Ensemble inequivalence in a mean-field XY model with ferromagnetic and nematic couplings

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We explore ensemble inequivalence in long-range interacting systems by studying an XY model of classical spins with ferromagnetic and nematic coupling. We demonstrate the inequivalence by mapping the microcanonical phase diagram onto the canonical one, and also by doing the inverse mapping. We show that the equilibrium phase diagrams within the two ensembles strongly disagree within the regions of first-order transitions, exhibiting interesting features like temperature jumps. In particular, we discuss the coexistence and forbidden regions of different macroscopic states in both the phase diagrams.

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Recent years have seen extensive studies of systems with long-range interactions that have the two-body potential in $d$ dimensions decaying at large separation $r$ as $1/r^\alpha$, $0 \leq \alpha \leq 1$ [1–4]. Examples span a wide variety, from bacterial population [5], plasmas [6], and dipolar ferroelectrics and ferromagnets [7], to two-dimensional geophysical vortices [8] and self-gravitating systems [9]. A striking feature of long-range systems distinct from short-range ones is that of nonadditivity, whereby thermodynamic quantities scale superlinearly with the system size. Nonadditivity manifests in static properties like negative microcanonical specific heat [10,11], inequivalence of statistical ensembles [12–19], and other rich possibilities [20]. For the dynamics, long-range systems often exhibit broken ergodicity [16,21] and slow relaxation towards equilibrium [8,16,22–25].

Here, we demonstrate ensemble inequivalence in a model of long-range systems that has mean-field interaction (i.e., $\alpha = 0$) and two coupling modes. This so-called generalized Hamiltonian mean-field (GHMF) model, a long-range version with added kinetic energy of the model of Ref. [26], has $N$ interacting particles with angular coordinates $\theta_i \in [0,2\pi]$ and momenta $p_i$, $i = 1,2,\ldots,N$, which are moving on a unit circle [27]. The GHMF Hamiltonian is

$$H = \frac{\sum_{i=1}^{N} p_i^2}{2} + \frac{1}{2N} \sum_{i,j=1}^{N} [1 - \Delta \cos \theta_{ij} - (1 - \Delta) \cos 2\theta_{ij}],$$

(1)

where $\theta_{ij} \equiv \theta_i - \theta_j$. Here, $\cos \theta_{ij}$ is an attractive interaction minimized by the particles forming a cluster, so that $\theta_{ij} = 0 \mod 2\pi$, while $\cos 2\theta_{ij}$ with two minima at $\theta_{ij} = 0, \pi \mod 2\pi$ promotes a two-cluster state. The parameter $\Delta \in [0,1]$ sets the relative strength of the two coupling modes. The potential energy in Eq. (1) is scaled by $N$ to make the energy extensive, following the Kac prescription [28], but the system remains nonadditive. In terms of the $XY$-spin vectors $S_i \equiv (\cos \theta_i, \sin \theta_i)$, the interactions have the form of a mean-field ferromagnetic interaction $\sim -\Delta S_i \cdot S_j$, and a mean-field coupling $\sim -(1 - \Delta)(S_i \cdot S_j)^2$ promoting nematic ordering.

For $XY$ lattice models with this type of ferro-nematic coupling, see Refs. [26,29–31]. The system (1) has Hamilton dynamics: $d\theta_i/dt = p_i$, $dp_i/dt = -\partial H/\partial \theta_i$. For $\Delta = 1$, when no nematic ordering exists, the GHMF model becomes the Hamiltonian-mean-field (HMF) model [22], a paradigmatic model of long-range systems [1].

In this work, we report on striking and strong inequivalence of statistical ensembles for the GHMF model. The system has three equilibrium phases: ferromagnetic, paramagnetic, and nematic, with first- and second-order transitions. Let us note that Ref. [32] studied another model with long-range interactions, which also shows paramagnetic, ferromagnetic, and nematic-like phases. For the GHMF model, by comparing the phase diagrams in the canonical and microcanonical ensembles (the latter is derived in Ref. [27]), we show in the regions of first-order transitions that the phase diagrams differ significantly. We analyze the inequivalence in two ways, by mapping the microcanonical phase diagram onto the canonical one, as is usually done [13–19], and also by doing the inverse mapping of the canonical onto the microcanonical one; in particular, we discuss the coexistence and forbidden regions of different macroscopic states. This study demonstrates the subtleties and intricacies of the presence of different stability regions of macroscopic states in long-range systems in microcanonical and canonical equilibria. It is worth noting that compared to the pure para-ferro transition, the phenomenology here due to the presence of the additional nematic phase is much richer. We show that the region where the three phases meet, within both microcanonical and canonical ensembles, is the one exhibiting ensemble inequivalence.

