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The Generalized Canonical Ensemble and Its Universal Equivalence with the Microcanonical Ensemble

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This paper shows for a general class of statistical mechanical models that when the microcanonical and canonical ensembles are nonequivalent on a subset of values of the energy, there often exists a generalized canonical ensemble that satisfies a strong form of equivalence with the microcanonical ensemble that we call universal equivalence. The generalized canonical ensemble that we consider is obtained from the standard canonical ensemble by adding an exponential factor involving a continuous function g of the Hamiltonian. For example, if the microcanonical entropy is C^2, then universal equivalence of ensembles holds with g taken from a class of quadratic functions, giving rise to a generalized canonical ensemble known in the literature as the Gaussian ensemble. This use of functions g to obtain ensemble equivalence is a counterpart to the use of penalty functions and augmented Lagrangians in global optimization. Generalizing the paper by Ellis *et al.* [*J. Stat. Phys.* **101**:999–1064 (2000)], we analyze the equivalence of the microcanonical and generalized canonical ensembles both at the level of equilibrium macrostates and at the thermodynamic level. A neat but not quite precise statement of one of our main results is that the microcanonical and generalized canonical ensembles are equivalent at the level of equilibrium macrostates if and only if they are equivalent at the thermodynamic level, which is the case if and only if the generalized microcanonical entropy $s-g$ is concave. This generalizes the work of Ellis *et al.*, who basically proved that the microcanonical and canonical ensembles are equivalent at the level of equilibrium macrostates if and only if they are equivalent at the thermodynamic level, which is the case if and only if the microcanonical entropy s is concave.

KEY WORDS: Generalized canonical ensemble; equivalence of ensembles; microcanonical entropy; large deviation principle.

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1. INTRODUCTION

1.1. Statement of the Problem

The problem of ensemble equivalence is a fundamental one lying at the foundations of equilibrium statistical mechanics. It forces us to re-evaluate a number of deep questions that have often been dismissed in the past as being physically obvious. These questions include the following. Is the temperature of a statistical mechanical system always related to its energy in a one-to-one fashion? Are the microcanonical equilibrium properties of a system calculated as a function of the energy always equivalent to its canonical equilibrium properties calculated as a function of the temperature? Is the microcanonical entropy always a concave function of the energy? Is the heat capacity always a positive quantity? Surprisingly, the answer to each of these questions is in general no.

Starting with the work of Lynden-Bell and Wood[41] and the work of Thirring,[51] physicists have come to realize in recent decades that systematic incompatibilities between the microcanonical and canonical ensembles can arise in the thermodynamic limit if the microcanonical entropy function of the system under study is nonconcave. The reason for this nonequivalence can be explained mathematically by the fact that, when applied to a nonconcave function, the Legendre–Fenchel transform is non-involutive; i.e., performing it twice does not give back the original function but gives back its concave envelope.[22,52] As a consequence of this property, the Legendre–Fenchel structure of statistical mechanics, traditionally used to establish a one-to-one relationship between the entropy and the free energy and between the energy and the temperature, ceases to be valid when the entropy is nonconcave.

From a more physical perspective, the explanation is even simpler. When the entropy is nonconcave, the microcanonical and canonical ensembles are nonequivalent because the nonconcavity of the entropy implies the existence of a nondifferentiable point of the free energy, and this, in turn, marks the presence of a first-order phase transition in the canonical ensemble.[19,29] Accordingly, the ensembles are nonequivalent because the canonical ensemble jumps over a range of energy values at a critical value of the temperature and is therefore prevented from entering a subset of energy values that can always be accessed by the microcanonical ensemble.[19,29,51] This phenomenon lies at the root of ensemble nonequivalence, which is observed in systems as diverse as lattice spin models, including mean-field versions of the Hamiltonian model,[13,37] the XY model,[14] the Curie–Weiss–Potts model,[11,12] and the Blume–Emery–Griffiths model;[1,2,22,23] in gravitational systems;[29,30,41,51] in models of coherent structures in turbulence;[7,19,20,24,35,46] in models of plasmas;[36,49] and in a model of the Lennard–Jones gas,[5] to mention only a few. Many of these models can be analyzed by the methods of ref. 19 and the present paper.

The problem that we solve in this paper generalizes the work in ref. 19, which studies the equivalence of the microcanonical and canonical ensembles. We will show that when the microcanonical ensemble is nonequivalent with the canonical ensemble on a subset of values of the energy, it is often possible to slightly modify the definition of the canonical ensemble so as to recover equivalence with the microcanonical ensemble. Specifically, we will give natural conditions under which one can construct a modified or generalized canonical ensemble that is equivalent with the microcanonical ensemble when the canonical ensemble is not. This is potentially useful if one wants to work out the equilibrium properties of a system in the microcanonical ensemble, a notoriously difficult problem because of the equality constraint appearing in the definition of this ensemble. In the case of ensemble equivalence, one circumvents the intractability of the microcanonical ensemble by using the more tractable canonical ensemble in order to obtain canonical results that are then transformed into microcanonical results via the Legendre–Fenchel transform. However, in the case of ensemble nonequivalence, this way of doing calculations is no longer available precisely because there are properties of the microcanonical ensemble that cannot be inferred using canonical techniques. The alternative that we propose here is to resort to a generalization of the canonical ensemble that is as tractable as the canonical ensemble itself, either analytically or numerically, and has the advantage that it can be proved to be equivalent with the microcanonical ensemble.

1.2. Overview of the Results

It is apparent that the problem of ensemble equivalence, when formulated in mathematical terms, also addresses a fundamental issue in global optimization. Namely, given a constrained minimization problem, under what conditions does there exist a related, unconstrained minimization problem having the same minimum points? This question will be the mathematical focus of this paper.

In order to explain the connection between ensemble nonequivalence and global optimization and in order to outline the contributions of this paper, we introduce some notation. Let $\mathcal{X}$ be a space, I a function mapping $\mathcal{X}$ into $[0, \infty]$, and $\tilde{H}$ a function mapping $\mathcal{X}$ into $\mathbb{R}^\sigma$, where σ is a positive integer. For $u \in \mathbb{R}^\sigma$ we consider the following constrained minimization problem:

$$\text{minimize } I(x) \text{ over } x \in \mathcal{X} \text{ subject to the contraint } \tilde{H}(x) = u. \quad (1.2.1)$$

A partial answer to the question posed at the end of the first paragraph can be found by introducing the following related, unconstrained minimization problem for $\beta \in \mathbb{R}^\sigma$:

$$\text{minimize } I(x) + \langle \beta, \tilde{H}(x) \rangle \text{ over } x \in \mathcal{X}, \quad (1.2.2)$$

where $\langle \cdot, \cdot \rangle$ denotes the Euclidean inner product on $\mathbb{R}^\sigma$. The theory of Lagrange multipliers outlines suitable conditions under which the solutions of the constrained problem (1.2.1) lie among the critical points of $I + \langle \beta, \tilde{H} \rangle$. However, it does not give, as we will do in Theorems 3.1 and 3.4, necessary and sufficient conditions for the solutions of (1.2.1) to coincide with the solutions of the unconstrained minimization problem (1.2.2) and with solutions of the unconstrained minimization problem appearing in (1.2.6).

By giving such necessary and sufficient conditions, we make contact with the duality theory of global optimization and the method of augmented Lagrangians (ref. 3; Section 2.2 and ref. 43; Section 6.4). In the context of global optimization the primal function and the dual function play the same roles that the (generalized) microcanonical entropy and the (generalized) canonical free energy play in statistical mechanics. Similarly, the replacement of the Lagrangian by the augmented Lagrangian in global optimization is paralleled by our replacement of the canonical ensemble by the generalized canonical ensemble.

The two minimization problems (1.2.1) and (1.2.2) arise in a natural way in the context of equilibrium statistical mechanics,[19] where in the case $\sigma = 1$, u denotes the energy and β the inverse temperature. We define $\mathcal{E}^u$ and $\mathcal{E}_\beta$ to be the respective sets of points solving the constrained problem (1.2.1) and the unconstrained problem (1.2.2); i.e.,

$$\mathcal{E}^u = \{x \in \mathcal{X} : I(x) \text{ is minimized subject to } \tilde{H}(x) = u\} \quad (1.2.3)$$

and

$$\mathcal{E}_\beta = \{x \in \mathcal{X} : I(x) + \langle \beta, \tilde{H}(x) \rangle \text{ is minimized}\}. \quad (1.2.4)$$

For a given statistical mechanical model $\mathcal{X}$ represents the set of all possible equilibrium macrostates. As we will outline in Section 2, the theory of large deviations allows one to identify $\mathcal{E}^u$ as the subset of $\mathcal{X}$ consisting of equilibrium macrostates for the microcanonical ensemble and $\mathcal{E}_\beta$ as the subset consisting of equilibrium macrostates for the canonical ensemble.

Defined by conditioning the Hamiltonian to have a fixed value, the microcanonical ensemble expresses the conservation of physical quantities such as the energy and is the more fundamental of the two ensembles. Among other reasons, the canonical ensemble was introduced by Gibbs(28) in the hope that in the limit $n \to \infty$ the two ensembles are equivalent; i.e., all asymptotic properties of the model obtained via the microcanonical ensemble could be realized as asymptotic properties obtained via the canonical ensemble. However, as numerous studies cited in Section 1.1 have shown, in general this is not the case. There are many examples of statistical mechanical models for which nonequivalence of ensembles holds over a wide range of model parameters and for which physically interesting microcanonical equilibria are often omitted by the canonical ensemble.

The paper(19) investigates this question in detail, analyzing equivalence of ensembles in terms of relationships between $\mathcal{E}^u$ and $\mathcal{E}_\beta$. In turn, these relationships are expressed in terms of support and concavity properties of the microcanonical entropy

$$s(u) = -\inf\{I(x) : x \in \mathcal{X}, \tilde{H}(x) = u\}.$$

The main results in ref. 19 are summarized in Theorem 3.1, which we now discuss under the simplifying assumption that $\operatorname{dom} s$ is an open subset of $\mathbb{R}^\sigma$.

We focus on $u \in \operatorname{dom} s$. Part (a) of Theorem 3.1 states that if s has a strictly supporting hyperplane at u, then full equivalence of ensembles holds in the sense that there exists a β such that $\mathcal{E}^u = \mathcal{E}_\beta$. In particular, if $\operatorname{dom} s$ is convex and open and s is strictly concave on $\operatorname{dom} s$, then s has a strictly supporting hyperplane at all u (Theorem 3.3(a)) and thus full equivalence of ensembles holds at all u. In this case we say that the microcanonical and canonical ensembles are *universally equivalent*.

