Non-extensive Entropy and Quasi-Equilibrium States in Hamiltonian Mean-Field Model

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Abstract

We investigate the thermodynamic properties of Hamiltonian mean-field (HMF) model as a prototypical long-range system by means of the non-extensive thermodynamics. Especially, the quasi-equilibrium state as extremum state of the generalized Tsallis entropy is studied and its thermodynamic stability is analyzed. Based on these analysis, the connection with quasi-stationary behaviors found in the numerical simulations is discussed.

Key words: non-extensive entropy, quasi-equilibrium state, Hamiltonian mean-field model, long-range system

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1 Introduction

There has been a lot of active debates on the non-extensive generalization of the standard Boltzmann-Gibbs statistical mechanics. In this subject, one important issue is the application of non-extensive statistics to the long-range systems. Since the extensivity or the additivity of the thermodynamic quantities no longer hold in this system, one expects that the long-range systems is one of the most preferable and interesting testing grounds for the framework of non-extensive statistics.

Among several well-known long-range system, the so-call Hamiltonian mean-field (HMF) model has attracted much attention because of the simplicity. The HMF model describes the motion of \( N \) rotators under the influence of the globally-coupled cosine interaction [1] (see also Ref.[2] for review). In the
case of the attractive interaction, the model exhibits the second-order phase transition[1].

Recently, numerical experiments of the HMF model have found that there exists the quasi-equilibrium (or the quasi-stationary) state near the transition point and the non-Gaussian momentum distribution could be described by the non-extensive statistics with Tsallis entropy[3]. Here, the term, quasi-equilibrium state means that due to the slow relaxation to the Boltzmann-Gibbs equilibrium, the non-equilibrium transient apparently seems equilibrium state. The dynamical study of the quasi-equilibrium state reveals that the timescale of the relaxation scales as $N^{1.7}$ and the relaxation proceeds through different stable stationary states of Vlasov equations[4].

While the existence of quasi-equilibrium state is really confirmed under a certain initial condition, the connection with non-extensive statistics is still under investigation. The one reason is that in most of the work, the non-Gaussian momentum distribution had been naively compared with the $q$-exponential distribution under the assumption of spatial homogeneity. However, in general, the weak clustering feature is manifest in quasi-equilibrium state and the magnetization cannot be neglected. Hence, to clarify the connection with non-extensive statistics, the spatially inhomogeneity of the quasi-equilibrium state must be fully taken into account in both numerical and theoretical analysis. In this paper, based on the Tsallis entropy, we construct the quasi-equilibrium state of the HMF model. Within the mean-field treatment, thermodynamic properties of HMF model are investigated and their thermodynamic stability is analyzed.

The paper is organized as follows · · ·.

2 Model

Hamiltonian

The model Hamiltonian is given by (e.g., [1]):

$$H = \frac{1}{2} \sum_{j=1}^{N} p_j^2 + \frac{1}{2N} \sum_{j,k=1}^{N} [1 - \cos (\theta_j - \theta_k)]$$  \hspace{1cm} (1)

Mean-field description

For large $N$, granularity of the particle distribution becomes negligible and the $N$-particle Hamiltonian dynamics is nearly equal to the Vlasov dynamics
characterized by the one-particle distribution function $f(\theta, p; t)$. Using this function, the number of particles $N$, total energy $E$ and the magnetization are expressed as follows:

\begin{align*}
\text{# of particles} & : \quad N = \int_{0}^{2\pi} d\theta \int_{-\infty}^{+\infty} dp \; f(\theta, p) \\
\text{Total energy} & : \quad E = \int_{0}^{2\pi} d\theta \int_{-\infty}^{+\infty} dp \left\{ \frac{1}{2} p^2 + \frac{1}{2} \Phi(\theta) \right\} f(\theta, p) \\
\text{Magnetization} & : \quad \vec{M} = \frac{1}{N} \int_{0}^{2\pi} d\theta \int_{-\infty}^{+\infty} dp \; (\cos \theta, \sin \theta) \; f(\theta, p)
\end{align*}

where $\Phi(\theta)$ is the potential defined by

$$
\Phi(\theta) = \frac{1}{N} \int_{0}^{2\pi} d\theta' \int_{-\infty}^{+\infty} dp' \; \{ 1 - \cos (\theta - \theta') \} \; f(\theta', p')
$$

Notice that irrespective of the distribution function, the potential (5) satisfies the following equation:

$$
\frac{d^2 \Phi}{d\theta^2} = 1 - \Phi(\theta)
$$

The general solution of (6) is given by

$$
\Phi(\theta) = 1 + B \cos (\theta + \gamma),
$$

where $B$ and $\gamma$ are the arbitrary constants. In what follows, we simply put $\gamma = 0$, since the translational invariance in the $\theta$-direction does always hold in the Hamiltonian (1). The constant $B$ characterizes the clustering feature of the particle distribution: uniform phase ($B = 0$) or cluster phase ($B \neq 0$).

For later analysis, we define the number distribution $\rho(\theta)$, the pressure $P(\theta)$ and the momentum distribution $F_p(p)$:

\begin{align*}
\text{Number distribution} & : \quad \rho(\theta) = \int dp \; f(\theta, p) \\
\text{Pressure} & : \quad P(\theta) = \int dp \; p^2 \; f(\theta, p)
\end{align*}
3 Equilibrium properties from Boltzmann-Gibbs entropy

Thermodynamic properties based on the Boltzmann-Gibbs entropy have been already investigated by Inagaki (1993). For notational convenience and later analysis, we repeat the same analysis as in Ref.

