Negative magnetic susceptibility and nonequivalent ensembles for the mean-field $\Phi^6$ spin model

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Abstract

We derive the thermodynamic entropy of the mean-field $\Phi^6$ spin model in the framework of microcanonical ensemble as a function of the energy and magnetization. Using the theory of large deviations and Rugh's microcanonical formalism we obtain the entropy and its derivatives and study the thermodynamic properties of $\Phi^6$ spin model. The interesting point we found is that like $\Phi^4$ model the entropy is a concave function of the energy for all values of the magnetization, but is nonconcave as a function of the magnetization for some values of the energy. This means that the magnetic susceptibility of the model can be negative for fixed values of the energy and magnetization in the microcanonical formalism. This leads to the inequivalence of the microcanonical and canonical ensembles. It is also shown that this mean-field model displays a first-order phase transition driven by the magnetic field. Finally we compare the results of the mean-field $\Phi^6$ and $\Phi^4$ spin models.

1 Introduction

The microcanonical and canonical ensembles are the two main probability distributions with respect to which the equilibrium properties of statistical mechanical models are calculated. Despite the two ensembles model two different physical situations, it is generally believed that the ensembles give equivalent results in the thermodynamic limit; i.e., in the limit in which the volume of the system tends to infinity. The equivalence of the microcanonical and canonical ensembles is most usually explained by saying that although the canonical ensemble is not a fixed-mean-energy ensemble like the microcanonical ensemble, it must 'converge' to a fixed-mean-energy ensemble in the thermodynamic limit, and so must become or must realize a microcanonical ensemble in that limit. This convergence can be proved to hold for noninteracting systems such as the
perfect gas and for a variety of weakly interacting systems. For general systems, however, neither is this convergence valid nor is the conclusion true concerning ensemble equivalence which this convergence is intended to motivate. In fact, in the past three and a half decades, numerous statistical models have been discovered having microcanonical equilibrium properties that cannot be accounted for within the framework of the canonical ensemble. For systems with short-range interactions, the choice of the statistical ensemble is typically of minor importance and could be considered a finitesize effect: differences between, say, microcanonical and canonical expectation values are known to vanish in the thermodynamic limit of large system size, and the various statistical ensembles become equivalent. In the presence of long-range interactions this is in general not the case, and microcanonical and canonical approaches can lead to different thermodynamic properties even in the infinite-system limit. In the astrophysical context, nonequivalence of ensembles and the importance of microcanonical calculations have long been known for gravitational systems. Although equivalence of ensembles had been proven only for short-range interactions, it was tacitly assumed by most physicists to hold in general. Therefore it came as a surprise to many that equivalence does not necessarily hold for long-range systems, in particular in the presence of a discontinuous phase transition. Until now, the phenomenon of nonequivalent ensembles has been identified and analyzed almost exclusively by determining regions of the mean energy where the microcanonical entropy function is anomalously nonconcave or by determining regions of the mean energy where the heat capacity, calculated microcanonically, is negative. The existence of such nonconcave anomalies invalidates yet another tacit principle of statistical mechanics which states that the one should always be able to express the microcanonical entropy, the basic thermodynamic function for the microcanonical ensemble, as the Legendre-Fenchel transform of the free energy, the basic thermodynamic function for the canonical ensemble. Indeed, if the microcanonical entropy is to be expressed as the Legendre-Fenchel transform of the canonical free energy, then the former function must necessarily be concave on its domain of definition. Hence, if the microcanonical entropy has nonconcave regions, then expressing it as a Legendre-Fenchel transform is impossible. When this occurs, we say that there is thermodynamic nonequivalence of ensembles. More recently, nonconcave anomalies in the microcanonical entropy as well as negative heat capacities have been observed in models of fluid turbulence and models of plasmas, in addition to long-range and mean-field spin models, including the mean-field XY model and the mean-field Blume-Emery-Griffiths (BEG) model.