The most surprising result, given in part (c), is that if s does not have a supporting hyperplane at u, then nonequivalence of ensembles holds in the strong sense that $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ for all $\beta \in \mathbb{R}^\sigma$. That is, if s does not have a supporting hyperplane at u — equivalently, if s is not concave at u — then microcanonical equilibrium macrostates cannot be realized canonically. This is to be contrasted with part (d), which states that for any $x \in \mathcal{E}_\beta$ there exists u such that $x \in \mathcal{E}^u$; i.e., canonical equilibrium macrostates can always be realized microcanonically. Thus of the two ensembles the microcanonical is the richer.

The starting point of the present paper is the following motivational question suggested by Theorem 3.1. If the microcanonical ensemble is not equivalent with the canonical ensemble on a subset of values of u, then is it possible to replace the canonical ensemble with a generalized canonical ensemble that is universally equivalent with the microcanonical ensemble; i.e., fully equivalent at all u?

The generalized canonical ensemble that we consider is a natural perturbation of the standard canonical ensemble, obtained from it by adding an exponential factor involving a continuous function g of the Hamiltonian. The special case in which g is quadratic plays a central role in the theory, giving rise to a generalized canonical ensemble known in the literature as the Gaussian ensemble.[8,9,31–33,50] As these papers discuss, an important feature of Gaussian ensembles is that they allow one to account for ensemble-dependent effects in finite systems. Although not referred to by name, the Gaussian ensemble also plays a key role in ref. 35, where it is used to address equivalence-of-ensemble questions for a point-vortex model of fluid turbulence.

Let us focus on the case of quadratic g because it illustrates nicely why the answer to the motivational question is yes in a wide variety of circumstances. In order to simplify the notation, we work with $u=0$ and the corresponding set $\mathcal{E}^0$ of equilibrium macrostates. We denote by $\|\cdot\|$ the Euclidean norm on $\mathbb{R}^\sigma$ and consider the Gaussian ensemble defined in (2.6) with $g(u)=\gamma\|u\|^2$ for $\gamma \geqslant 0$. As we will outline in Section 2, the theory of large deviations allows one to identify the subset of $\mathcal{X}$ consisting of equilibrium macrostates for the Gaussian ensemble with the set

$$\mathcal{E}(\gamma)_\beta = \left\{ x \in \mathcal{X} : I(x) + \langle \beta, \tilde{H}(x) \rangle + \gamma \|\tilde{H}(x)\|^2 \text{ is minimized} \right\}. \quad (1.2.5)$$

$\mathcal{E}(\gamma)_\beta$ can be viewed as an approximation to the set $\mathcal{E}^0$ of equilibrium macrostates for the microcanonical ensemble. This follows from the calculation:

$$\left\{ x \in \mathcal{X} : \lim_{\gamma \to \infty} \left(I(x) + \langle \beta, \tilde{H}(x) \rangle + \gamma \|\tilde{H}(x)\|^2 \right) \text{ is minimized} \right\}$$
$$= \{ x \in \mathcal{X} : I(x) \text{ is minimized subject to } \tilde{H}(x) = 0 \} = \mathcal{E}^0.$$

This observation makes it plausible that for sufficiently large γ there exists a β such that $\mathcal{E}^0$ equals $\mathcal{E}(\gamma)_\beta$; i.e., the microcanonical ensemble and the Gaussian ensemble are fully equivalent. As we will see, under suitable hypotheses this and much more are true.

Our results apply to a much wider class of generalized canonical ensembles, of which the Gaussian ensemble is a special case. Given a continuous function g mapping $\mathbb{R}^\sigma$ into $\mathbb{R}$, the associated set of equilibrium macrostates is defined as

$$\mathcal{E}(g)_\beta = \{x \in \mathcal{X} : I(x) + \langle \beta, \tilde{H}(x) \rangle + g(\tilde{H}(x)) \text{ is minimized}\}. \quad (1.2.6)$$

This set reduces to (1.2.5) when $g(u) = \gamma \|u\|^2$.

The utility of the generalized canonical ensemble rests on the simplicity with which the function g defining this ensemble enters the formulation of ensemble equivalence. Essentially all the results in ref. 19 concerning ensemble equivalence, including Theorem 3.1, generalize to the setting of the generalized canonical ensemble by replacing the microcanonical entropy s by the generalized microcanonical entropy $s - g$. The generalization of Theorem 3.1 is stated in Theorem 3.4, which gives all possible relationships between the set $\mathcal{E}^u$ of equilibrium macrostates for the microcanonical ensemble and the set $\mathcal{E}(g)_\beta$ of equilibrium macrostates for the generalized canonical ensemble. These relationships are expressed in terms of support and concavity properties of $s - g$. The proof of Theorem 3.4 shows how easily it follows from Theorem 3.1, in which all equivalence and nonequivalence relationships between $\mathcal{E}^u$ and $\mathcal{E}_\beta$ are expressed in terms of support and concavity properties of s.

For the purpose of applications the most important consequence of Theorem 3.4 is given in part (a), which we now discuss under the simplifying assumption that $\operatorname{dom} s$ is an open subset of $\mathbb{R}^\sigma$. We focus on $u \in \operatorname{dom} s$. Part (a) states that if $s - g$ has a strictly supporting hyperplane at u, then full equivalence of ensembles holds in the sense that there exists a β such that $\mathcal{E}^u = \mathcal{E}(g)_\beta$. In particular, if $\operatorname{dom} s$ is convex and open and if $s - g$ is strictly concave on $\operatorname{dom} s$, then $s - g$ has a strictly supporting hyperplane at all u (Theorem 3.6(a)) and thus full equivalence of ensembles holds at all u. In this case we say that the microcanonical and generalized canonical ensembles are *universally equivalent*.

The only requirement on the function g defining the generalized canonical ensemble is that g is continuous. The considerable freedom that one has in choosing g makes it possible to define a generalized canonical ensemble that is universally equivalent with the microcanonical ensemble when the microcanonical and standard canonical ensembles are not equivalent on a subset of values of u. In Theorems 5.2–5.4 several examples of universal equivalence are derived under natural smoothness and boundedness conditions on s, while Theorem 5.5 derives a weaker form of universal equivalence under other conditions. In the first, second, and fourth of these theorems g is taken from a set of quadratic functions, and the associated ensembles are Gaussian.

Theorem 5.2, which applies when the dimension $\sigma = 1$, is particularly useful. It shows that if s is C^2 and s'' is bounded above on the interior of $\operatorname{dom} s$, then for any

$$\gamma > \frac{1}{2} \cdot \sup_{u \in \text{int}(\text{dom}\, s)} s''(u),$$

$s(u) - \gamma u^2$ is strictly concave on dom s. By part (b) of Theorem 3.6 and part (a) of Theorem 3.4, it follows that the microcanonical ensemble and the Gaussian ensemble defined in terms of γ are universally equivalent. The strict concavity of $s(u) - \gamma u^2$ also implies that the generalized canonical free energy is differentiable on $\mathbb{R}$ (Theorem 4.1(c)), a condition guaranteeing the absence of a discontinuous, first-order phase transition with respect to the Gaussian ensemble. Theorem 5.3 is the analogue of Theorem 5.2 that treats arbitrary dimension $\sigma \geqslant 2$. Again, we prove that for all sufficiently large γ, the microcanonical ensemble and the Gaussian ensemble defined in terms of γ are universally equivalent. These two theorems are particularly satisfying because they make rigorous the intuition underlying the introduction of the Gaussian ensemble: because it approximates the microcanonical ensemble in the limit $\gamma \to \infty$, universal ensemble equivalence should hold for all sufficiently large γ.

The criterion in Theorem 5.2 that s'' is bounded above on the interior of dom s is essentially optimal for the existence of a fixed quadratic function g guaranteeing the strict concavity of $s - g$ on dom s. The situation in which $s''(u) \to \infty$ as u approaches a boundary point can often be handled by Theorem 5.5, which is a local version of Theorem 5.2. The second derivative $s''(u)$ has this behavior in the Curie–Weiss–Potts model, which is introduced as the second model in Example 2.1. As we show in ref. 11 by explicit calculation of the canonical and microcanonical equilibrium macrostates, the microcanonical and canonical ensembles are not equivalent for all values of the energy. Specifically, there exists a subset of energy values for which the microcanonical entropy is nonconcave and for which the microcanonical equilibrium macrostates are not realized canonically. In ref. 12, we use the methods of the present paper together with special features of the model to show, among other results, that for any energy v for which the ensembles are nonequivalent and for any $u \leqslant v$ there exists a Gaussian ensemble that is fully equivalent with the microcanonical ensemble at u. A related feature of the Curie–Weiss–Potts model is discussed in the second paragraph before Theorem 5.5.

Besides studying ensemble equivalence at the level of equilibrium macrostates, one can also analyze it at the thermodynamic level. This level focuses on Legendre–Fenchel–transform relationships involving the basic thermodynamic functions in the three ensembles: the microcanonical entropy $s(u)$, on the one hand, and the canonical free energy and generalized canonical free energy, on the other. The analysis is carried out in Section 4, where we also relate ensemble equivalence at the two levels.

A neat but not quite precise statement of the main result proved in that section is that the microcanonical ensemble and the canonical ensemble (resp., generalized canonical ensemble) are equivalent at the level of equilibrium macrostates if and only if they are equivalent at the thermodynamic level, which is the case if and only s (resp., $s-g$) is concave.