3.1 Extremum state of Boltzmann-Gibbs entropy

Let us first consider the equilibrium configuration based on the Boltzmann-Gibbs entropy $S_{BG}$:

$$S_{BG} = -N \int_0^{2\pi} d\theta \int dp \left\{ \frac{f(\theta, p)}{N} \right\} \ln \left\{ \frac{f(\theta, p)}{N} \right\}$$

Denoting the distribution function as $f(\theta, p) = N h(\theta, p)$, extremization of the entropy (11) under keeping the energy and the number of particles fixed implies

$$\delta \left[ S_{BG} - \alpha \left\{ \int d\theta \int dp \, h(\theta, p) - 1 \right\} - \beta \left\{ \int d\theta \int dp \left( \frac{1}{2}p^2 + \frac{1}{2}\Phi \right) f - E \right\} \right] = 0,$$

where $\alpha$ and $\beta$ are the Lagrange multiplier. The variation with respect to the function $h(\theta, p)$ leads to

$$\int d\theta \int dp \left[ -N(\ln h + 1) - \alpha - \beta N \left( \frac{1}{2}p^2 + \Phi \right) \right] \delta h = 0,$$

Since the above equation must be satisfied independently of the choice of the variation $\delta h$, one obtains

$$f(\theta, p) = N \, h(\theta, p) = A e^{-\beta[p^2/2 + \Phi(\theta)]} ; \quad A = Ne^{-1-\alpha/N}.$$  

The numerical constant $A$ in equation (13) is related to the constant $B$ in the potential $\Phi$. Using the equation (7), substitution of (13) into (2) yields (see
eq.[A.2] in Appendix A):

\[
N = \sqrt{\frac{2\pi}{\beta}} A \int_0^{2\pi} d\theta \ e^{-\beta(B\cos\theta+1)} \iff \frac{A}{N} = \sqrt{\frac{\beta}{(2\pi)^3}} \frac{1}{e^{-\beta} I_0(\beta B)}, \tag{14}
\]

where \(I_0(x)\) denotes the zeroth modified Bessel function of the first kind. Further, substitution of (13) into (5) gives

\[
B \cos \theta = -\sqrt{\frac{2\pi}{\beta}} \frac{A}{N} \int d\theta' \cos(\theta - \theta') \ e^{-\beta(B\cos\theta'+1)}
\left\{
\begin{aligned}
B &= -\sqrt{\frac{2\pi}{\beta}} \frac{A}{N} \int d\theta' \cos \theta' \ e^{-\beta(B\cos\theta'+1)} , \\
0 &= -\sqrt{\frac{2\pi}{\beta}} \frac{A}{N} \int d\theta' \sin \theta' \ e^{-\beta(B\cos\theta'+1)} .
\end{aligned}
\right. \tag{15}
\]

In the last line, while the second equation is an identity and is always satisfied, the first equation leads to a non-trivial relation. Rewriting the factor \(A/N\) with (14), we have

\[
B = -\frac{2\pi}{\beta} \frac{A}{N} \int d\theta' \cos \theta' \ e^{-\beta(B\cos\theta'+1)} = \frac{I_1(\beta B)}{I_0(\beta B)}. \tag{16}
\]

The above equation is the most important equation in determining the equilibrium configuration. For a given \(\beta\), numerical value of the constant \(B\) is obtained by solving (16). Then, the potential profile is completely specified. Note that the equation (16) has a solution \(B = 0\), in addition to the non-zero solution \((B \neq 0)\).

3.2 Equilibrium configuration

Provided the numerical value of \(B\) from equation (16), all the macroscopic quantities such as energy and magnetization are determined. Denoting the solution of (16) by \(B = B_*(\beta)\), we here explicitly write down the analytic expressions for these quantities.

Energy

Substituting (13) into the definition (3), the total energy becomes
\[ E = \frac{1}{2} \int d\theta \int dp \{ p^2 + (B_\ast \cos \theta + 1) \} \ A e^{-\beta(p^2/2 + B_\ast \cos \theta + 1)} \]
\[ = \frac{A}{2} \sqrt{\frac{2\pi}{\beta}} \left[ (\beta^{-1} + 1) \int_0^{2\pi} d\theta \ e^{-\beta(B_\ast \cos \theta + 1)} + B_\ast \int_0^{2\pi} d\theta \ \cos \theta \ e^{-\beta(B_\ast \cos \theta + 1)} \right] \]
\[ = \frac{N}{2\beta} \left\{ 1 + \beta(1 - B_\ast^2) \right\}, \quad (17) \]

where we have used the relation (15) in the last line.