One of the motivations for the study of $\Phi^6$ models is the search for soliton. Another reason for interest is that $\Phi^6$ models are the simplest systems with continuous variables that exhibit a rich phase diagram, with first- and second-order phase transitions and a tricritical point. This structure was observed in the study of the quantum mechanics of a single site, three-well potential when classical, perturbative and mean-field arguments were used and bubble solutions, their relation to the phase transitions and the question of their stability, both relativistically and non-relativistically. In recent years the $\Phi^6$ model and its
application in different physical systems including the following problems have been studied extensively: the crossover from a quantum $\phi^6$ theory to a renormalized two-dimensional classical nonlinear sigma model, alpha matter on a lattice, first-order electroweak phase transition (EWPT) due to a dimension-six operator in the effective Higgs potential, first-order phase transitions in confined systems, effective Potential and spontaneous symmetry breaking in the noncommutative $\Phi^6$ model, bubble dynamics in quantum phase transitions, the canonical transformation and duality in the $\Phi^6$ theory, hermitian matrix model $\Phi^6$ for 2D quantum gravity, phase structure of the generalized two dimensional Yang-Mills theories on sphere, tricritical Ising model near criticality, spontaneous symmetry breaking at two Loop in 3D massless scalar electrodynamics, Ising model in the ferromagnetic phase, statistical mechanics of nonlinear coherent structures, kinks in the $\Phi^6$ model, growth kinetics in the $\Phi^6$ N-Component model, stability of Q-balls, the liquid states of pion condensate and hot pion matter, instantons and conformal holography, first-order phase transitions in superconducting films, field-theoretic description of ionic crystallization in the restricted primitive mode.

This increasing interest in $\Phi^6$ model and its many application in physics, motivated us to study the statistical mechanics of $\Phi^6$ spin models.

2 The mean-field $\Phi^6$ model and its thermodynamic

The Hamiltonian of the mean-field $\Phi^6$ model is given by the following expression

$$H = \sum_{i=1}^{N} \frac{P_i^2}{2} - \frac{q_i^2}{4} + \frac{q_i^4}{4} + \frac{q_i^6}{6} - \frac{1}{4N} \sum_{i,j=1}^{N} q_i q_j$$

(1)

where $q_i$ and $p_i$ are the canonical coordinates of unit mass, moving on a line $(q_i, p_i)$. The entropy of the system in terms of its mean energy and magnetization is defined as\(^1\)

$$S(\epsilon, m) = \lim_{N \to \infty} \frac{1}{N} \ln \int \delta(\epsilon(x) - \epsilon)\delta(m(x) - m) dx$$

(2)

As is sated in [1], if $S(\epsilon, m)$ were concave, then one would calculate this function from the point of view of the canonical ensemble using the following steps

- Calculate the partition function:

$$Z(\beta, \eta) = \int \exp [-\beta H(x) - \eta M(x)] dx$$

(3)

where $M = Nm(x)$

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\(^1\)In this paper we choose $k_B = 1$
• Calculate the thermodynamic potential defined by

\[ \varphi(\beta, \eta) = -\lim_{N \to \infty} \frac{1}{N} \ln Z(\beta, \eta) \]  

where \( \varphi(\beta, \eta) = \beta F(\beta, \eta) \), where \( F \) is the free energy of the system.

• Obtain \( S(\epsilon, m) \) by taking the legendre transform of the free energy function \( \varphi(\beta, \eta) \):

\[ S(\epsilon, m) = \beta \epsilon + \eta m - \varphi(\beta, \eta) \]  

with \( \beta \) and \( \eta \) determined by the equations

\[ \frac{\partial}{\partial \beta} \varphi(\beta, \eta) = \epsilon, \quad \frac{\partial}{\partial \eta} \varphi(\beta, \eta) = m \]  

As mentioned earlier these steps are valid only when the entropy is concave. For nonconcave entropies we use two methods i.e., a) method of large deviation. b) Rugh’s method, and compare the results.