1.3. Background

One of the seeds out of which the present paper germinated is the paper,[20] in which we study the equivalence of the microcanonical and canonical ensembles for statistical equilibrium models of coherent structures in two-dimensional and quasi-geostrophic turbulence. Numerical computations demonstrate that nonequivalence of ensembles occurs over a wide range of model parameters and that physically interesting microcanonical equilibria are often omitted by the canonical ensemble. In addition, in Section 5 of ref. 20, we establish the nonlinear stability of the steady mean flows corresponding to microcanonical equilibria via a new Lyapunov argument. The associated stability theorem refines the well-known Arnold stability theorems, which do not apply when the microcanonical and canonical ensembles are not equivalent. The Lyapunov functional appearing in this new stability theorem is defined in terms of a generalized thermodynamic potential similar in form to

$$I(x) + \langle \beta, \tilde{H}(x) \rangle + \gamma \|\tilde{H}(x)\|^2$$

the minimum points of which define the set of equilibrium macrostates for the Gaussian ensemble (see (1.2.5)). Such Lyapunov functionals arise in the study of constrained optimization problems, where they are known as augmented Lagrangians.[3,43]

Another seed out of which the present paper germinated is the work of Hetherington and coworkers[8,9,31,32,50] on the Gaussian ensemble. Reference 31 is the first paper that defined the Gaussian ensemble as a modification of the canonical ensemble in which the standard exponential Boltzmann term involving the energy is augmented by an additional term involving the square of the energy. As shown in refs. 8, 9, 32, 50, such a modified canonical ensemble arises when a sample system is in contact with a finite heat reservoir. From this point of view, the Gaussian ensemble can be viewed as an intermediate ensemble between the microcanonical, whose definition involves no reservoir, and the canonical ensemble, which is defined in terms of an infinite reservoir. The Gaussian ensemble is used in refs. 8, 9, 32, 50, to study microcanonical-canonical discrepancies in finite-size systems; such discrepancies are generally present near first-order phase transitions.

Gaussian ensembles are also considered in ref. 33 and more or less implicitly in ref. 35. Reference 33 is a theoretical study of the Gaussian ensemble which derives it from the maximum entropy principle and studies its stability properties. Reference 35 uses some mathematical methods that are reminiscent of the Gaussian ensemble to study a point-vertex model of fluid turbulence. By sending $\gamma \to \infty$ after the fluid limit $n \to \infty$, the authors recover the special class of nonlinear, stationary Euler flows that is expected from the microcanonical ensemble. Their use of Gaussian ensembles improves previous studies in which either the logarithmic singularities of the Hamiltonian must be regularized or equivalence of ensembles must be assumed. As they point out, the latter is not a satisfactory assumption because the ensembles are nonequivalent in certain geometries in which conditionally stable configurations exist in the microcanonical ensemble but not in the canonical ensemble. Their paper motivated in part the analysis of ensemble equivalence in the present paper, which focuses on generalized canonical ensembles with a fixed function g and, as a special case, Gaussian ensembles in which γ is fixed and is not sent to ∞.

In addition to the connections with refs. 8, 9, 33, 35, the present paper also builds on the wide literature concerning equivalence of ensembles in statistical mechanics. An overview of this literature is given in the introduction of ref. 40. A number of papers on this topic, including refs. 15, 19, 24, 27, 39, 40, 48, investigate equivalence of ensembles using the theory of large deviations. In ref. 39, Section 7 and ref. 40, Section 7.3 there is a discussion of nonequivalence of ensembles for the simplest mean-field model in statistical mechanics; namely, the Curie-Weiss model of a ferromagnet. However, despite the mathematical sophistication of these and other studies, none of them except for our paper(19) explicitly addresses the general issue of the nonequivalence of ensembles, which seems to be the typical behavior for a wide class of models arising in various areas of statistical mechanics.

The study of ensemble equivalence at the level of equilibrium macrostates involves relationships among the sets $\mathcal{E}^u$, $\mathcal{E}_\beta$, and $\mathcal{E}(g)_\beta$ of equilibrium macrostates for the three ensembles. These sets are subsets of $\mathcal{X}$, which in many cases, including short-range spin models and models of coherent structures in turbulence, is an infinite-dimensional space. The most important discovery in our work on this topic is that all relationships among these possibly infinite dimensional sets are completely determined by support and concavity properties of the finite-dimensional, and in many applications, one-dimensional functions s and $s - g$. The main tools for analyzing ensemble equivalence are the theory of large deviations and the theory of concave functions, both of which exhibit an analogous conceptual structure. On the one hand, the two theories provide powerful, investigative methodologies in which formal manipulations or geometric intuition can lead one to the correct answer. On the other hand, both theories are fraught with numerous technicalities which, if emphasized, can obscure the big picture. In the present paper we emphasize the big picture by relegating a number of technicalities to Appendix A. Reference 10 treats in greater detail some of the material in the present paper including background on concave functions.

In Section 3 of this paper, we state the hypotheses on the statistical mechanical models to which the theory of the present paper applies, give a number of examples of such models, and then present the results on ensemble equivalence at the level of equilibrium macrostates for the three ensembles. In Section 4 we relate ensemble equivalence at the level of equilibrium macrostates and at the thermodynamic level via the Legendre–Fenchel transform and a mild generalization suitable for treating quantities arising in the generalized canonical ensemble. In Section 5 we present a number of results giving conditions for the existence of a generalized canonical ensemble that is universally equivalent to the microcanonical ensemble. In all but one of these results the generalized canonical ensemble is Gaussian. Appendix A contains a number of technical results on concave functions needed in the main body of the paper.

2. DEFINITIONS OF MODELS AND ENSEMBLES

The main contribution of this paper is that when the canonical ensemble is nonequivalent to the microcanonical ensemble on a subset of values of u, it can often be replaced by a generalized canonical ensemble that is equivalent to the microcanonical ensemble at all u. Before introducing the various ensembles as well as the methodology for proving this result, we first specify the class of statistical mechanical models under consideration. The models are defined in terms of the following quantities.

- A sequence of probability spaces $(\Omega_n, \mathcal{F}_n, P_n)$ indexed by $n \in \mathbb{N}$, which typically represents a sequence of finite dimensional systems. The Ω_n are the configuration spaces, $\omega \in \Omega_n$ are the microstates, and the P_n are the prior measures.

- A sequence of positive scaling constant $a_n \to \infty$ as $n \to \infty$. In general a_n equals the total number of degrees of freedom in the model. In many cases a_n equals the number of particles.

- A positive integer σ and for each $n \in \mathbb{N}$ measurable functions $H_{n,1}, \ldots, H_{n,\sigma}$ mapping Ω_n into $\mathbb{R}$. For $\omega \in \Omega_n$ we define

$$h_{n,i}(\omega) = \frac{1}{a_n} H_{n,i}(\omega) \quad \text{and} \quad h_n(\omega) = (h_{n,1}(\omega), \ldots, h_{n,\sigma}(\omega)).$$

The $H_{n,i}$ include the Hamiltonian and, if $\sigma \geqslant 2$, other dynamical invariants associated with the model.

A large deviation analysis of the general model is possible provided that there exist, as specified in the next four items, a space of macrostates, macroscopic variables, and interaction representation functions and provided that the macroscopic variables satisfy the large deviation principle (LDP) on the space of macrostates.

1. *Space of macrostates*. This is a complete, separable metric space $\mathcal{X}$, which represents the set of all possible macrostates.

2. *Macroscopic variables.* These are a sequence of random variables Y_n mapping Ω_n into $\mathcal{X}$. These functions associate a macrostate in $\mathcal{X}$ with each microstate $\omega \in \Omega_n$.

3. *Interaction representation functions.* These are bounded, continuous functions $\tilde{H}_1, \ldots, \tilde{H}_\sigma$ mapping $\mathcal{X}$ into $\mathbb{R}$ such that as $n \to \infty$

$$h_{n,i}(\omega) = \tilde{H}_i(Y_n(\omega)) + \mathrm{o}(1) \quad \text{uniformly for } \omega \in \Omega_n; \tag{2.1}$$

i.e.,

$$\lim_{n\to\infty} \sup_{\omega\in\Omega_n} |h_{n,i}(\omega) - \tilde{H}_i(Y_n(\omega))| = 0.$$

We define $\tilde{H} = (\tilde{H}_1, \ldots, \tilde{H}_\sigma)$. The functions $\tilde{H}_i$ enable us to write the $h_{n,i}$, either exactly or asymptotically, as functions of the macrostate via the macroscopic variables Y_n.

4. *LDP for the macroscopic variables.* There exists a function I mapping $\mathcal{X}$ into $[0, \infty]$ and having compact level sets such that with respect to P_n the sequence Y_n satisfies the LDP on $\mathcal{X}$ with rate function I and scaling constants a_n. In other words, for any closed subset F of $\mathcal{X}$

$$\limsup_{n\to\infty} \frac{1}{a_n} \log P_n\{Y_n \in F\} \leqslant -\inf_{x\in F} I(x)$$

and for any open subset G of $\mathcal{X}$

$$\liminf_{n\to\infty} \frac{1}{a_n} \log P_n\{Y_n \in G\} \geqslant -\inf_{x\in G} I(x).$$

It is helpful to summarize the LDP by the formal notation $P_n\{Y_n \in dx\} \asymp \exp[-a_n I(x)]$. This notation expresses the fact that, to a first degree of approximation, $P_n\{Y_n \in dx\}$ behaves like an exponential that decays to 0 whenever $I(x) > 0$.

As specified in item 3, the functions $\tilde{H}_i$ are bounded on $\mathcal{X}$, and because of (2.1) the functions $h_{n,i}$ are also bounded on $\mathcal{X}$. In ref. 10 it is shown that all the results in this paper are valid under much weaker hypotheses on $\tilde{H}_i$, including $\tilde{H}$ that are not bounded on $\mathcal{X}$.

The assumptions on the statistical mechanical models just stated, as well as a number of definitions to follow, are valid for lattice spin and other models. These assumptions differ slightly from those in ref. 19, where they are adapted for applications to statistical mechanical models of coherent structures in turbulence. The major difference is that H_n in ref. 19 is replaced by h_n here in several equations: the asymptotic relationship (2.1), the definition (2.3) of the microcanonical ensemble $P_n^{u,r}$, and the definition (2.4) of the canonical ensemble $P_{n,\beta}$. In addition, in ref. 19 the LDP for Y_n is studied with respect to $P_{n,a_n\beta}$, in which β is scaled by a_n; here the LDP for Y_n is studied with respect to $P_{n,\beta}$. With only such superficial changes in notation, all the results in ref. 19 are applicable here, and, in turn, all the results derived here are applicable to the models considered in ref. 19.

A wide variety of statistical mechanical models satisfy the hypotheses listed at the start of this section and so can be studied by the methods of ref. 19 and the present paper. We next give six examples. The first two are long-range spin systems, the third a class of short-range spin systems, the fourth a model of two-dimensional turbulence, the fifth a model of quasi-geostrophic turbulence, and the sixth a model of dispersive wave turbulence.

Example 2.1.