**Magnetization**

Using the relation (15), equation (4) becomes

\[ \vec{M} = \frac{A}{N} \sqrt{\frac{2\pi}{\beta}} \int_0^{2\pi} d\theta \ (\cos \theta, \sin \theta) \ e^{-\beta(B_\ast \cos \theta + 1)} = (-B_\ast, \ 0) \quad (18) \]

**Microscopic quantities**

Distribution function:

\[ f(\theta, p) = \rho(\theta) \sqrt{\frac{\beta}{2\pi}} e^{-\beta p^2/2}, \quad (19) \]

Number distribution/Pressure:

\[ \rho(\theta) = \beta P(\theta) = N \frac{e^{-\beta B_\ast \cos \theta}}{2\pi I_0(\beta B_\ast)}, \quad (20) \]

Momentum distribution:

\[ F_p(p) = N \sqrt{\frac{\beta}{2\pi}} e^{-\beta p^2/2}. \quad (21) \]

**4 Quasi-equilibrium structure based on Tsallis entropy**

**4.1 Extremum state of Tsallis entropy**

We now consider the quasi-equilibrium state characterized by the Tsallis entropy \( S_q \). In the framework of the Tsallis statistics using the normalized \( q \)-values, the one-particle distribution function \( f(\theta, p) \) should be expressed as
the escort distribution $^1$ [6]:

$$f(\theta, p) = N \frac{\{h(\theta, p)\}^q}{\int d\theta \int dp \{h(\theta, p)\}^q},$$

(22)

where $h(\theta, p)$ is a fundamental probability distribution characterizing the phase-space structure and coincides with the one defined in Section 3.1 in the limit $q \rightarrow 1$. Using this, the Tsallis entropy is defined by

$$S_q = -\frac{1}{q-1} \int d\theta \int dp \left[ \{h(\theta, p)\}^q - h(\theta, p) \right].$$

(23)

Note that the probability distribution $h(\theta, p)$ satisfies the normalization condition:

$$\int d\theta \int dp \ h(\theta, p) = 1.$$  

(24)

Similar to the equation (12) in the Boltzmann-Gibbs case, the variational problem for the Tsallis entropy under keeping the normalization and the total energy fixed becomes $^2$

$$\delta \left[ S_q - \alpha \left( \int d\theta \int dp \ h - 1 \right) - \beta \left( \frac{1}{2}p^2 + \frac{1}{2}\Phi \right) f - E \right] = 0.$$  

(25)

The variation with respect to the probability $h(\theta, p)$ leads to

$$\int d\theta \int dp \left[ -\frac{1}{q-1} (qh^{q-1} - 1) \delta h - \alpha \delta h - \beta \left( \frac{1}{2}p^2 + \Phi \right) \delta f \right] = 0,$$

(26)

where the variation $\delta f$ is given by

$$\delta f(\theta, p) = q f(\theta, p) \left\{ \frac{\delta h(\theta, p)}{h(\theta, p)} - \frac{1}{N} \int d\theta' \int dp' f(\theta', p') \frac{\delta h(\theta', p')}{h(\theta', p')} \right\}.$$  

(27)

Substituting the above equation into (26) and exchanging the role of the variables $(\theta, p) \leftrightarrow (\theta', p')$ in the phase-space integral, we obtain

$^1$ Within this treatment, the normalized $q$-values are naturally incorporated into the mean-field description of HMF model and are indeed consistent with the definitions (2)-(4).

$^2$ This extremization procedure is the one proposed by Tsallis, Mendes & Plastino (1998). see Ref.[7].
\[ \int d\theta \int dp \left[ \frac{1}{q-1} (qh^{q-1} - 1) - \alpha - \beta N_q \frac{h^{q-1}}{N_q} \left( \frac{1}{2} p^2 + \Phi - \epsilon \right) \right] \delta h = 0, \quad (28) \]

where we defined:

\[ \epsilon = \frac{1}{N} \int d\theta \int dp \left( \frac{1}{2} p^2 + \Phi \right) f(\theta, p), \quad (29) \]
\[ N_q = \int d\theta \int dp \{h(\theta, p)\}^q. \quad (30) \]

Equation (28) should be satisfied independently of the choice of the variation \( \delta h \). Thus, we obtain the power-law distribution:

\[ f(\theta, p) = N \frac{\{h(\theta, p)\}^q}{N_q} = A \left[ \Phi_0 - \frac{1}{2} p^2 - \Phi(\theta) \right]^{q/(1-q)} \quad (31) \]

with the constants \( A \) and \( \Phi \) respectively being

\[ A = \frac{N}{N_q} \left\{ \frac{q(1-q)}{\alpha(1-q) + 1} \frac{\beta N}{N_q} \right\}^{q/(1-q)}, \quad (32) \]
\[ \Phi_0 = \frac{N_q}{\beta N(1-q)} + \epsilon. \quad (33) \]

From the expression (31), we readily see that the extremum state of the Tsallis entropy satisfies the polytropic equation of state as follows. Using the formula,

\[ \int dp \ p^j f(\theta, p) = 2^{(j-1)/2} B \left( \frac{j+1}{2}, \frac{1}{1-q} \right) A \{\Phi_0 - \Phi(\theta)\}^{q/(1-q)+(j+1)/2} \quad (34) \]

with \( B(a, b) \) being the \( \beta \) function, the number distribution and the pressure defined by (8) and (9) respectively become

\[ \rho(\theta) = \frac{A}{\sqrt{2}} B \left( \frac{1}{2}, \frac{1}{1-q} \right) \{\Phi_0 - \Phi(\theta)\}^{q/(1-q)+1/2}, \quad (35) \]
\[ P(\theta) = \sqrt{2} A B \left( \frac{3}{2}, \frac{1}{1-q} \right) \{\Phi_0 - \Phi(\theta)\}^{q/(1-q)+3/2}, \quad (36) \]

which yield the polytropic relation:

\[ P(\theta) = K_n \rho(\theta)^{1+1/n}. \quad (37) \]
The polytrope index \( n \) and the coefficient \( K_n \) are respectively given by

\[
n = \frac{q}{1 - q} + \frac{1}{2}, \quad (38)
\]

\[
K_n = \frac{1}{n + 1} \left[ \frac{A}{\sqrt{2}} B \left( \frac{1}{2}, n + \frac{1}{2} \right) \right]^{-1/n}. \quad (39)
\]