We now turn to derive our results. Rotational symmetry of the Hamiltonian (1) allows us to choose, without loss of generality, the ordering direction in the equilibrium stationary state to be along $x$ (there are no stationary states with a nonzero angle between the directions of ferromagnetic and nematic order) and to define as order parameters the equilibrium averages

$$R_m \equiv \langle \cos m\theta \rangle, \quad m = 1,2,$$

(2)
that maximizes the entropy [27]:

\[
\frac{1}{2} \ln 2 \pi + \frac{1}{2} \ln q(\epsilon) - \frac{1}{2} \left( \frac{\Delta R_1^2 + (1 - \Delta) R_2^2}{q(\epsilon)} \right) + \ln \int d\theta \exp \left[ \frac{\Delta R_1 \cos \theta + (1 - \Delta) R_2 \cos 2\theta}{q(\epsilon)} \right].
\]

(8)

The averages (7) are the same as Eq. (3) on making the identification of the microcanonical energy \(\epsilon\) with the average energy \(\langle \epsilon \rangle\) in the canonical ensemble, so that the inverse temperature \(\beta\) in Eq. (3) is

\[
\beta^{-1} = q(\epsilon) = 2\epsilon - 1 + \Delta R_1^2 + (1 - \Delta) R_2^2.
\]

(9)

This constitutes a link between the phase diagrams in the two ensembles. Using then the integrals (3), we get the following parametric representation in the \(\Delta-\epsilon\) plane for the microcanonical ensemble: After finding \(R_1 = C_1(R, \alpha)\) and \(R_2 = C_2(R, \alpha)\), we get

\[
R \cos \alpha = \Delta R_1 / q(\epsilon), \quad R \sin \alpha = (1 - \Delta) R_2 / q(\epsilon),
\]

and, explicitly,

\[
\Delta = \frac{R_2 \cos \alpha}{R_2 \cos \alpha + R_1 \sin \alpha},
\]

\[
\epsilon = \frac{1}{2} \left[ \left( 1 - \Delta \right) R_2^2 - \Delta R_1^2 - (1 - \Delta) R_2^2 + 1 \right].
\]

(10)

Once \(R_{1,2}, \alpha, \epsilon, \Delta\) have been determined, one can use Eq. (8) to find the entropy of the solution. For the pure nematic phase, \(\alpha = \pi/2\), and \(R_2^2 = 1 + (1 - 2\epsilon) / (1 - \Delta)\).

Summarizing, expressions (3), (6), (7), and (10) provide self-consistent stationary state solutions for the order parameters in the canonical and the microcanonical ensembles, respectively. Stable branches of these solutions correspond respectively to the minimum of the free energy (4) and to the maximum of the entropy (8).

We now present results of the phase diagrams for the two ensembles in Fig. 1. Both diagrams are qualitatively similar, with three phases: paramagnetic, ferromagnetic, and nematic. For large values of the parameter \(\Delta\), on decreasing the energy or temperature, one observes a second-order transition from the paramagnetic to the ferromagnetic phase; only at lower values of \(\Delta\) does this phase transition become of first order. For low values of \(\Delta\), decreasing the energy or temperature results in a second-order transition from the paramagnetic to the purely nematic phase for which \(R_1\) is zero; a further decrease results in either a second-order transition (for very small values of \(\Delta\) or a first-order transition (for \(\Delta \approx 1/2\)) to the ferromagnetic phase that has nonzero \(R_1\).
FIG. 1. (Color online) Comparison of the canonical and the microcanonical phase diagrams. Here, pf1 means first-order para-ferro transition, etc. (a) Phase diagram in the $\Delta$-E plane in the microcanonical ensemble, Eqs. (7) and (8). The two tricritical points are at $\Delta \approx 0.545$, $\epsilon \approx 0.636$, and at $\Delta \approx 0.477$, $\epsilon \approx 0.628$, while there is a critical end point at $\Delta \approx 0.487$, $\epsilon \approx 0.628$. The inset shows a zoom into the central part. (b) Phase diagram in the $\Delta$-T plane in the canonical ensemble, Eqs. (3) and (4). There are two tricritical points, at $\Delta \approx 0.667$, $T \approx 0.333$, and at $\Delta \approx 0.34$, $T \approx 0.267$. The critical end point is at $\Delta \approx 0.441$, $T \approx 0.279$.