1. *Mean-field Blume–Emery–Griffiths model.* The Blume–Emery–Griffiths model[(4)] is one of the few and certainly one of the simplest lattice-spin models known to exhibit, in the mean-field approximation, both a continuous, second-order phase transition and a discontinuous, first-order phase transition. Defined on the set $\{1, 2, \ldots, n\}$, the mean-field model coincides with the Blume–Emery–Griffiths model on the complete graph on n vertices. The spin at site $j \in \{1, 2, \ldots, n\}$ is denoted by ω_j, a quantity taking values in $\Lambda = \{-1, 0, 1\}$. The configuration spaces for the model are $\Omega_n = \Lambda^n$, the prior measures P_n are product measures on Ω_n with identical one-dimensional marginals $\rho = \frac{1}{3}(\delta_{-1} + \delta_0 + \delta_1)$, and for $\omega = (\omega_1, \ldots, \omega_n) \in \Omega_n$ the Hamiltonian is given by

$$H_n(\omega) = \sum_{j=1}^{n} \omega_j^2 - \frac{K}{n}\left(\sum_{j=1}^{n} \omega_j\right)^2,$$

where K is a fixed positive number. The space of macrostates for this model is the set of probability measures on Λ, the macroscopic variables are the empirical measures associated with the spin configurations ω, and the associated LDP is Sanov's Theorem, for which the rate function is the relative entropy with respect to ρ. The large deviation analysis of the model is given in ref. 22, which also analyzes the phase transition in the model. Equivalence and nonequivalence of ensembles for this model is studied at the thermodynamic level in refs. 1, 2, 23 and at the level of equilibrium macrostates in ref. 23. Phase transitions in the model are studied in ref. 22.

2. *Curie-Weiss-Potts model.* The Curie–Weiss–Potts model is a mean-field approximation to the nearest–neighbor Potts model.(53) Defined on the set $\{1, 2, \dots, n\}$, it coincides with the Potts model on the complete graph on n vertices. The spin at site $j \in \{1, 2, \dots, n\}$ is denoted by ω_j, a quantity taking values in the set Λ consisting of q distinct vectors $\theta^i \in \mathbb{R}^q$, where $q \geqslant 3$ is a fixed integer. The configuration spaces for the model are $\Omega_n = \Lambda^n$, the prior measures P_n are product measures on Ω_n with identical one-dimensional marginals $(1/q)\sum_{i=1}^{q} \delta_{\theta^i}$, and for $\omega = (\omega_1, \dots, \omega_n) \in \Omega_n$ the Hamiltonian is given by

$$H_n(\omega) = -\frac{1}{2n} \sum_{j,k=1}^{n} \delta(\omega_j, \omega_k).$$

As in the case of the mean-field Blume–Emery–Griffiths model, the space of macrostates for the Curie–Weiss–Potts model is the set of probability measures on Λ, the macroscopic variables are the empirical measures associated with ω, and the associated LDP is Sanov's Theorem, for which the rate function is the relative entropy with respect to ρ. The large deviation analysis of the model is summarized in ref. 11, which together with ref. 12 gives a complete analysis of ensemble equivalence and nonequivalence at the level of equilibrium macrostates. Further details are given in the next-to-last paragraph of Section 1.2.

3. *Short-range spin systems.* Short-range spin systems such as the Ising model on $\mathbb{Z}^d$ and numerous generalizations can also be handled by the methods of this paper. The large deviation techniques required to analyze these models are much more subtle than in the case of the long-range,

mean-field models considered in items 1 and 2. The already complicated large deviation analysis of one-dimensional models is given in Section IV.7 of ref. 17. The even more sophisticated analysis of multi-dimensional models is carried out in refs. 25 and 44. For these spin systems the space of macrostates is the space of translation-invariant probability measures on $\mathbb{Z}^d$, the macroscopic variables are the empirical processes associated with the spin configurations, and the rate function in the associated LDP is the mean relative entropy.

4. *A model of two-dimensional turbulence.* The Miller–Robert model is a model of coherent structures in an ideal, two-dimensional fluid that includes all the exact invariants of the vorticity transport equation.[42,45] In its original formulation, the infinite family of enstrophy integrals is imposed microcanonically along with the energy. If this formulation is slightly relaxed to include only finitely many enstrophy integrals, then the model can be put in the general form described above; that form can also be naturally extended to encompass complete enstrophy conservation. The space of macrostates is the space of Young measures on the vorticity field; that is, a macrostate has the form $\nu(x, dz)$, where $x \in \Lambda$ runs over the fluid domain Λ, z runs over the range of the vorticity field $\zeta(x)$, and for almost all x, $\nu(x, dz)$ is a probability measure in z. The large deviation analysis of this model, developed first in ref. 45 and more recently in ref. 6, gives a rigorous derivation of maximum entropy principles governing the equilibrium behavior of the ideal fluid.

5. *A model of quasi-geostrophic turbulence.* In later formulations, especially in geophysical applications, another version of the model in item 4 is preferred, in which the enstrophy integrals are treated canonically and the energy and circulation are treated microcanonically.[20] In those formulations, the space of macrostates is $L^2(\Lambda)$ or $L^\infty(\Lambda)$ depending on the contraints on the vorticity field. The large deviation analysis for such a formulation is carried out in ref. 18. Numerical results given in ref. 20 illustrate key examples of nonequivalence with respect to the energy and circulation invariants. In addition, this paper shows how the nonlinear stability of the steady mean flows arising as equilibriums macrostates in these models can be established by utilizing the appropriate generalized thermodynamic potentials.

6. *A model of dispersive wave turbulence.* A statistical equilibrium model of solitary wave structures in dispersive wave turbulence governed by a nonlinear Schrödinger equation is studied in ref. 21. In this model the energy is treated canonically while the particle number invariant is imposed microcanonically; without the microcanonical constraint on particle number the ensemble is not normalizable for focusing nonlinearities.

The large deviation analysis given in ref. 21 derives rigorously the concentration phenomenon observed in long-time numerical simulations and predicted by mean-field approximations.[34,38] The space of macrostates is $L^2(\Lambda)$, where Λ is a bounded interval or more generally a bounded domain in $\mathbb{R}^d$. ▮

We now return to the general theory, first introducing the function whose support and concavity properties completely determine all aspects of ensemble equivalence and nonequivalence. This function is the microcanonical entropy, defined for $u \in \mathbb{R}^\sigma$ by

$$s(u) = -\inf\{I(x) : x \in \mathcal{X}, \tilde{H}(x) = u\}. \tag{2.2}$$

Since I maps $\mathcal{X}$ into $[0, \infty]$, s maps $\mathbb{R}^\sigma$ into $[-\infty, 0]$. Moreover, since I is lower semicontinuous and $\tilde{H}$ is continuous on $\mathcal{X}$, s is upper semicontinuous on $\mathbb{R}^\sigma$. We define $\operatorname{dom} s$ to be the set of $u \in \mathbb{R}^\sigma$ for which $s(u) > -\infty$. In general, $\operatorname{dom} s$ is nonempty since $-s$ is a rate function (ref. 19, Proposition 3.1(a)). For each $u \in \operatorname{dom} s$, $r > 0$, $n \in \mathbb{N}$, and set $B \in \mathcal{F}_n$ the microcanonical ensemble is defined to be the conditioned measure

$$P_n^{u,r}\{B\} = P_n\{B \mid h_n \in \{u\}^{(r)}\}, \tag{2.3}$$

where $\{u\}^{(r)} = [u_1 - r, u_1 + r] \times \cdots \times [u_\sigma - r, u_\sigma + r]$. As shown in ref. 19, p. 1027, if $u \in \operatorname{dom} s$, then for all sufficiently large n, $P_n\{h_n \in \{u\}^{(r)}\} > 0$; thus the conditioned measures $P_n^{u,r}$ are well defined.

A mathematically more tractable probability measure is the canonical ensemble. Let $\langle \cdot, \cdot \rangle$ denote the Euclidian inner product on $\mathbb{R}^\sigma$. For each $n \in \mathbb{N}$, $\beta \in \mathbb{R}^\sigma$, and set $B \in \mathcal{F}_n$ we define the partition function

$$Z_n(\beta) = \int_{\Omega_n} \exp[-a_n \langle \beta, h_n \rangle] \, dP_n,$$

which is well defined and finite, and the probability measure

$$P_{n,\beta}\{B\} = \frac{1}{Z_n(\beta)} \cdot \int_B \exp[-a_n \langle \beta, h_n \rangle] \, dP_n. \tag{2.4}$$

The measures $P_{n,\beta}$ are Gibbs states that define the canonical ensemble for the given model.

The generalized canonical ensemble is a natural perturbation of the canonical ensemble, defined in terms of a continuous function g mapping

$\mathbb{R}^\sigma$ into $\mathbb{R}$. For each $n \in \mathbb{N}$ and $\beta \in \mathbb{R}^\sigma$ we define the generalized partition function

$$Z_{n,g}(\beta) = \int_{\Omega_n} \exp[-a_n \langle \beta, h_n \rangle - a_n g(h_n)]\, dP_n. \tag{2.5}$$

This is well defined and finite because the h_n are bounded and g is bounded on the range of the h_n. For $B \in \mathcal{F}_n$ we also define the probability measure

$$P_{n,\beta,g}\{B\} = \frac{1}{Z_{n,g}(\beta)} \cdot \int_B \exp[-a_n \langle \beta, h_n \rangle - a_n g(h_n)]\, dP_n, \tag{2.6}$$

which we call the generalized canonical ensemble. The special case in which g equals a quadratic function gives rise to the Gaussian ensemble.[8,9,31–33,50]

In order to define the set of equilibrium macrostates for each ensemble, we summarize two large deviation results proved in ref. 19 and extend one of them. It is proved in ref. 19, Theorem 3.2 that with respect to the microcanonical ensemble $P_n^{u,r}$, Y_n satisfies the LDP on $\mathcal{X}$, in the double limit $n \to \infty$ and $r \to 0$, with rate function

$$I^u(x) = \begin{cases} I(x) + s(u) & \text{if } \tilde{H}(x) = u, \\ \infty & \text{otherwise.} \end{cases} \tag{2.7}$$

I^u is nonnegative on $\mathcal{X}$, and for $u \in \operatorname{dom} s$, I^u attains its infimum of 0 on the set

$$\begin{aligned} \mathcal{E}^u &= \{x \in \mathcal{X} : I^u(x) = 0\} \\ &= \{x \in \mathcal{X} : I(x) \text{ is minimized subject to } \tilde{H}(x) = u\}. \end{aligned} \tag{2.8}$$