### 4.2 Macroscopic quantities

Quasi-equilibrium distribution obtained in section 4.1 has several numerical constants, which can be determined as follows. For the overall factor \( A \) in the distribution function (31), the definition (2) leads to

\[
N = \frac{A}{\sqrt{2}} B \left( \frac{1}{2}, n + \frac{1}{2} \right) \int_{0}^{2\pi} d\theta (\Phi_0 - 1 - B \cos \theta)^n
\]

\[
\iff \quad \frac{A}{N} = \frac{\sqrt{2}}{B(1/2, n+1/2) \int_{0}^{2\pi} d\theta (\Phi_0 - 1 - B \cos \theta)^n} \quad (40)
\]

As for the quantity \( B \) in the potential (7), a direct substitution of (31) into (7) gives

\[
B \cos \theta = -\frac{A}{\sqrt{2} N} B \left( \frac{1}{2}, n + \frac{1}{2} \right) \int d\theta' \cos (\theta - \theta') (\Phi_0 - 1 - B \cos \theta)^n
\]

\[
\implies \begin{cases} B = -\frac{A}{\sqrt{2} N} B \left( \frac{1}{2}, n + \frac{1}{2} \right) \int d\theta' \cos \theta' \ (\Phi_0 - 1 - B \cos \theta)^n \\ 0 = -\frac{A}{\sqrt{2} N} B \left( \frac{1}{2}, n + \frac{1}{2} \right) \int d\theta \sin \theta \ (\Phi_0 - 1 - B \cos \theta)^n \end{cases} \quad (41)
\]

Since the second equation in the last line is an identity and always holds, the non-trivial relation is obtained through the first equation. Eliminating the factor \( A/N \) from (40), we have

\[
B = -\frac{2\pi}{\int_{0}^{2\pi} d\theta (\Phi_0 - 1 - B \cos \theta)^n}. \quad (42)
\]
Note that another important relation is obtained through the definition (29). As examined in the three-dimensional self-gravitating case[6], this non-trivial relation yields a definition of the thermodynamic temperature in the non-extensive statistics. Using the definitions of number distribution and pressure, equation (29) is rewritten with

\[
\epsilon = \frac{1}{N} \int d\theta \left\{ \frac{1}{2} P(\theta) + \rho(\theta) \Phi(\theta) \right\} \\
= \frac{1}{N} \int d\theta \left[ \frac{1}{2} P(\theta) - \rho(\theta) \{ \Phi_0 - \Phi(\theta) \} \right] + \Phi_0. \tag{43}
\]

From (35) and (36), one finds \( \Phi_0 - \Phi(\theta) = (n+1)P(\theta)/\rho(\theta) \). Using this relation and substituting the definition of \( \Phi_0 \) (eq.[33]) into the above equation, the variable \( \epsilon \) is canceled out and one obtains

\[
\frac{N_q}{\beta} = \int d\theta \ P(\theta). \tag{44}
\]

As will be discussed in Appendix B, the quantity \( N_q/(\beta N) \) can be recognized as the thermodynamic temperature (see also Ref.[6] in the case of the self-gravitating system). We therefore denote \( N_q/(\beta N) \) by \( T_{\text{phys}} \), hereafter. The right-hand side of the equation (44) is explicitly evaluated using the functional form of \( P(\theta) \), (36). We have

\[
T_{\text{phys}} = \frac{1}{N} \int d\theta \ P(\theta) \\
= \frac{A}{N} \sqrt{2} B \left( \frac{3}{2}, n + \frac{1}{2} \right) \frac{2\pi}{0} d\theta \ (\Phi_0 - 1 - B \cos \theta)^{n+1} \\
= \frac{1}{n + 1} \frac{2\pi}{0} d\theta \ (\Phi_0 - 1 - B \cos \theta)^{n+1} \frac{2\pi}{0} d\theta \ (\Phi_0 - 1 - B \cos \theta)^n. \tag{45}
\]

In the last line, we used the relation (40) to eliminate the factor \( A/N \).

Using the above relations, the total energy and the magnetization can be simply expressed as follows. The total energy \( E \) is rewritten with the aid of (7), (35) and (45):

\[
E = \int d\theta \int dp \ \left\{ \frac{1}{2} P(\theta) + \frac{1}{2} \Phi(\theta) \rho(\theta) \right\}
\]
\[\begin{align*}
    &= \frac{N}{2} T_{\text{phys}} + \frac{N}{2} + \frac{A}{2\sqrt{2}} B \left( \frac{1}{2}, n + \frac{1}{2} \right) B \int_0^{2\pi} d\theta \cos \theta (\Phi_0 - 1 - B \cos \theta)^n \\
    &= \frac{N}{2} (T_{\text{phys}} + 1 - B^2)
\end{align*}\]

In the second line, we used the first equation in (41). Thus, the energy per particle becomes

\[\frac{E}{N} = \frac{T_{\text{phys}}}{2} \left\{ 1 + \frac{1}{T_{\text{phys}}} (1 - B^2) \right\}. \quad (46)\]

As for the magnetization, the relation (41) leads to

\[\vec{M} = \frac{A}{\sqrt{2}N} B \left( \frac{1}{2}, n + \frac{1}{2} \right)^{2\pi} \int_0^{2\pi} d\theta \left( \cos \theta, \sin \theta \right) (\Phi_0 - 1 - B \cos \theta)^n
\]

\[= (-B, 0). \quad (47)\]

Comparing the above expressions with the Boltzmann-Gibbs results (eq.[17][18]), the resultant expressions for \(E\) and \(\vec{M}\) are shown to be form-invariant. Provided the temperature \(T_{\text{phys}}\) and the constant \(B\), specific values of \(E\) and \(\vec{M}\) are obtained.

