Generalised thermostatistics using hyperensembles

Jan Naudts

Department of Physics, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerpen, Belgium

Abstract. The hyperensembles, introduced by Crooks in a context of non-equilibrium statistical physics, are considered here as a tool for systems in equilibrium. Simple examples like the ideal gas, the mean-field model, and the Ising interaction on small square lattices, are worked out to illustrate the concepts.

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INTRODUCTION

The starting point of superstatistics [1, 2] is the assumption that the inverse temperature $\beta$ of the Boltzmann-Gibbs distribution

$$q_\beta(x) = \frac{1}{Z(\beta)} e^{-\beta H(x)}$$

may itself be a fluctuating quantity, governed by a probability density $f(\beta)$. The resulting probability distribution is then determined by

$$p_f(x) = \int_0^\infty d\beta \, f(\beta) q_\beta(x).$$

The choice of the hyperdistribution $f(\beta)$ (called the entropic distribution in [3]) depends on the application at hand. Recently, Crooks [3] suggested that this distribution should be determined by means of the Maximum Entropy Principle (MEP) because, in general, information is lacking about what choice of $f(\beta)$ is appropriate. Additional constraints, introduced when applying the MEP, then lead to a parametrised family of probability distributions. The latter he called a hyperensemble.

The choice of constraints is crucial. Crooks proposes to use three constraints: the normalisation, the mean energy and the mean entropy. The result of applying the MEP is that the hyperdistribution is of the form

$$f(\beta) = \frac{c(\beta)}{Z(\theta, \lambda)} \exp \left( \lambda \mathcal{S}(\beta) - \theta \langle H \rangle_\beta \right).$$

Here, $\theta$ is the Lagrange multiplier controlling the mean energy, $\lambda$ controls the mean entropy. The canonical entropy is denoted $\mathcal{S}(\beta)$ to distinguish it from the entropy of the
hyperensemble. The normalisation is given by

\[ Z(\theta, \lambda) = \int_{0}^{\infty} c(\beta) d\beta \exp \left( \lambda \tilde{S}(\beta) - \theta \langle H \rangle_\beta \right). \]  

(4)

The intention of Crooks is to use the notion of hyperensembles to study systems out of equilibrium. The present paper shows the usefulness of hyperensembles as a unifying concept for systems in equilibrium. In this context the parameter \( \lambda \) plays no important role and may be taken equal to 1.

**THE IDEAL GAS**

Consider only the momenta \( p_1, p_2, \cdots, p_N \) of an ideal gas containing \( N \) particles. The Hamiltonian is

\[ H(p) = \frac{1}{2m} \sum_{n=1}^{N} \sum_{\alpha=1}^{3} p_{n\alpha}^2. \]  

(5)

The canonical probability distribution is

\[ q_\beta(p) = \frac{1}{(2\pi mk_BT)^{3N/2}} e^{-\beta H(p)}. \]  

(6)

The entropy and energy equal

\[ \tilde{S}(\beta) = -\frac{3N}{2} \ln \beta, \quad \langle H \rangle_\beta = \frac{3N}{2} \beta^{-1}. \]  

(7)

After optimisation, the hyperdistribution becomes

\[ f(\beta) = \frac{c(\beta)}{Z(\theta)} \exp \left( -\frac{3N}{2} \ln \beta - \theta \frac{3N}{2\beta} \right). \]  

(8)

This is the inverse Gamma distribution, also called the inverse \( \chi^2 \)-distribution. It has a maximum at \( \beta = \theta \). Hence, the canonical probability distribution \( q_\beta(p) \), with \( \beta = \theta \), is the most likely distribution at inverse hypertemperature \( \theta \).

The ideal gas, together with the above hyperdistribution, was already considered in the context of superstatistics [4, 5].

**THE MEAN-FIELD APPROXIMATION**

Consider spin variables \( \sigma_1, \sigma_2, \cdots, \sigma_n \), taking on values \( \pm 1 \). The equilibrium states of the ideal paramagnet are the product states

\[ q_\epsilon(\sigma) = \prod_{n=1}^{N} \epsilon^{\frac{1}{2}(1+\sigma_n)} (1-\epsilon)^{\frac{1}{2}(1-\sigma_n)}, \]  

(9)
 FIGURE 1. Hyperdistribution $f_{\beta,h}(\epsilon)$ of the mean-field model with $J = 1$, $N = 5$, $h = 0$, and $\beta = 0.6$ and $\beta = 1.2$, respectively.

with $0 \leq \epsilon \leq 1$. The total magnetisation is $\langle M \rangle_\epsilon = N(2\epsilon - 1)$. The entropy is

$$\hat{S}(\epsilon) = -N\epsilon \ln \epsilon - N(1 - \epsilon) \ln(1 - \epsilon).$$

(10)

Here, we use $\epsilon$ as a parameter instead of $\beta$. Introduce the ferromagnetic Hamiltonian

$$H = -\frac{1}{2} \sum_{m,n=1}^{N} J_{m,n} \sigma_m \sigma_n - h \sum_{m=1}^{N} \sigma_m.$$  

(11)

Its average, using the equilibrium distribution of the paramagnet and assuming $J_{mm} = 0$, equals $\langle H \rangle_\epsilon = -\frac{1}{2}NJ(2\epsilon - 1)^2 - hN(2\epsilon - 1)$, with

$$J = \frac{1}{N} \sum_{m,n=1}^{N} J_{m,n}.$$  

(12)