In order to state the LDPs for the other two ensembles, we bring in the canonical free energy, defined for $\beta \in \mathbb{R}^\sigma$ by

$$\varphi(\beta) = -\lim_{n \to \infty} \frac{1}{a_n} \log Z_n(\beta),$$

and the generalized canonical free energy, defined by

$$\varphi_g(\beta) = -\lim_{n \to \infty} \frac{1}{a_n} \log Z_{n,g}(\beta).$$

Clearly $\varphi_0(\beta)=\varphi(\beta)$. It is proved in ref. 19, Theorem 2.4 that the limit defining $\varphi(\beta)$ exists and is given by

$$\varphi(\beta)=\inf_{y\in\mathcal{X}}\{I(y)+\langle\beta,\tilde{H}(y)\rangle\} \tag{2.9}$$

and that with respect to $P_{n,\beta}$, Y_n satisfies the LDP on $\mathcal{X}$ with rate function

$$I_\beta(x)=I(x)+\langle\beta,\tilde{H}(x)\rangle-\varphi(\beta). \tag{2.10}$$

I_β is nonnegative on $\mathcal{X}$ and attains its infimum of 0 on the set

$$\begin{aligned}\mathcal{E}_\beta &= \{x\in\mathcal{X}: I_\beta(x)=0\}\\ &= \{x\in\mathcal{X}: I(x)+\langle\beta,\tilde{H}(x)\rangle \text{ is minimized}\}.\end{aligned} \tag{2.11}$$

A straightforward extension of these results shows that the limit defining $\varphi_g(\beta)$ exists and is given by

$$\varphi_g(\beta)=\inf_{y\in\mathcal{X}}\{I(y)+\langle\beta,\tilde{H}(y)\rangle+g(\tilde{H}(y))\} \tag{2.12}$$

and that with respect to $P_{n,\beta,g}$, Y_n satisfies the LDP on $\mathcal{X}$ with rate function

$$I_{\beta,g}(x)=I(x)+\langle\beta,\tilde{H}(x)\rangle+g(\tilde{H}(x))-\varphi_g(\beta). \tag{2.13}$$

$I_{\beta,g}$ is nonnegative on $\mathcal{X}$ and attains its infimum of 0 on the set

$$\begin{aligned}\mathcal{E}(g)_\beta &= \{x\in\mathcal{X}: I_{\beta,g}(x)=0\}\\ &= \{x\in\mathcal{X}: I(x)+\langle\beta,\tilde{H}(x)\rangle+g(\tilde{H}(x)) \text{ is minimized}\}.\end{aligned} \tag{2.14}$$

For $u\in\operatorname{dom} s$, let x be any element of $\mathcal{X}$ satisfying $I^u(x)>0$. The formal notation

$$P_n^{u,r}\{Y_n\in dx\}\asymp e^{-a_n I^u(x)}$$

suggests that x has an exponentially small probability of being observed in the limit $n\to\infty$, $r\to 0$. Hence it makes sense to identify $\mathcal{E}^u$ with the set of microcanonical equilibrium macrostates. In the same way we identify with $\mathcal{E}_\beta$ the set of canonical equilibrium macrostates and with $\mathcal{E}(g)_\beta$ the set of generalized canonical equilibrium macrostates. A rigorous justification of these identifications is given in ref. 19, Theorem 2.4(d).

3. ENSEMBLE EQUIVALENCE AT THE LEVEL OF EQUILIBRIUM MACROSTATES

Having defined the sets of equilibrium macrostates $\mathcal{E}^u$, $\mathcal{E}_\beta$, and $\mathcal{E}(g)_\beta$ for the microcanonical, canonical, and generalized canonical ensembles, we now come to the main point of this paper, which is to show how these sets relate to one another. In Theorem 3.1 we state the results proved in ref. 19 concerning equivalence and nonequivalence at the level of equilibrium macrostates for the microcanonical and canonical ensembles. Then in Theorem 3.4 we extend these results to the generalized canonical ensemble.

Parts (a)–(c) of Theorem 3.1 give necessary and sufficient conditions, in terms of support properties of s, for ensemble equivalence and nonequivalence of $\mathcal{E}^u$ and $\mathcal{E}_\beta$. These assertions are proved in Theorems 4.4 and 4.8 in ref. 19. Part (a) states that s has a strictly supporting hyperplane at u if and only if full equivalence of ensembles holds; i.e., if and only if there exists a β such that $\mathcal{E}^u = \mathcal{E}_\beta$. The most surprising result, given in part (c), is that s has no supporting hyperplane at u if and only if nonequivalence of ensembles holds in the strong sense that $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ for all $\beta \in \mathbb{R}^\sigma$. Part (c) is to be contrasted with part (d), which states that for any $\beta \in \mathbb{R}^\sigma$ canonical equilibrium macrostates can always be realized microcanonically. Part (d) is proved in Theorem 4.6 in ref. 19. Thus one conclusion of this theorem is that at the level of equilibrium macrostates the microcanonical ensemble is the richer of the two ensembles. The concept of a relative boundary point, which arises in part (c), is defined after the statement of the theorem. For $\beta \in \mathbb{R}^\sigma$, $[\beta, -1]$ denotes the vector in $\mathbb{R}^{\sigma+1}$ whose first σ components agree with those of β and whose last component equals -1.

Theorem 3.1. In parts (a)–(c), u denotes any point in $\operatorname{dom} s$.

(a) *Full equivalence.* There exists $\beta \in \mathbb{R}^\sigma$ such that $\mathcal{E}^u = \mathcal{E}_\beta$ if and only if s has a strictly supporting hyperplane at u with normal vector $[\beta, -1]$; i.e.,

$$s(v) < s(u) + \langle \beta, v - u \rangle \quad \text{for all } v \neq u.$$

(b) *Partial equivalence.* There exists $\beta \in \mathbb{R}^\sigma$ such that $\mathcal{E}^u \subset \mathcal{E}_\beta$ but $\mathcal{E}^u \neq \mathcal{E}_\beta$ if and only if s has a nonstrictly supporting hyperplane at u with normal vector $[\beta, -1]$; i.e.,

$$s(v) \leqslant s(u) + \langle \beta, v - u \rangle \quad \text{for all } v \text{ with equality for some } v \neq u.$$

(c) *Nonequivalence.* For all $\beta \in \mathbb{R}^\sigma$, $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ if and only if s has no supporting hyperplane at u; i.e.,

$$\text{for all } \beta \in \mathbb{R}^\sigma \text{ there exists } v \text{ such that } s(v) > s(u) + \langle \beta, v - u \rangle.$$

Except possibly for relative boundary points of $\operatorname{dom} s$, the latter condition is equivalent to the nonconcavity of s at u (Theorem A.5(c)).

(d) *Canonical is always realized microcanonically.* For any $\beta \in \mathbb{R}^\sigma$ we have $\tilde{H}(\mathcal{E}_\beta) \subset \operatorname{dom} s$ and

$$\mathcal{E}_\beta = \bigcup_{u \in \tilde{H}(\mathcal{E}_\beta)} \mathcal{E}^u.$$

We highlight several features of the theorem in order to illuminate their physical content. In part (a) we assume that for a given $u \in \operatorname{dom} s$ there exists a unique β such that $\mathcal{E}^u = \mathcal{E}_\beta$. If s is differentiable at u and s and the double–Legendre–Fenchel transform s^{**} are equal in a neighborhood of u, then β is given by the standard thermodynamic formula $\beta = \nabla s(u)$ (Theorem A.4(b)). The inverse relationship can be obtained from part (d) of the theorem under the assumption that $\mathcal{E}_\beta$ consists of a unique macrostate or more generally that for all $x \in \mathcal{E}_\beta$ the values $\tilde{H}(x)$ are equal. Then $\mathcal{E}_\beta = \mathcal{E}^{u(\beta)}$, where $u(\beta) = \tilde{H}(x)$ for any $x \in \mathcal{E}_\beta$; $u(\beta)$ denotes the mean energy realized at equilibrium in the canonical ensemble. The relationship $u = u(\beta)$ inverts the relationship $\beta = \nabla s(u)$. Partial ensemble equivalence can be seen in part (d) under the assumption that for a given β, $\mathcal{E}_\beta$ can be partitioned into at least two sets $\mathcal{E}_{\beta,i}$ such that for all $x \in \mathcal{E}_{\beta,i}$ the values $\tilde{H}(x)$ are equal but $\tilde{H}(x) \neq \tilde{H}(y)$ whenever $x \in \mathcal{E}_{\beta,i}$ and $y \in \mathcal{E}_{\beta,j}$ for $i \neq j$. Then $\mathcal{E}_\beta = \bigcup_i \mathcal{E}^{u_i(\beta)}$, where $u_i(\beta) = \tilde{H}(x)$, $x \in \mathcal{E}_{\beta,i}$. Clearly, for each i, $\mathcal{E}^{u_i(\beta)} \subset \mathcal{E}_\beta$ but $\mathcal{E}^{u_i(\beta)} \neq \mathcal{E}_\beta$. Physically, this corresponds to a situation of coexisting phases that normally takes place at a first-order phase transition.[52]

Theorem 4.10 in ref. 19 states an alternative version of part (d) of Theorem 3.1, in which the set $\tilde{H}(\mathcal{E}_\beta)$ of canonical equilibrium mean-energy values is replaced by another set. We next present a third version of part (d) that could be useful in applications. This corollary is also aesthetically pleasing because like parts (a)–(c) of Theorem 3.1 it is formulated in terms of support properties of s.