As Fig. 2(a) shows, mapping of the canonical phase diagram onto the $\Delta$-E plane yields a gap. In the domain of $\Delta$ where a first-order canonical transition occurs, the canonical transition line splits into two lines when mapped onto the $\Delta$-E plane. Between these lines, there is no stable canonical state for a given $\epsilon$ (cf. Fig. 3).

A more nontrivial situation arises due to the mapping of the microcanonical phase diagram onto the $\Delta$-T plane, as shown in Fig. 2(b). Here, two features are evident. First, in regions where the microcanonical transition is of second order but the canonical transition is of first order, there are three microcanonically stable values of $R_{1,2}$ at temperatures between the lines $T^{(1)}_{\max}$ (green line) and $T^{(1)}_{\min}$ (red line), and those between the lines $T^{(2)}_{\max}$ and $T^{(2)}_{\min}$ (brown line). Second, in regions of a first-order microcanonical transition, the transition line splits into two lines, denoted $T^{(1,0)}_{\max}$ (blue line) and $T^{(1,0)}_{\min}$ (black dashed line), with the latter coinciding with either $T^{(1)}_{\min}$ or $T^{(2)}_{\max}$ such that for temperatures in between there are two microcanonically stable values of $R_{1,2}$; see the inset of Fig. 2(b) and cuts of the $\Delta$-T phase diagram at fixed values of $\Delta$ in Fig. 3. Thus, in the whole domain of $\Delta$ where the canonical transition is of first order, one observes a multiplicity of microcanonically stable states in the $\Delta$-T plane. Remarkably, the tricritical points are different in the two ensembles.

In Fig. 4, we employ relation (9) to draw the temperature-energy relation $T(\epsilon)$ for $\Delta = 0.5$. For both microcanonical and canonical ensembles, this curve has two branches: a high-energy branch and a low-energy branch. At the point where the two branches intersect, the two entropies in the microcanonical ensemble and the two free energies in the canonical ensemble become equal. In the region where the canonical curve shows a jump in the energy at a given temperature, characteristic of a first-order transition that here occurs between the paramagnetic and the ferromagnetic phase [see Fig. 1(b)], the microcanonical curve shows a region of negative specific heat $(\partial T/\partial \epsilon < 0)$. Since the canonical specific heat is always positive, being given by the fluctuations in the energy of the system, the negative microcanonical specific heat is a further indication of ensemble inequivalence for the model under study.

To conclude, we addressed the issue of ensemble inequivalence in long-range interacting systems by studying an $XY$ model of classical spins with linear and quadratic coupling, and evolving under Hamilton dynamics. In this so-called generalized Hamiltonian mean-field model, we compared exact equilibrium phase diagrams in the microcanonical and canonical ensembles. We showed that, within the region of...
paramagnetic, ferromagnetic, and nematic phases. The phase (1) relaxes to quasistationary states (QSSs) which also have
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transition lines is similar in the phase diagrams of the two
appropriate variables, the arrangement of critical points and
behaviors. Nevertheless, let us remark that when plotted using
first-order transitions, the two ensembles show very different
behaviors. Nevertheless, let us remark that when plotted using
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diffs in the two ensembles, a behavior investigated earlier in
the microcanonical ensemble in Ref. [27]. In that paper, it was
shown that an isolated system described by the Hamiltonian
(1) relaxes to quasistationary states (QSSs) which also have
paramagnetic, ferromagnetic, and nematic phases. The phase
diagram of a QSS, however, is very different from the one
predicted by the equilibrium statistical mechanics in the
microcanonical ensemble, Fig. 1. Nevertheless, we expect
that since the lifetime of the QSS scales with the number
of particles in the system, a finite system will eventually relax
to the Boltzmann-Gibbs equilibrium. In the thermodynamic
limit, however, this relaxation might take longer than the age
of the universe. It will be of interest to explore such dynamical
behavior in the canonical ensemble.

Finally, we mention that an overdamped nonequilibrium
version of the GHMF is a Kuramoto-type model of synchroniza-
tion of globally coupled oscillators (just as an overdamped
nonequilibrium version of the HMF model is the standard
Kuramoto model [34,35]), where transitions to synchroniza-
tion are of major interest. In the context of synchronization,
nematic and ferromagnetic phases correspond respectively
to two-cluster and one-cluster synchronization patterns (see
Ref. [33]), but their stability is obtained from dynamical and
not from free energy or entropy considerations.

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