### 4.3 Quasi-equilibrium structure in cluster phase

The macroscopic quantities \(E\) and \(|\vec{M}|\) derived in previous subsection (eqs.[46] [47]) seem difficult to evaluate because of the complicated integrals in (42) and (45). However, it is easy to find that equation (42) has a particular solution \(B = 0\), corresponding to the uniform phase. In this case, we have \(E/N = (T_{\text{phys}} + 1)/2\) and \(|\vec{M}| = 0\), irrespective of the polytrope index \(n\). The equation (45) becomes trivial and is given by \(T_{\text{phys}} = (\Phi_0 - 1)/(n + 1)\), which merely determines the numerical value of \(\Phi_0\). Thus, in the uniform phase, the thermodynamic properties of quasi-equilibrium state is indistinguishable to those from the Boltzmann-Gibbs entropy.

On the other hand, differences are manifest in the cluster phase\((B \neq 0)\). Introducing the new variable \(c \equiv (\Phi_0 - 1)/B\)\((-1 \leq c < +\infty)\), the equations (42) and (45) can be expressed in terms of the Gauss hyper-geometric function (see Eqs. [A.3]–[A.6] in Appendix A):
\begin{align}
B &= \frac{n}{2c} \frac{F\left(\frac{1-n}{2}, \frac{1-n}{2}, \frac{1}{2}; \frac{1}{c^2}\right)}{F\left(\frac{1-n}{2}, \frac{-n}{2}, \frac{1}{2}; \frac{1}{c^2}\right)}, \quad (48) \\
T_{\text{phys}} &= \frac{n}{2(n+1)} \frac{F\left(\frac{1-n}{2}, \frac{1-n}{2}, \frac{1}{2}; \frac{1}{c^2}\right) F\left(\frac{-n}{2}, \frac{n+1}{2}, \frac{1}{c^2}\right)}{\left\{F\left(\frac{1-n}{2}, -\frac{n}{2}, \frac{1}{c^2}\right)\right\}^2}, \quad (49)
\end{align}

for \(c \geq 1\) and

\begin{align}
B &= \frac{1-c}{2} \frac{F\left(-\frac{1}{2}, n, \frac{n+3}{2}; \frac{c+1}{c-1}\right)}{F\left(\frac{1}{2}, n+1, n+\frac{3}{2}; \frac{c+1}{c-1}\right)}, \quad (50) \\
T_{\text{phys}} &= \frac{c^2-1}{2n+3} \frac{F\left(-\frac{1}{2}, n, \frac{n+3}{2}; \frac{c+1}{c-1}\right) F\left(\frac{1}{2}, n+2, n+\frac{5}{2}; \frac{c+1}{c-1}\right)}{\left\{F\left(\frac{1}{2}, n+1, n+\frac{3}{2}; \frac{c+1}{c-1}\right)\right\}^2}, \quad (51)
\end{align}

for \(-1 < c < 1\). For a given parameter set \((c, n)\), the variables \(B\) and \(T_{\text{phys}}\) are determined from the above equations. Thus, the macroscopic quantities \(E/N\) and \(|\vec{M}|\) are explicitly evaluated and given by the functions of \((c, n)\).

In Fig.1, we plot the inverse of temperature (black), the energy per particle (blue) and the magnetization (red) as function of the parameter \(c\) for polytrope index \(n = 2, 5\), and 10 (from left to right). While the non-monotonic behavior appears in the inverse of the temperature in \(n = 2\) case, all the variables in the \(n = 5\) and 10 cases behave monotonically. Notice that in the limit \(c \to +\infty\), the inverse of the temperature converges to a finite value for any \(n\) and \(E/N\) and \(|\vec{M}|\) respectively approach to a critical value \(E_{\text{crit}}/N\) and 0. This implies that similar to the Boltzmann-Gibbs case, the cluster phase in quasi-equilibrium state ceases to exist at some values of the high temperature, depending on the polytrope index \(n\). Based on this result, we next plot the energy per particle and the magnetization as function of \(1/T_{\text{phys}}\) (Figs.2 and 3). As expected from Fig.1, the quantities \(E/N\) \(|\vec{M}|\) become multi-variate for the index \(n < 4\) and show somewhat curious behavior. These pathological behavior might be partially ascribed to the definition of the temperature.