Corollary 3.2. For $\beta \in \mathbb{R}^\sigma$ we define A_β to be the set of $u \in \operatorname{dom} s$ such that s has a supporting hyperplane at u with normal vector $[\beta, -1]$. Then

$$\mathcal{E}_\beta = \bigcup_{u \in A_\beta} \mathcal{E}^u.$$

Proof. Part (d) of Theorem 3.1 implies that if $u \in \tilde{H}(\mathcal{E}_\beta)$, then $\mathcal{E}^u \subset \mathcal{E}_\beta$. From parts (a) and (b) of the theorem it follows that s has a supporting hyperplane at u with normal vector $[\beta, -1]$. Hence $\tilde{H}(\mathcal{E}_\beta) \subset A_\beta$ and

$$\mathcal{E}_\beta = \bigcup_{u \in \tilde{H}(\mathcal{E}_\beta)} \mathcal{E}^u \subset \bigcup_{u \in A_\beta} \mathcal{E}^u.$$

The reverse inclusion is also a consequence of parts (a) and (b) of the theorem, which imply that if $u \in A_\beta$, then $\mathcal{E}^u \subset \mathcal{E}_\beta$ and thus that

$$\bigcup_{u \in A_\beta} \mathcal{E}^u \subset \mathcal{E}_\beta.$$

This completes the proof. ▮

Before continuing with our analysis of ensemble equivalence, we introduce several sets that play a central role in the theory. Let $f \not\equiv -\infty$ be a function mapping $\mathbb{R}^\sigma$ into $\mathbb{R} \cup \{-\infty\}$. The relative interior of $\operatorname{dom} f$, denoted by $\operatorname{ri}(\operatorname{dom} f)$, is defined as the interior of $\operatorname{dom} f$ when considered as a subset of the smallest affine set that contains $\operatorname{dom} f$. Clearly, if the smallest affine set that contains $\operatorname{dom} f$ is $\mathbb{R}^\sigma$, then the relative interior of $\operatorname{dom} f$ equals the interior of $\operatorname{dom} f$, which we denote by $\operatorname{int}(\operatorname{dom} f)$. This is the case if, for example, $\sigma = 1$ and $\operatorname{dom} f$ is a nonempty interval. The relative boundary of $\operatorname{dom} f$ is defined as $\operatorname{cl}(\operatorname{dom} f) \setminus \operatorname{ri}(\operatorname{dom} f)$.

We continue by giving several definitions for concave functions on $\mathbb{R}^\sigma$ when σ is an arbitrary positive integer. We then specialize to the case $\sigma = 1$, for which all the concepts can be easily visualized. Additional material on concave functions is contained in Appendix A. Let f be a concave function on $\mathbb{R}^\sigma$. For $u \in \mathbb{R}^\sigma$ the superdifferential of f at u, denoted by $\partial f(u)$, is defined to be the set of $\beta \in \mathbb{R}^\sigma$ such that $[\beta, -1]$ is the normal vector to a supporting hyperplane of f at u; i.e.,

$$f(v) \leqslant f(u) + \langle \beta, v - u \rangle \quad \text{for all } v \in \mathbb{R}^\sigma.$$

Any such β is called a supergradient of f at u. The domain of ∂f, denoted by $\operatorname{dom} \partial f$, is then defined to be the set of u for which $\partial f(u) \neq \emptyset$. A basic fact is that $\operatorname{dom} \partial f$ is a subset of $\operatorname{dom} f$ and differs from it, if at all, only in a subset of the relative boundary of $\text{dom}\, f$; a precise statement is given in part (a) of Theorem A.1. By definition of $\text{dom}\, \partial f$, it follows that f has a supporting hyperplane at all points of $\text{dom}\, f$ except possibly relative boundary points.

We now specialize to the case $\sigma = 1$, considering a concave function f mapping $\mathbb{R}$ into $\mathbb{R} \cup \{-\infty\}$ for which $\text{dom}\, f$ is a nonempty interval L. For $u \in L$, $\partial f(u)$ is defined to be the set of $\beta \in \mathbb{R}$ such that β is the slope of a supporting line of f at u. Thus, if f is differentiable at $u \in \text{int}\, L$, then $\partial f(u)$ consists of the unique point $\beta = f'(u)$. If f is not differentiable at $u \in \text{int}\, L$, then $\text{dom}\, \partial f$ consists of all β satisfying the inequalities

$$(f')^+(u) \leqslant \beta \leqslant (f')^-(u),$$

where $(f')^-(u)$ and $(f')^+(u)$ denote the left-hand and right-hand derivatives of f at u.

Complications arise because $\text{dom}\, \partial f$ can be a proper subset of $\text{dom}\, f$, as the situation in one dimension clearly shows. Let b be a boundary point of $\text{dom}\, f$ for which $f(b) > -\infty$. Then b is in $\text{dom}\, \partial f$ if and only if the one-sided derivative of f at b is finite. For example, if b is a left hand boundary point of $\text{dom}\, f$ and $(f')^+(b)$ is finite, then $\partial f(b) = [(f')^+(b), \infty)$; any $\beta \in \partial f(b)$ is the slope of a supporting line at b. The possible discrepancy between $\text{dom}\, \partial f$ and $\text{dom}\, f$ introduces unavoidable technicalities in the statements of many results concerning the existence of supporting hyperplanes.

One of our goals is to find concavity and support conditions on the microcanonical entropy guaranteeing that the microcanonical and canonical ensembles are fully equivalent at all points $u \in \text{dom}\, s$ except possibly relative boundary points. If this is the case, then we say that the ensembles are *universally equivalent*. Here is a basic result in that direction.

Theorem 3.3. Assume that $\text{dom}\, s$ is a convex subset of $\mathbb{R}^\sigma$ and that s is strictly concave on $\text{ri}(\text{dom}\, s)$ and continuous on $\text{dom}\, s$. The following conclusions hold.

(a) s has a strictly supporting hyperplane at all $u \in \text{dom}\, s$ except possibly relative boundary points.

(b) The microcanonical and canonical ensembles are universally equivalent; i.e., fully equivalent at all $u \in \text{dom}\, s$ except possibly relative boundary points.

(c) s is concave on $\mathbb{R}^\sigma$, and for each u in part (b) the corresponding β in the statement of full equivalence is any element of $\partial s(u)$.

(d) If s is differentiable at some $u \in \operatorname{dom} s$, then the corresponding β in part (b) is unique and is given by the standard thermodynamic formula $\beta = \nabla s(u)$.

Proof.

(a) This is a consequence of part (c) of Theorem A.4.

(b) The universal equivalence follows from part (a) of Theorem 3.1.

(c) By Proposition A.3 the continuity of s on $\operatorname{dom} s$ allows us to extend the strict concavity of s on *ri*($\operatorname{dom} s$) to the concavity of s on $\operatorname{dom} s$. Since s equals $-\infty$ on the complement of $\operatorname{dom} s$, s is also concave on $\mathbb{R}^\sigma$. The second assertion in part (c) is the definition of supergradient.

(d) This is a consequence of part (c) of the present theorem and part (b) of Theorem A.1. ▮

We now come to the main result of this paper, which extends Theorem 3.1 by giving equivalence and nonequivalence results involving $\mathcal{E}^u$ and $\mathcal{E}(g)_\beta$. The proof of the theorem makes it transparent why s in Theorem 3.1 is replaced here by $s-g$. In ref. 10 an independent proof of Theorem 3.4 is derived from first principles rather than from Theorem 3.1. As we point out after the statement of Theorem 3.4, for the purpose of applications part (a) is its most important contribution. In order to illuminate its physical content, we note that if $s-g$ is differentiable at some $u \in \operatorname{dom} s$ and $s-g=(s-g)^{**}$ in a neighborhood of u, then β is unique and is given by the thermodynamic formula $\beta = \nabla(s-g)(u)$ (Theorem A.4(b)).

Theorem 3.4. Let g be a continuous function mapping $\mathbb{R}^\sigma$ into $\mathbb{R}$, in terms of which the generalized canonical ensemble (2.6) is defined. The following conclusions hold. In parts (a)–(c), u denotes any point in $\operatorname{dom} s$.

(a) *Full equivalence.* There exists $\beta \in \mathbb{R}^\sigma$ such that $\mathcal{E}^u = \mathcal{E}(g)_\beta$ if and only if $s-g$ has a strictly supporting hyperplane at u with normal vector $[\beta, -1]$.

(b) *Partial equivalence.* There exists $\beta \in \mathbb{R}^\sigma$ such that $\mathcal{E}^u \subset \mathcal{E}(g)_\beta$ but $\mathcal{E}^u \neq \mathcal{E}_\beta$ if and only if $s-g$ has a nonstrictly supporting hyperplane at u with normal vector $[\beta, -1]$.

(c) *Nonequivalence.* For all $\beta \in \mathbb{R}^\sigma$, $\mathcal{E}^u \cap \mathcal{E}(g)_\beta = \emptyset$ if and only if $s-g$ has no supporting hyperplane at u. Except possibly for relative boundary points of $\operatorname{dom} s$, the latter condition is equivalent to the nonconcavity of $s-g$ at u (Theorem A.5(c)).

(d) *Generalized canonical is always realized microcanonically.* For any $\beta \in R^\sigma$ we have $\tilde{H}(\mathcal{E}(g)_\beta) \subset \operatorname{dom} s$ and

$$\mathcal{E}(g)_\beta = \bigcup_{u \in \tilde{H}(\mathcal{E}(g)_\beta)} \mathcal{E}^u.$$

Proof. For $B \in \mathcal{F}_n$ we define a new probability measure

$$P_{n,g}\{B\} = \frac{1}{\int_{\Omega_n} \exp[-a_n g(h_n)]\, dP_n} \cdot \int_B \exp[-a_n g(h_n)]\, dP_n.$$

Replacing the prior measure P_n in the standard canonical ensemble with $P_{n,g}$ gives the generalized canonical ensemble $P_{n,\beta,g}$; i.e.,

$$P_{n,\beta,g}\{B\} = \frac{1}{\int_{\Omega_n} \exp[-a_n \langle \beta, h_n \rangle]\, dP_{n,g}} \cdot \int_B \exp[-a_n \langle \beta, h_n \rangle]\, dP_{n,g}.$$

We also introduce a new conditioned measure

$$P^{u,r}_{n,g}\{B\} = P_{n,g}\{B \mid h_n \in \{u\}^{(r)}\},$$

obtained from the microcanonical ensemble $P^{u,r}_n$ by replacing P_n with $P_{n,g}$. Since g is continuous, for ω in the set $\{h_n \in \{u\}^{(r)}\}$, $g(h_n(\omega))$ converges to $g(u)$ uniformly in ω and n as $r \to 0$. It follows that with respect to $P^{u,r}_{n,g}$, Y_n satisfies the LDP on $\mathcal{X}$, in the double limit $n \to \infty$ and $r \to 0$, with the same rate function I^u as in the LDP for Y_n with respect to $P^{u,r}_n$. As a result, the set $\mathcal{E}(g)^u$ of equilibrium macrostates corresponding to $P^{u,r}_{n,g}$ coincides with the set $\mathcal{E}^u$ of microcanonical equilibrium macrostates.