The optimised hyperdistribution with parameters $\beta$ (instead of $\theta$) and $h$ is

$$f_{\beta,h}(\epsilon) = \frac{1}{Z(\beta,h)} \exp \left( \hat{S}(\epsilon) - \beta \langle H \rangle_\epsilon \right)$$

$$= \frac{1}{Z(\beta,h)} \exp \left( N \left[ -\epsilon \ln \epsilon - (1 - \epsilon) \ln(1 - \epsilon) + \frac{1}{2} \beta J(2\epsilon - 1)^2 + \beta h(2\epsilon - 1) \right] \right).$$

(13)

For $\beta > \beta_{\text{mf}} = J^{-1}$ and $h = 0$ the hyperdistribution has two maxima, corresponding to two equally likely states. See the Figure 1. At high temperature the paramagnetic state $q_\epsilon(\sigma)$ with $\epsilon = 1/2$ is the most likely state. At low temperature the two states with $\epsilon \neq 1/2$, maximising $f_{\beta,h}(\epsilon)$, are the most likely ones. This bifurcation from a paramagnetic state to a pair of ferromagnetic states as a function of the temperature $\beta^{-1}$ involves a spontaneous magnetisation of the system.
In the quantum case the ideal paramagnet is described by a density matrix of the product form $\rho^\otimes N$, with

$$\rho = \frac{1}{2} + \sum_{k=1}^{3} \theta_k \sigma_k.$$  \hspace{1cm} (14)

The $\sigma_k$ are the Pauli matrices. The Hamiltonian of the Heisenberg model reads

$$H = -\frac{1}{2} \sum_{m,n=1}^{N} J_{m,n} \sum_{k=1}^{3} \sigma_{mk} \sigma_{nk} - h \sum_{n=1}^{N} \sigma_n.$$  \hspace{1cm} (15)

The matrix $\sigma_{mk}$ is a copy of $\sigma_k$ at site $m$. Without restriction, assume $J_{nn} = 0$. Then the average energy in the product state is

$$\langle H \rangle_{\theta} = -NJ|\theta|^2 + Nh\theta_3,$$

with $J$ as in the classical case. The von Neumann entropy of the product state equals

$$S(\rho^\otimes N) = -\frac{N}{2} (1 + |\theta|) \ln \frac{1}{2} (1 + |\theta|) - \frac{N}{2} (1 - |\theta|) \ln \frac{1}{2} (1 - |\theta|).$$ \hspace{1cm} (16)

One can now calculate the hyperdistribution $f_{\beta, h}(\theta)$. Note that this is a classical distribution, not an operator. A maximum is attained when the following three equations are satisfied

$$\frac{1}{2} \theta_k \ln \frac{1 + |\theta|}{1 - |\theta|} = -2\beta J \theta_k - h \delta_{k,3}, \hspace{1cm} k = 1, 2, 3.$$ \hspace{1cm} (17)

Assuming $h \neq 0$, the solution requires $\theta_2 = \theta_3 = 0$. The third parameter $\theta_3$ must be a solution of the usual mean-field equation $\theta_3 = \tanh(\beta J \theta_3 + \theta_3 h)$.

**THE MICROCANONICAL ENSEMBLE**

Following Boltzmann, the probability distribution of the microcanonical ensemble equals

$$q_E(x) = \frac{c(x)}{\rho(E)} \delta(E - H(x)),$$ \hspace{1cm} (18)

with the density of states $\rho(E)$ given by $\rho(E) = \int dx c(x) \delta(E - H(x))$. The Boltzmann entropy is $\hat{S}(E) = k_B \ln \rho(E)$. The optimised hyperdistribution becomes

$$f_{\theta}(E) = \frac{1}{Z(\theta)} \exp \left( \hat{S}(E) - \theta E \right) = \frac{\rho(E)}{Z(\theta)} e^{-\theta E}.$$ \hspace{1cm} (19)

The probability distribution $p_{\theta}(x)$ of the hyperensemble coincides with the canonical Boltzmann-Gibbs distribution

$$p_{\theta}(x) \equiv \int_0^\infty dE f_{\theta}(E) q_E(x).$$
The parameter $\theta$ is the inverse temperature $\beta$.

As an example, involving a discrete phase space, let us consider the 2-dimensional Ising model on a square lattice of $n \times n$ Ising spins. Count the number of configurations $C(m, n)$ with $m$ spins up and $n$ pairs of unequal nearest neighbours. See the Figure 2.

The entropy is $\mathcal{S}(m, n) = \ln C(m, n)$. The hyperdistribution is

$$f_{\beta, h}(m, n) = \frac{C(m, n)}{Z(\beta, h)} \exp\left(2\beta J(N - n) - \beta h(N - 2m)\right).$$

(21)

At constant $n$ and $h = 0$ it is proportional to $C(m, n)$. See the Figure 3. It shows two maxima, corresponding with the spin up and spin down phases.

**DISCUSSION**

The aim of the paper is to show that the concept of hyperensembles, as introduced by Crooks [3] in a context of non-equilibrium systems, fits well into the standard theory of equilibrium statistical physics. Several situations have been considered. In the example of the ideal gas the hyperensemble approach coincides with the superstatistical treatment of [4, 5]. In the mean-field theory one starts from a simple model, such as the
ideal paramagnet, to solve more complex models under the constraint that the state of the system is an equilibrium state of the simple model. The present formulation in terms of hyperensembles is a mere reformulation of what is known since long. However, it can be applied in a very general context. Such an application beyond the traditional scope of mean-field theory can be found in [6], where a random walk model is used to model polymer behaviour. In the microcanonical ensemble the probability distribution of the hyperensemble coincides with the canonical Boltzmann-Gibbs distribution. The maximum of the hyperdistribution may be degenerate. This is for instance the case in finite spin lattices with ferromagnetic Ising interaction. Hence, the most-likely microcanonical state is non-unique. Such a feature also occurs in mean-filed models and may be interpreted as a precursor of the phase transition occurring in the thermodynamic limit.

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