Fig.4 shows the combined results of Figs.2 and 3, i.e., the magnetization as function of \(E/N\). In contrast to Figs.2 and 3, non-monotonic behavior disappears in the cluster phase. The critical energy \(E_{\text{crit}}\), which separates the quasi-equilibrium state into the uniform and the cluster phases, slightly changes with
the polytrope index $n$:

$$\frac{E_{\text{crit}}}{N} = \frac{E}{N} \Big|_{c \to +\infty} = \frac{1}{2} \left\{ \frac{n}{2(n+1)} + 1 \right\},$$

which reproduces the Boltzmann-Gibbs result, $E_{\text{crit}}/N = 3/4$, in the limit $n \to \infty$.

Finally, we address the microscopic quantities characterizing the quasi-equilibrium state in the cluster phase. In the expressions for distribution function (31), the factor $A$ is eliminated by using (40). With a help of integral formula (A.3) (A.5), the explicit expression for distribution function becomes

$$f(\theta, p) = N \frac{\sqrt{2}}{B\left(\frac{1}{2}, n + \frac{1}{2}\right)} \frac{1}{\int d\theta (c - \cos \theta)^n} \frac{(\Phi_0 - \varepsilon)^{n-1/2}}{B^n}$$

with the quantity $\varepsilon$ being the specific energy given by $\varepsilon \equiv p^2/2 + \Phi(\theta)$. In similar way, from (35) and (40), the number distribution $\rho(\theta)$ is expressed as

$$\rho(\theta) = N \frac{(c - \cos \theta)^n}{\int d\theta (c - \cos \theta)^n}.$$ 

Further, one obtains the momentum distribution $F_p(p)$:

$$F_p(p) = \int d\theta f(\theta, p)$$
\[
= N \frac{\sqrt{2/B}}{B(\frac{1}{2}, n + \frac{1}{2})} \int d\theta \left\{ b(p, c) - \cos \theta \right\}^{n-1/2} \int d\theta (c - \cos \theta)^n,
\]

(55)

Using the formulas (A.3)–(A.6), the integrals in the above equation can be expressed in terms of the Gauss hyper-geometric functions. Here, the function \(b(p, c)\) is given by

\[
b(p, c) = c - \frac{p^2}{2B}
\]

(56)

The expression in the distribution function \(f\) includes the numerical constant \(\Phi_0 - 1\), which can be evaluated through the definition \(c = (\Phi_0 - 1)/B\). Using (48), we have

\[
\Phi_0 - 1 = c B = \frac{n}{2} \frac{F\left(\frac{1-n}{2}, 1 - \frac{n}{2}, 2; \frac{1}{c^2}\right)}{F\left(\frac{1-n}{2}, -\frac{n}{2}, 1; \frac{1}{c^2}\right)}
\]

(57)

for \(c \geq 1\) and

\[
\Phi_0 - 1 = \frac{c(1-c)}{2} \frac{F\left(-\frac{1}{2}, n, n + \frac{3}{2}; \frac{c+1}{c-1}\right)}{F\left(\frac{1}{2}, n + 1, n + \frac{3}{2}; \frac{c+1}{c-1}\right)}
\]

(58)

for \(-1 < c < 1\). Thus, provided the parameters \((c, n)\), functional forms of the distribution functions \(f(\theta, p), \rho(\theta)\) and \(F_p(p)\) are completely specified, which can be compare with the quasi-stationary state seen in the simulations quantitatively.

As a demonstration, varying the parameter \(c\), the number distribution and the momentum distribution are depicted for the specific values of the polytrope indices, \(n = 2\) and \(5\) (Figs.5 and 6). Figures show that the clustering features becomes appreciable as decreasing \(c\) and the momentum distribution \(F_p\) has a cutoff at the tails with a finite value of \(p\). Compared to the \(q\)-exponential function \([1 - \beta'(1 - q)p^2/2]^{1/(1-q)}\), which has been naively used to fit to the numerical simulations, the momentum distribution is continuous.
5 Thermodynamic stability of quasi-equilibrium state

6 Conclusion and Discussion
Fig. 2. Energy per particle as function of $1/T_{\text{phys}}$. In each panel, the black lines means the uniform phase ($B = 0$), while the red lines represents the cluster phase ($B \neq 0$). Note that the $n = \infty$ case corresponds to the Boltzmann-Gibbs result.

Fig. 3. Magnetization as function of $1/T_{\text{phys}}$. The meaning of the color in each line is the same as in Fig.2.
Fig. 4. Magnetization as function of energy per particle for various polytrope indices: $n = 2$ (black), 3 (blue), 4 (cyan), 5 (yellow), 8 (green), 10 (magenta), and 15 (red). The thick solid line represents the result obtained from the Boltzmann-Gibbs entropy ($n = \infty$).
Fig. 5. Number distribution in the cluster phase for $n = 2$ (upper-left & upper-right) and $n = 5$ (lower-left & lower-right). Here, we artificially set $N = 1$. 
Fig. 6. Momentum distribution in cluster phase for $n = 2$ (upper-left & upper-right) and $n = 5$ (lower-left & lower-right). Similar to Fig. 5, we artificially set $N = 1$. 
A Integral formulas

\[ \int_{0}^{2\pi} d\theta \cos \theta e^{-\beta(B\cos \theta + 1)} = -2\pi e^{-\beta} I_1(\beta B) \]  \hspace{1cm} (A.1)

\[ \int_{0}^{2\pi} d\theta e^{-\beta(B\cos \theta + 1)} = 2\pi e^{-\beta} I_0(\beta B) \]  \hspace{1cm} (A.2)

\[ \int_{0}^{2\pi} (c - \cos \theta)^n = 2 \int_{-1}^{+1} dx (1 - x^2)^{-1/2}(c - x)^n \]
\[ = 2\pi c^n F \left( \frac{1 - n}{2} , -\frac{n}{2} , 1 ; \frac{1}{c^2} \right) . \]  \hspace{1cm} (A.3)

\[ \int_{0}^{2\pi} \cos \theta (c - \cos \theta)^n = 2 \int_{-1}^{+1} dx (1 - x^2)^{-1/2}x(c - x)^n \]
\[ = -n\pi c^{n-1} F \left( \frac{1 - n}{2} , 1 - \frac{n}{2} , 1 ; \frac{1}{c^2} \right) . \]  \hspace{1cm} (A.4)