3 Calculation of the entropy using large deviation method

We are looking for a set of macro variables or mean-fields such that the energy per particle \( \epsilon(x) \) and the mean magnetization \( m(x) \) can be considered as a function of these variables:

\[ \epsilon(x) = \bar{\epsilon}(\mu(x)) \quad , \quad m(x) = \bar{m}(\mu(x)) \]  

Here we have used \( \mu(x) \) to denote the macro variables collectively. Correspondingly the entropy can be expressed as a function of these macro variables or mean fields:

\[ \tilde{S}(\mu) = \lim_{N \to \infty} \frac{1}{N} \ln \int \delta(\mu(x) - \mu) dx \]  

In this method the entropy \( S(\epsilon, m) \) can be obtained by solving the following constrained maximization problem:

\[ S(\epsilon, m) = \sup_{\mu : \bar{\epsilon}(\mu) = \epsilon, \bar{m}(\mu) = m} \tilde{S}(\mu) \]  

If \( \tilde{S}(\mu) \) is a concave function of the given macrostate \( M \), then \( \tilde{S}(\mu) \) is the legendre transform of the free energy function defined by:

\[ \tilde{Z}(\lambda) = \int_{\Gamma} \exp \left[ -N \lambda \cdot \mu(x) \right] dx \]  

If \( \tilde{S}(\mu) \) is concave, one can find it using the so called macrostate generalization of the legendre transform presented in Eqs. (5) and (6)

\[ \tilde{S}(\mu) = \inf_{\lambda} \{ \lambda \mu - \bar{\varphi}(\lambda) \} \]
Now, let us return to the mean-field $\phi^6$ model. An appropriate choice of macrostate is the vector $M(m, k, \nu)$, where $m$, $k$ and $\nu$ are the mean magnetization, the mean kinetic energy and the mean potential energy, respectively:

$$ k = \frac{1}{2N} \sum_i (P_i^2) $$

$$ \nu = \frac{1}{N} \sum_i \left( \frac{q_i^6}{6} + \frac{q_i^4 - q_i^2}{4} \right) $$

So we can write $\bar{\epsilon}(\mu)$ as follows:

$$ \bar{\epsilon}(\mu) = k + \nu - \frac{m^2}{4} $$

To calculate the entropy $\bar{S}(\mu)$, we use the Legendre transformation. It is shown in [2] that the $S(\epsilon, m)$ is given by the following expression:

$$ S(\epsilon, m) = \sup_{\nu} \left\{ \frac{1}{2} \ln(\epsilon - \nu + \frac{m^2}{4}) + \frac{1}{2} \ln 4\pi e + \bar{S}(m, \nu) \right\} $$

### 4 Rugh’s formalism for the mean-field $\phi^6$ model

Rugh’s microcanonical formalism has been discussed in [1,2]. We assume the Hamiltonian $H(x; M)$ in which $M$ is the total magnetization. The microcanonical entropy of the system is given by:

$$ S(E, M) = \ln \int_{\Gamma} \delta(H(x; M) - E) dx $$

where $E$ is the total energy of the system. In Rugh’s method the thermodynamic quantities are defined through derivatives of the entropy [1,2], and calculated by introducing a vector $Y$ in $\Gamma$ in such a way that, $Y \cdot \nabla H = 1$, so we have:

$$ \frac{\partial}{\partial E} S(E, M) = \langle \nabla . Y \rangle_{E,M} = \frac{1}{T(E, M)} $$

and

$$ \frac{\partial}{\partial M} S(E, M) = - \langle \nabla . (\frac{\partial H}{\partial M} Y) \rangle_{E,M} $$

In general for an arbitrary observable $A(x)$, we have [1]:

$$ \frac{\partial}{\partial E} \langle A \rangle_{E,M} = \langle \nabla . (AY) \rangle_{E,M} - \frac{1}{T(E,M)} \langle A \rangle_{E,M} $$

and

$$ \frac{\partial}{\partial M} \langle A \rangle_{E,M} = - \langle \nabla . (\frac{\partial H}{\partial M} Y) \rangle_{E,M} + \langle \nabla . (\frac{\partial H}{\partial M} Y) \rangle_{E,M} \langle A \rangle_{E,M} + \langle \frac{\partial A}{\partial M} \rangle_{E,M} $$
where $\langle A \rangle$ denotes the average of the abserable $A$. By incorporating the magnetization constraint into the Hamiltonian $H(x)$ one can obtain the Hamiltonian $H(x;M)$. This can be done by eliminating one of the $q_i$, for example $q_N = M - \sum_{i=1}^{N-1} q_i$. For the mean-field $\phi^6$ model we have:

$$H(x;M) = \sum_{i=1}^{N-1} \frac{p_i^2}{2} - \frac{1}{2N} \sum_{i,j} p_ip_j - \sum_{i=1}^{N-1} \left( \frac{q_i^2 - q_i^4}{4} - \frac{1}{6} q_i^6 \right)$$

$$- \frac{1}{4} (M - \sum_{i=1}^{N-1} q_i)^2 + \frac{1}{4} (M - \sum_{i=1}^{N-1} q_i)^4 - \frac{1}{6} (M - \sum_{i=1}^{N-1} q_i)^6$$

(21)

(22)

Following Rugh[1], we choose the vector $Y$ as: $Y = \frac{1}{2K_c} (p_1, ..., p_{N-1}, 0, ..., 0)$ where $K_c$ is the kinetic part of $H(x;M)$. From Eq.(17) we have:

$$\frac{1}{T(E,M)} = \langle \frac{N-3}{2k_c} \rangle \big|_{E,M}$$

(23)

and from Eq.(18) we have:

$$\frac{\partial}{\partial M} S(E,M) = \frac{m_1}{T(E,M)} - \langle (m_3 - m_5) \frac{N-3}{2k_c} \rangle \big|_{E,M}$$

(24)

Here $m_3 = \frac{1}{N} \sum_{i=1}^{N} q_i^3$ and $m_5 = \frac{1}{N} \sum_{i=1}^{N} q_i^5$. We define the effective mean-field $h(E, M)$ as follows:

$$h(E, M) = -T(E, M) \frac{\partial S(E, M)}{\partial M}$$

(25)

using Eq.(24), we have:

$$h(E, M) = -m + T(E, M) \langle (m_3 - m_5) \frac{N-3}{2k_c} \rangle \big|_{E,M}$$

(26)

magnetic susceptibility and the heat capacity can be calculated by differentiating of $h(E, M)$ and $T(E, M)$, see Eqs.(19) and (20).
5 Results of the large deviation method for mean-field $\phi^6$ model

The entropy density $S(\epsilon, m)$ of the mean-field $\phi^6$ model has been shown as a function of mean energy $\epsilon$ and mean magnetization $m$ for five different values of $\epsilon$ in fig.1. One of them is above the critical value $\epsilon_c \approx 0.102$ and the rest are below. The effective magnetic field $b(E, M)$ has been plotted as a function of $m$ for different values of $\epsilon$, in fig.2. It is worth mentioning that the data in fig.1 and fig.2 are obtained using the large deviation method i.e., Eq.(15). In fig.3 the magnetic susceptibility has been plotted as a function of magnetization $m$ for different values of $\epsilon$. 

Figure 1: Entropy as a function of the mean magnetization $m$ for different values of the mean energy $\epsilon=0.16, 0.08, 0.04, 0.00$ and $-0.04$ (from top to bottom).
Figure 2: Effective magnetic field as a function of magnetization $m$ for different values of $\epsilon=0.16, 0.08, 0.04, 0.00$ and $-0.04$ (from top to bottom).

6 Ensemble inequivalence for mean-field $\phi^6$ model

Now, we study the inequivalence of microcanonical and canonical ensemble, for the case of $\phi^6$ model. This is in close relation with nonconcavity of the entropy $S(\epsilon, m)$. The effective magnetic field $h(E, M)$ is shown in fig 2. We observe that $h(E, M)$ can be negative for positive values of $m$ when $\epsilon < \epsilon_c$. In the canonical ensemble, the magnetization $m(\beta, h)$ and the magnetic field $h$ have the same sign. This means that, in the canonical ensemble, the magnetization of the mean-field $\phi^6$ model is always in the direction of the magnetic field. But in the microcanonical ensemble the situation is different. $h(E, M)$ and $m$ can have opposite signs, so the canonical and microcanonical ensembles are inequivalent.