At this point we recall that according to parts (a)–(c) of Theorem 3.1, all equivalence and nonequivalence relationships between $\mathcal{E}^u$ and $\mathcal{E}_\beta$ are expressed in terms of support properties of

$$s(u) = -\inf\{I(x) : x \in \mathcal{X}, \tilde{H}(x) = u\},$$

where I is the rate function in the LDP for Y_n with respect to the prior measures P_n. With respect to the new prior measures $P_{n,g}$, Y_n satisfies the LDP on $\mathcal{X}$ with rate function

$$I_g(x) = I(x) + g(\tilde{H}(x)) - \text{const.}$$

It follows that all equivalence and nonequivalence relationships between $\mathcal{E}(g)^u$ and $\mathcal{E}(g)_\beta$ are expressed in terms of support properties of the function s_g obtained from s by replacing the rate function I by the new rate function I_g. The function s_g is given by

$$\begin{aligned} s_g(u) &= -\inf\{I_g(x) : x \in \mathcal{X}, \tilde{H}(x) = u\} \\ &= -\inf\{I(x) + g(\tilde{H}(x)) : x \in \mathcal{X}, \tilde{H}(x) = u\} + \text{const} \\ &= s(u) - g(u) + \text{const.} \end{aligned}$$

Since $\mathcal{E}(g)^u = \mathcal{E}^u$ and since s_g differs from $s - g$ by a constant, we conclude that all equivalence and nonequivalence relationships between $\mathcal{E}^u$ and $\mathcal{E}(g)_\beta$ are expressed in terms of the same support properties of $s - g$. This completes the derivation of parts (a)–(c) of Theorem 3.4 from parts (a)–(c) of Theorem 3.1. Similarly, part (d) of Theorem 3.4 follows from part (d) of Theorem 3.1. ∎

The relationships between $\mathcal{E}^u$ and $\mathcal{E}(g)_\beta$ in Theorem 3.4 are valid under much weaker assumptions on both g and $\tilde{H}_i$ that guarantee that these sets are nonempty. For example, the continuity of g is not needed. Of course, if one does not have the LDPs for Y_n with respect to $P_n^{u,r}$ and $P_{n,\beta,g}$, then one cannot interpret $\mathcal{E}^u$ and $\mathcal{E}(g)_\beta$ as sets of equilibrium macrostates for the two ensembles. A similar comment applies to Theorem 3.1.

The next corollary gives an alternative version of part (d) of Theorem 3.4. It follows from the theorem in the same way that Corollary 3.2 follows from Theorem 3.1, which is the analog of Theorem 3.4 for the canonical ensemble.

Corollary 3.5. Let g be a continuous function mapping $\mathbb{R}^\sigma$ into $\mathbb{R}$, in terms of which the generalized canonical ensemble (2.6) is defined. For $\beta \in \mathbb{R}^\sigma$ we define $A(g)_\beta$ to be the set of $u \in \operatorname{dom} s$ such that $s - g$ has a supporting hyperplane at u with normal vector $[\beta, -1]$. Then

$$\mathcal{E}(g)_\beta = \bigcup_{u \in A(g)_\beta} \mathcal{E}^u.$$

The importance of part (a) of Theorem 3.4 in applications is emphasized by the following theorem, which will be applied several times in the sequel. This theorem is the analog of Theorem 3.3 for the generalized canonical ensemble, replacing s in that theorem with $s - g$. Since g takes values in $\mathbb{R}$, the domain of $s-g$ equals the domain of s. Theorem 3.6 is proved exactly like Theorem 3.3.

Theorem 3.6. Assume that $\mathrm{dom}\, s$ is a convex subset of $\mathbb{R}^\sigma$ and that $s-g$ is strictly concave on ri(dom s) and continuous on dom s. The following conclusions hold:

(a) $s-g$ has a strictly supporting hyperplane at all $u \in \mathrm{dom}\, s$ except possibly relative boundary points.

(b) The microcanonical and generalized canonical ensembles defined in terms of this g are universally equivalent; i.e., fully equivalent at all $u \in \mathrm{dom}\, s$ except possibly relative boundary points.

(c) $s-g$ is concave on $\mathbb{R}^\sigma$, and for each u in part (b) the corresponding β in the statement of full equivalence is any element of $\partial(s-g)(u)$.

(d) If $s-g$ is differentiable at some $u \in \mathrm{dom}\, s$, then the corresponding β in part (b) is unique and is given by the thermodynamic formula $\beta = \nabla(s-g)(u)$.

The most important repercussion of Theorem 3.6 is the ease with which one can prove that the microcanonical and generalized canonical ensembles are universally equivalent in those cases in which microcanonical and standard canonical ensembles are not fully or partially equivalent. In order to achieve universal equivalence, one merely chooses g so that $s-g$ is strictly concave on *ri*(dom s). One has considerable freedom doing this since the only requirement is that g be continuous. Section 5 is devoted to this and related issues. In Theorems 5.2–5.5 we will give several useful examples, three of which involve quadratic functions g.

In the next section we introduce the thermodynamic level of ensemble equivalence and discuss its relationship to ensemble equivalence at the level of equilibrium macrostates.

4. ENSEMBLE EQUIVALENCE AT THE THERMODYNAMIC LEVEL

The thermodynamic level of ensemble equivalence is formulated in terms of the Legendre–Fenchel transform for concave, upper semicontinuous functions. Such transforms arise in a natural way via the variational formula (2.9) for the canonical free energy φ. Replacing the infimum over $y \in \mathcal{X}$ by the infimum over $y \in \mathcal{X}$ satisfying $\tilde{H}(y) = u$ followed by the infimum over $u \in \mathbb{R}^\sigma$ and using the definition (2.2) of the microcanonical entropy s, we see that for all $\beta \in \mathbb{R}^\sigma$

$$\varphi(\beta) = \inf_{u \in \mathbb{R}^\sigma} \{\langle \beta, u \rangle + \inf\{I(y) : y \in \mathcal{X}, \tilde{H}(y) = u\}\}$$
$$= \inf_{u \in \mathbb{R}^\sigma} \{\langle \beta, u \rangle - s(u)\} = s^*(\beta).$$

This calculation shows that φ, the basic thermodynamic function in the canonical ensemble, can always be expressed as the Legendre–Fenchel transform s^* of s, the basic thermodynamic function in the microcanonical ensemble. However, the converse need not be true. In fact, by the theory of Legendre–Fenchel transforms $s(u) = \varphi^*(u)$ for all $u \in \mathbb{R}^\sigma$, or equivalently $s(u) = s^{**}(u)$ for all u, if and only if s is concave and upper semicontinuous on $\mathbb{R}^\sigma$. While the upper semicontinuity is automatic from the definition of s, the concavity does not hold in general. This state of affairs concerning φ and s makes it clear that the thermodynamic level reveals what we have already seen at the level of equilibrium macrostates; namely, of the two ensembles the microcanonical ensemble is the more fundamental.

Similar considerations apply to the relationship between s and φ_g, the generalized canonical free energy, defined in terms of a continuous function g mapping $\mathbb{R}^\sigma$ into $\mathbb{R}$. Making the same changes in the variational formula (2.12) for φ_g as we just did in the variational formula for φ shows that for all $\beta \in \mathbb{R}^\sigma$

$$\varphi_g(\beta) = \inf_{u \in \mathbb{R}^\sigma} \{\langle \beta, u \rangle + g(u) + \inf\{I(y) : y \in \mathbb{R}^\sigma, \tilde{H}(y) = u\}\}$$
$$= \inf_{u \in \mathbb{R}^\sigma} \{\langle \beta, u \rangle + g(u) - s(u)\}$$
$$= (s - g)^*(\beta).$$

As in the case when $g \equiv 0$, this relationship can be inverted to give $(s - g)(u) = \varphi_g^*(u)$ for all $u \in \mathbb{R}^\sigma$, or equivalently $(s - g)(u) = (s - g)^{**}(u)$, if and only if $s - g$ is concave on $\mathbb{R}^\sigma$.

In order to be able to express these relationships in forms similar to those relating φ and s, we define for β and u in $\mathbb{R}^\sigma$

$$s^\sharp(g, \beta) = \inf_{u \in \mathbb{R}^\sigma} \{\langle \beta, u \rangle + g(u) - s(u)\} = (s - g)^*(\beta) \tag{4.1}$$

and

$$s^{\sharp\sharp}(g, u) = g(u) + \inf_{\beta \in \mathbb{R}^\sigma} \{\langle \beta, u \rangle - s^\sharp(g, \beta)\} = g(u) + (s - g)^{**}(u). \tag{4.2}$$

Thus for all β, $\varphi_g(\beta) = s^\sharp(g, \beta)$ while for all u, $s^{\sharp\sharp}(g, u) = s(u)$ if and only if $(s - g)(u) = (s - g)^{**}(u) = \varphi_g^*(u)$, and this holds if and only if $s - g$ is concave on $\mathbb{R}^\sigma$.

Theorem 4.1 records these facts in parts (a) and (b). Part (c) introduces a new theme proved in Theorem 26.3 in ref. 47. The strict concavity of $s-g$ on $\text{dom}\, s$ implies that φ_g is essentially smooth; i.e., φ_g is differentiable on $\mathbb{R}^\sigma$ and

$$\lim_{n\to\infty} \|\nabla\varphi_g(\beta_n)\| = \infty \text{ whenever } \|\beta_n\| \to \infty.$$

Setting $g \equiv 0$ implies a similar result relating s and $\varphi_0 = \varphi$. The differentiability of $\varphi(\beta)$ or $\varphi_g(\beta)$ implies that the corresponding ensemble does not exhibit a discontinuous, first-order phase transition.

Theorem 4.1. Let g be a continuous function mapping $\mathbb{R}^\sigma$ into $\mathbb{R}$, in terms of which the generalized canonical ensemble (2.6) is defined. The choice $g \equiv 0$ gives the standard canonical ensemble (2.4). The following conclusions hold:

(a) For all $\beta \in \mathbb{R}^\sigma$, $\varphi_g(\beta) = s^\sharp(g, \beta) = (s-g)^*(\beta)$.

(b) For all $u \in \mathbb{R}^\sigma$

$$s(u) = g(u) + (s-g)^{**}(g, u) = g(u) + \varphi_g^*(u)$$

if and only if $s-g$ is concave on $\mathbb{R}^\sigma$. Both of these are equivalent to $(s-g)(u) = (s-g)^{**}(u)$ and to $s(u) = s^{\sharp\sharp}(g, u)$.