Notice that equations (A.3) and (A.4) are valid only if \( c \geq 1 \). In cases with \(-1 < c < 1\), the range of integration should be restricted to \(-1 \leq \cos \theta \leq c\), or \(-1 \leq x \leq c\). We then have

\[ \int d\theta (c - \cos \theta)^n = 2\sqrt{\pi} (c + 1)^n \sqrt{\frac{1 + c}{1 - c}} \frac{\Gamma(n + 1)}{\Gamma(n + 3/2)} \]
\[ \times F \left( \frac{1}{2} , n + 1 , n + \frac{3}{2} ; \frac{c + 1}{c - 1} \right) , \]  \hspace{1cm} (A.5)

\[ \int d\theta \cos \theta (c - \cos \theta)^n = -\sqrt{\pi} (c + 1)^n \sqrt{1 - c^2} \frac{\Gamma(n + 1)}{\Gamma(n + 3/2)} \]
\[ \times F \left( -\frac{1}{2} , n , n + \frac{3}{2} ; \frac{c + 1}{c - 1} \right) . \]  \hspace{1cm} (A.6)

B On the thermodynamic temperature in quasi-equilibrium state

In this appendix, we consider the thermodynamic temperature in quasi-equilibrium state.

In the framework of the non-extensive thermostatistics with Tsallis entropy, the physically plausible thermodynamic temperature \( T_{\text{phys}} \) is defined through
the zero-th law of thermodynamics[8]. Accordingly, the thermodynamic temperature differs from the usual one, i.e., the inverse of the Lagrange multiplier $\beta$. This means that the relation between the heat transfer and the entropy change in a quasi-static treatment is also modified. We have [8]

$$\frac{dS_q}{1 + (1 - q)S_q} = \frac{1}{T_{\text{phys}}} \, d'Q.$$  \hspace{1cm} (B.1)

If the above relation is applied to the mean-field analysis of the HMF model, the variation $d'Q$ should be regarded as the heat change per particle, since the entropy defined in (23) is the specific entropy, i.e., the entropy per particle. Then, using the fact that the HMF model has no specific volume size ($dV = 0$), the first-law of thermodynamics becomes $d'Q = dE/N$. Thus, the relation (B.1) is rewritten with

$$\frac{dS_q}{1 + (1 - q)S_q} = \frac{1}{T_{\text{phys}}} \, \frac{dE}{N}.$$ \hspace{1cm} (B.2)

As a consistency check, assuming that the correct thermodynamic temperature is given by $T_{\text{phys}} = N_q/(\beta N)$ (Eq.[45]), we will show that the relation (B.2) indeed holds in the HMF model.

Let us first write down the entropy of the extremum state:

$$S_q = \left(n + \frac{1}{2}\right) (N_q - 1)$$ \hspace{1cm} (B.3)

from the definition (30). Here the quantity $N_q$ is given by (see Appendix C for derivation):

$$N_q = D_n \, B^{-1/(2n+1)} \frac{\int d\theta \, (c - \cos \theta)^n}{\left\{ \int d\theta \, (c - \cos \theta)^{n+1} \right\}^{(n-1/2)/(n+1/2)}}$$ \hspace{1cm} (B.4)

with the quantity being $D_n = \left\{B(1/2, n + 1/2)/\sqrt{2}\right\}^{1/(n+1/2)}$. On the other hand, the energy of the extremum state is expressed as (Eq.[46]):

$$E = \frac{N}{2} \left\{ T_{\text{phys}} + (1 - B^2) \right\}.$$ \hspace{1cm} (B.5)

For a given polytrope index $n$, the quantities $B$ and $T_{\text{phys}}$ are whole expressed as function of the parameter $c$ (Eqs.[42][45]). Hence, the thermodynamic quantities $S_q$ and $E$ can be regarded as the function of $c$ and the variations of these
quantities are invoked from the variation of parameter $c$ along a sequence of quasi-equilibrium states. We have

\[ dS_q = \left( n + \frac{1}{2} \right) \left( \frac{dN_q}{dc} \right) dc, \quad \text{(B.6)} \]

\[ \frac{dE}{N} = \left\{ \frac{1}{2} \left( \frac{dT_{\text{phys}}}{dc} \right) - B \left( \frac{dB}{dc} \right) \right\} dc \quad \text{(B.7)} \]

To calculate the derivatives $dN_q/dc$, $dT_{\text{phys}}/dc$ and $dB/dc$, we introduce the quantity:

\[ f_n(c) = \int d\theta \ (c - \cos \theta)^n. \quad \text{(B.8)} \]