For more understanding of the this problem in microcanonical ensemble and its relation with nonconcavity of the entropy $S(\epsilon, m)$, we have plotted the magnetic susceptibility and $m$ derivative of the entropy in figs.(3) and (4) respectively. Since $T(E, M)$ is directly proportional to the kinetic energy, it is always positive and this means that the sign of $h(E, M)$ is always opposite to the sign of $\frac{\partial S(\epsilon, m)}{\partial m}$. Then $h(E, M)$ is negative for $m > 0$. By comparing figs.(3) and (4), we find that this happens when the entropy $S(\epsilon, m)$ is a concave function of the magnetization e.g., the case for which $\epsilon = 0.16$, then $\frac{\partial S(\epsilon, m)}{\partial m}$ is necessarily negative when $m > 0$ (fig.4), which implies that $h(E, M)$ is necessarily positive (for $m > 0$).

This is in agreement with the results of canonical ensemble. Let us now study the magnetic susceptibility in the microcanonical and canonical ensemble. In the canonical ensemble, the magnetic susceptibility at the constant temperature
Figure 3: Magnetic susceptibility as a function of magnetization $m$ calculated using the large deviation method for different values of $\epsilon=0.16$, 0.08, 0.04, 0.00 and -0.04 (from top to bottom).

Figure 4: $\frac{\partial S(\epsilon, m)}{\partial m}$ for different values of $\epsilon=0.16$, 0.08, 0.04, 0.00 and -0.04 (from top to bottom), calculated using the large deviation method.
is defined by the following expression:

\[
\chi^T(\beta, h) = \frac{\partial m(\beta, h)}{\partial h}
\]  

(27)

It is easy to show that \(\chi^T(\beta, h)\) is always positive. In the microcanonical ensemble \(\chi^T\) is a function of \(\epsilon\) and \(m\), and given by:

\[
\chi^T(E, M) = \left[\frac{\partial h(\epsilon, m)}{\partial m} \mid_{T(\epsilon, m)}\right]^{-1}
\]  

(28)

where \(h(\epsilon, m)\) is given by Eq.(25). Using Eq.(25) and (28) one can show that:

\[
\chi^T(\epsilon, m) = -T^{-1}(\epsilon, m) \frac{\partial^2 S}{\partial \epsilon^2} \left[ \frac{\partial^2 S}{\partial m^2} \frac{\partial^2 S}{\partial \epsilon^2} - \left(\frac{\partial^2 S}{\partial m \partial \epsilon}\right)^2 \right]^{-1}
\]  

(29)

For the mean-field \(\phi^6\) model, \(\frac{\partial^2 S}{\partial \epsilon^2}\) is always negative, so if for some values of \(m\) (when \(\epsilon < \epsilon_c\), see fig.3), \(\frac{\partial^2 S}{\partial m^2}\) is positive, then \(\chi^T\) will be negative as can be checked by Eq.(29). But we already shown that in the canonical ensemble \(\chi^T\) is always positive, this again means that microcanonical and canonical ensembles are nonequivalent. It is worth to mention that this is a consequence of nonconcavity of the entropy \(S(\epsilon, m)\).

7 conclusion

The entropy of the mean-field \(\phi^6\) model is concave as a function of the energy, but is nonconcave as a function of the energy and magnetization. This leads to a very important difference between the thermodynamic properties of this model in the microcanonical and canonical ensembles. We shown that the effective magnetic field in the microcanonical ensemble can have a sign opposite to that of the magnetization \(m\), which is in contrast to the case of canonical ensemble for which the magnetization \(m\) is always in the direction of the applied magnetic field. The magnetic susceptibility which in microcanonical ensemble is a function of the energy and magnetization can be negative but it is always positive in the canonical ensemble. These are two important differences between microcanonical and canonical ensemble which make them nonequivalent. The mean-field \(\phi^6\) model like \(\phi^4\) model displays a first-order phase transition driven by the magnetic field in the canonical ensemble which is a consequence of the nonconcavity of the entropy, as a function of magnetization (for certain values of the energy). In addition to display a first-order phase transition driven by the magnetic field the mean-field \(\phi^6\) model displays a second order phase transition driven by the temperature or the energy.
8 References.

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