)}\sqrt{k_i}$$



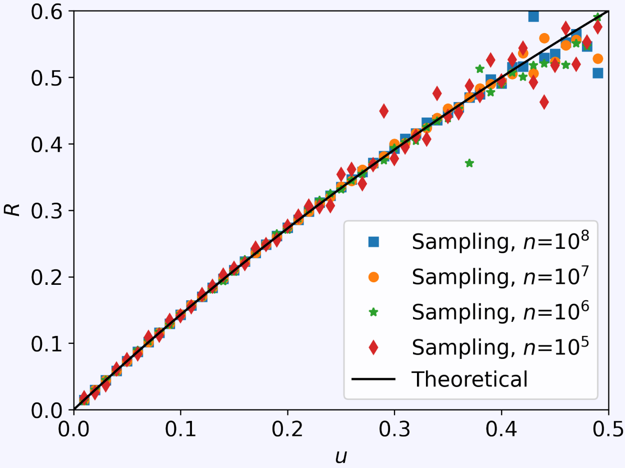
Joint distribution of kinetic energies

$$P(k_1, k_2|u, \beta_S) = \frac{4}{\pi}(\beta_S)^3(1+u)(1+2u)\sqrt{k_1 k_2}\Big[1+u\beta_S(k_1+k_2)\Big]^{-\left(\frac{1}{u}+3\right)}$$



Pearson correlation between kinetic energies

$$R(u) = \frac{\langle \delta k_1 \delta k_2 \rangle_{u,\beta_S}}{\langle (\delta k_1)^2 \rangle_{u,\beta_S}} = \frac{3u}{2+u} = \frac{3}{2\kappa}$$



Mutual information

The mutual information $\mathcal{I}_{XY}$ between two variables X and Y is defined by

$$\boxed{\mathcal{I}_{XY}(\boldsymbol{\lambda}) := \left\langle \ln\left[\frac{P(X, Y|\boldsymbol{\lambda})}{P(X|\boldsymbol{\lambda})P(Y|\boldsymbol{\lambda})}\right]\right\rangle_{\boldsymbol{\lambda}}}$$

and measures the correlation between them. For any pair of variables X, Y it holds that

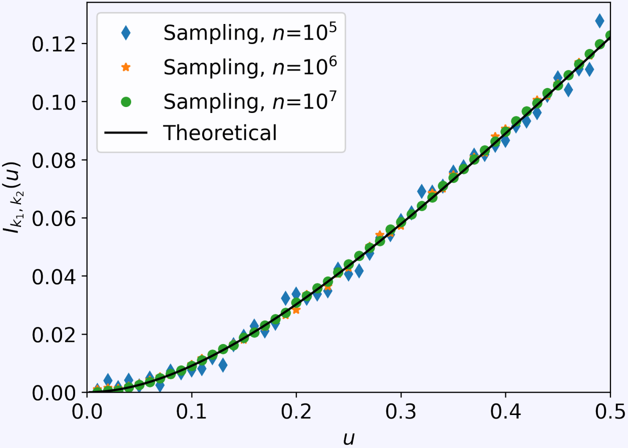
$$\mathcal{I}_{XY}(\boldsymbol{\lambda}) \geq 0, \tag{8}$$

being zero only in the case where X and Y are independent, that is, if

$$P(X, Y|\boldsymbol{\lambda}) = P(X|\boldsymbol{\lambda})P(Y|\boldsymbol{\lambda}). \tag{9}$$

Mutual information between kinetic energies

$$\mathcal{I}_{k_1,k_2}(u) = 2F\left(\frac{1}{u}+\frac{3}{2}\right) - F\left(\frac{1}{u}\right) - F\left(\frac{1}{u}+3\right), \quad \text{con} \quad F(z) := z\frac{\partial}{\partial z}\ln\Gamma(z) - \ln\Gamma(z)$$



Concluding remarks

- Superstatistics provides an elegant formulation of kappa distributions
- Kappa distributions can be written in terms of invariant parameters *u* and β_S, where *u* measures the uncertainty about the temperature
- Using Gibbs sampling it is possible to generate kappa velocities efficiently and preserving interparticle correlations
- This method only requires generation of Gaussian and gamma (pseudo)random numbers

For more information:

(1) *Single-particle velocity distributions of collisionless, steady-state plasmas must follow Superstatistics.* Sergio Davis, Gonzalo Avaria, Biswajit Bora, Jalaj Jain, José Moreno, Cristian Pavez, Leopoldo Soto.
Physical Review E **100**, 023205 (2019).

(2) *Kappa distribution from particle correlations in non-equilibrium, steady-state plasmas.*
Sergio Davis, Gonzalo Avaria, Biswajit Bora, Jalaj Jain, José Moreno, Cristian Pavez, Leopoldo Soto.
Physical Review E **108**, 065207 (2023).

(3) *Kappa distributions in the framework of superstatistics.*
Sergio Davis, Biswajit Bora, Cristian Pavez, Leopoldo Soto.
Physica A **682**, 131191 (2026).

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