In terms of this, the quantities $N_q$, $T_{\text{phys}}$ and $B$ becomes

\[ N_q = D_n \left\{ \frac{f_{n+1}(c)}{f_n(c)} - c \right\}^{-1/(2n+1)} \frac{f_n(c)}{\{f_{n+1}(c)\}^{(n-1)/2(n+1/2)}}, \quad \text{(B.9)} \]

\[ T_{\text{phys}} = \frac{1}{n + 1} f_{n+1}(c) \left\{ \frac{f_{n+1}(c)}{f_n(c)} - c \right\}, \quad \text{(B.10)} \]

\[ B = \frac{f_{n+1}(c)}{f_n(c)} - c. \quad \text{(B.11)} \]

Using the fact that $df_n/dc = n f_{n-1}$, we obtain

\[ \frac{dN_q}{dc} = \left( \frac{1}{2n + 1} \frac{d\ln B}{dc} + \frac{d\ln f_n}{dc} - \frac{n - 1/2}{n + 1/2} \frac{d\ln f_{n+1}}{dc} \right) N_q \]
\[ = \frac{1}{n + 1/2} \left\{ n \frac{f_{n+1}^2 f_{n-1}}{f_n^3} - \frac{n(n + 1/2)}{n + 1} \frac{c f_{n+1} f_{n-1}}{f_n^2} \right. \]
\[ + \left. (n - 1/2) c - \frac{2n^2 + 2n - 1}{2(n + 1)} \frac{f_{n+1}}{f_n} \right\} \frac{N_q}{T_{\text{phys}}}, \quad \text{(B.12)} \]

\[ \frac{dT_{\text{phys}}}{dc} = \frac{1}{n + 1} \frac{f_{n+1}}{f_n} + c \left( \frac{n}{n + 1} \frac{f_{n+1} f_{n-1}}{f_n^2} - 1 \right), \quad \text{(B.13)} \]

\[ \frac{dB}{dc} = n \left( 1 - \frac{f_{n+1} f_{n-1}}{f_n^2} \right). \quad \text{(B.14)} \]
Substituting these equations into (B.6) and (B.7), after some manipulations, the variations of entropy and the energy respectively become

\[
dS_q = \frac{N_q}{T_{\text{phys}}} \left\{ n \frac{f_{n+1}^2 f_{n-1}}{f_n^3} - \frac{n(n+1/2)}{n+1} \frac{c f_{n+1} f_{n-1}}{f_n^2} \right. \\
+ \left. (n-1/2) c - \frac{2n^2 + 2n - 1}{2(n+1)} \frac{f_{n+1}}{f_n} \right\} dc, \tag{B.15}
\]

\[
d\tilde{E} = \left\{ n \frac{f_{n+1}^2 f_{n-1}}{f_n^3} - \frac{n(n+1/2)}{n+1} \frac{c f_{n+1} f_{n-1}}{f_n^2} \right. \\
+ \left. (n-1/2) c - \frac{2n^2 + 2n - 1}{2(n+1)} \frac{f_{n+1}}{f_n} \right\} dc. \tag{B.16}
\]

which immediately lead to the following relation:

\[
dS_q = \frac{N_q}{T_{\text{phys}}} \frac{d\tilde{E}}{N}. \tag{B.17}
\]

From (38) and (B.3), one has \(N_q = 1 + (1 - q) S_q\). Thus, we obtain

\[
dS_q = \frac{1}{T_{\text{phys}}} \left\{ 1 + (1 - q) S_q \right\} \frac{d\tilde{E}}{N}, \tag{B.18}
\]

which exactly matches the equation (B.1). Therefore, the temperature defined in (45) is fully consistent with the arguments in Ref.[8] and thereby it can be regarded as the plausible physical temperature.

C Derivation of Eq.(B.4)

The non-trivial relation (B.4) can be obtained from the normalization condition for the primitive distribution \(h(\theta, p)\) (see Eq.[24]):

\[
\int d\theta \int dp \ h(\theta, p) = 1.
\]

which can be rewritten with

\[
1 = \left( \frac{N_q}{N} \right)^{1/q} \int d\theta \int dp \ \{ f(\theta, p) \}^{1/q}. \tag{C.1}
\]
Substituting the explicit form of the distribution function (31) into the above equation, one has

\[
1 = \left( \frac{A}{N} N_q \right)^{1/q} \int d\theta \int dp \left( \Phi_0 - 1 - B \cos \theta - \frac{1}{2} p^2 \right)^{1/(1-q)},
\]

\[
= \left( \frac{A}{N} N_q \right)^{1/q} \frac{B(1/2, n + 1/2)}{\sqrt{2}} \int d\theta \left( \Phi_0 - 1 - B \cos \theta \right)^{n+1}. \quad (C.2)
\]

Further substituting the equation (40) leads to

\[
N_q = \left( \frac{A}{N} \right) \frac{1}{\left\{ B(1/2, n + 1/2) \right\}^{1/\sqrt{2}} \int d\theta \left( \Phi_0 - 1 - B \cos \theta \right)^{n+1}^{1/\sqrt{2}}}
\]

\[
= \left\{ \frac{B(1/2, n + 1/2)}{\sqrt{2}} \right\}^{1/\sqrt{2}} \int d\theta \left( \Phi_0 - 1 - B \cos \theta \right)^n \left\{ \int d\theta \left( \Phi_0 - 1 - B \cos \theta \right)^{n+1} \right\}^{1/\sqrt{2}}, \quad (C.3)
\]

which finally reduces to equation (B.4).

References