(c) If $\text{dom}\, s$ is convex and $s-g$ is strictly concave on $\text{dom}\, s$, then φ_g is essentially smooth; in particular, φ_g is differentiable on $\mathbb{R}^\sigma$.

Theorem 4.1 is the basis for defining equivalence and nonequivalence of ensembles at the thermodynamic level. The microcanonical and canonical ensembles are said to be thermodynamically equivalent at $u \in \text{dom}\, s$ if $s(u) = s^{**}(u)$ and to be thermodynamically nonequivalent at u if $s(u) \neq s^{**}(u)$; the latter inequality holds if and only if $s(u) < s^{**}(u)$ (Propostition A.2). Similarly, the microcanonical and generalized canonical ensembles are said to be thermodynamically equivalent at u if $(s-g)(u) = (s-g)^{**}(u)$ — equivalently, $s(u) = s^{\sharp\sharp}(g, u)$ — and to be thermodynamically nonequivalent at u if $(s-g)(u) \neq (s-g)^{**}(u)$; the latter inequality holds if and only if $(s-g)(u) < (s-g)^{**}(u)$ (Proposition A.2).

The relationship between ensemble equivalence at the thermodynamic level and at the level of equilibrium macrostates is formulated in Theorem 4.2 for the microcanonical and generalized canonical ensembles. Setting $g \equiv 0$ gives the corresponding relationships between ensemble equivalence at the two levels for the microcanonical and canonical ensembles. Ensemble equivalence at the thermodynamic level involves concavity properties of $s-g$ while ensemble equivalence at the level of equilibrium macrostates involves support properties of $s-g$. Except possibly for relative boundary points, $s-g$ is concave at $u \in \text{dom}\, s$ if and only if $s-g$ has a supporting hyperplane at u. Hence if $\text{dom}\, s$ is open and so contains no relative boundary points, then the relationship between the two levels of ensemble equivalence is elegantly symmetric. This is given in part (a). In part (b) we state the less symmetric relationship between the two levels when $\text{dom}\, s$ is not open and so contains relative boundary points.

Theorem 4.2. Let g be a continuous function mapping $\mathbb{R}^\sigma$ into $\mathbb{R}$, in terms of which the generalized canonical ensemble (2.6) is defined. The choice $g \equiv 0$ gives the standard canonical ensemble. The following conclusions hold.

(a) Assume that $\text{dom}\, s$ is an open subset of $\mathbb{R}^\sigma$. Then the microncanonical and generalized canonical ensembles are thermodynamically equivalent at $u \in \text{dom}\, s$ if and only if the ensembles are either fully or partially equivalent at u.

(b) Assume that $\text{dom}\, s$ is not an open subset of $\mathbb{R}^\sigma$. If the microcanonical and generalized canonical ensembles are thermodynamically equivalent at $u \in \text{ri}(\text{dom}\, s)$, then the ensembles are either fully or partially equivalent at u. Conversely, if the ensembles are either fully or partially equivalent at $u \in \text{dom}\, s$, then the ensembles are thermodynamically equivalent at u.

Proof. (a) If $\text{dom}\, s$ is open, then since $\text{dom}\, s$ contains no relative boundary points, the sets $\text{dom}\, s$ and $ri(\text{dom}\, s)$ coincide. Hence part (a) is a consequence of part (b).

(b) If the ensembles are thermodynamically equivalent at $u \in ri(\text{dom}\, s)$, then $(s-g)(u) = (s-g)^{**}(u)$. Applying the first inclusion in part (b) of Theorem A.5 to $f = s-g$, we conclude the existence of β such that s has a supporting hyperplane at u with normal vector $[\beta, -1]$. Parts (a) and (b) of Theorem 3.4 then imply that the ensembles are either fully or partially equivalent at u. Conversely, if the ensembles are either fully or partially equivalent at $u \in \text{dom}\, s$, then by parts (a) and (b) of Theorem 3.4 there exists β such that s has a supporting hyperplane at u with normal vector $[\beta, -1]$. Applying part (a) of Theorem A.4 to $f = (s-g)$, we conclude that $(s-g)(u) = (s-g)^{**}(u)$; i.e., the ensembles are thermodynamically equivalent at u. This completes the proof. ∎

In the next section we isolate a number of scenarios arising in applications for which the microcanonical and generalized canonical ensembles are universally equivalent. This rests mainly on part (b) of Theorem 3.6, which states that universal equivalence of ensembles holds if there exists a g such that $s-g$ is strictly concave on $ri(\text{dom}\, s)$.

5. UNIVERSAL EQUIVALENCE VIA THE GENERALIZED CANONICAL ENSEMBLE

This section addresses a basic foundational issue in statistical mechanics. In Theorems 5.2–5.5, we show that when the standard canonical ensemble is nonequivalent to the microcanonical ensemble on a subset of values of u, it can often be replaced by a generalized canonical ensemble that is univerally equivalent to the microcanonical ensemble. In three of these four theorems, the function g defining the generalized canonical ensemble is a quadratic function, and the ensemble is Gaussian.

In these three theorems our strategy is to find a quadratic function g such that $s-g$ is strictly concave on $ri(\text{dom}\, s)$ and continuous on $\text{dom}\, s$. Part (b) of Theorem 3.6 then yields the universal equivalence. As Proposition 5.1 shows, an advantage of working with quadratic functions is that support properties of $s-g$ involving a supporting hyperplane are equivalent to support properties of s involving a supporting paraboloid defined in terms of g. This observation gives a geometrically intuitive way to find a quadratic function g guaranteeing universal ensemble equivalence.

In order to state the proposition, we need a definition. Let f be a function mapping $\mathbb{R}^\sigma$ into $\mathbb{R}\cup\{-\infty\}$, u and β points in $\mathbb{R}^\sigma$, and $\gamma \geqslant 0$. We say that f has a supporting paraboloid at $u \in \mathbb{R}^\sigma$ with parameters (β, γ) if

$$f(v) \leqslant f(u) + \langle \beta, v-u \rangle + \gamma \|v-u\|^2 \quad \text{for all } v \in \mathbb{R}^\sigma.$$

The paraboloid is said to be strictly supporting if the inequality is strict for all $v \neq u$.

Proposition 5.1. f has a (strictly) supporting paraboloid at u with parameters (β, γ) if and only if $f - \gamma\|\cdot\|^2$ has a (strictly) supporting hyperplane at u with normal vector $[\tilde{\beta}, -1]$. The quantities β and $\tilde{\beta}$ are related by $\tilde{\beta} = \beta - 2\gamma u$.

Proof. The proof is based on the identity $\|v-u\|^2 = \|v\|^2 - 2\langle u, v-u\rangle - \|u\|^2$. If f has a strictly supporting paraboloid at u with parameters (β, γ), then for all $v \neq u$

$$f(v) - \gamma\|v\|^2 < f(u) - \gamma\|u\|^2 + \langle \tilde{\beta}, v-u \rangle,$$

where $\tilde{\beta}=\beta-2\gamma u$. Thus $f-\gamma\|\cdot\|^2$ has a strictly supporting hyperplane at u with normal vector $[\tilde{\beta},-1]$. The converse is proved similarly, as is the case in which the supporting hyperplane or paraboloid is supporting but not strictly supporting. ∎

The first application of Theorem 3.6 is Theorem 5.2, which is formulated for dimension $\sigma=1$. The theorem gives a criterion guaranteeing the existence of a quadratic function g such that $s-g$ is strictly concave on $\operatorname{dom} s$. The criterion — that s'' is bounded above on the interior of $\operatorname{dom} s$ — is essentially optimal for the existence of a fixed quadratic function g guaranteeing the strict concavity of $s-g$. The situation in which s'' is not bounded above on the interior of $\operatorname{dom} s$ can often be handled by Theorem 5.5, which is a local version of Theorem 5.2.

The strict concavity of $s-g$ on $\operatorname{dom} s$ has several important consequences concerning universal equivalence of ensembles at the level of equilibrium macrostates and equivalence of ensembles at the thermodynamic level — i.e., $s^{\sharp\sharp}(g,u)=s(u)$ for all u. As we note in part (e) of Theorem 5.2, the strict concavity of $s-g$ also implies that the generalized canonical free energy $\varphi_g=(s-g)^*$ is differentiable on $\mathbb{R}$, a condition guaranteeing the absence of a discontinuous, first-order phase transition with respect to the Gaussian ensemble.

Theorem 5.3 is the analog of Theorem 5.2 that treats arbitrary dimension $\sigma\geqslant 2$. When $\sigma\geqslant 2$, in general the results are weaker than when $\sigma=1$.

Theorem 5.2. Assume that the dimension $\sigma=1$ and that $\operatorname{dom} s$ is a nonempty interval. Assume also that s is continuous on $\operatorname{dom} s$, s is twice continuously differentiable on $\operatorname{int}(\operatorname{dom} s)$, and s'' is bounded above on $\operatorname{int}(\operatorname{dom} s)$. Then for all sufficiently large $\gamma\geqslant 0$ and $g(u)=\gamma u^2$, conclusions (a)–(e) hold. Specifically, if s is strictly concave on $\operatorname{dom} s$, then we choose any $\gamma\geqslant 0$, and otherwise we choose

$$\gamma>\gamma_0=\frac{1}{2}\cdot\sup_{u\in\operatorname{int}(\operatorname{dom} s)} s''(u). \tag{5.1}$$

(a) $s-g$ is strictly concave and continuous on $\operatorname{dom} s$.

(b) $s-g$ has a strictly supporting line, and s has a strictly supporting paraboloid, at all $u\in\operatorname{dom} s$ except possibly boundary points. At a boundary point $s-g$ has a strictly supporting line, and s has a strictly supporting parabola, if and only if the one-sided derivative of $s-g$ is finite at that boundary point.

(c) The microcanonical and Gaussian ensembles defined in terms of this g are universally equivalent; i.e., fully equivalent at all $u\in\operatorname{dom} s$

except possibly boundary points. For all $u \in$ int(dom s) the value of β defining the universally equivalent Gaussian ensemble is unique and is given by $\beta = s'(u) - 2\gamma u$.

(d) For all $u \in \mathbb{R}$, $s^{\sharp\sharp}(g, u) = s(u)$ or equivalently $(s - g)^{**}(u) = (s - g)(u)$.

(e) The generalized canonical free energy $\varphi_g = (s - g)^*$ is essentially smooth; in particular, φ_g is differentiable on $\mathbb{R}$.

Proof. (a) If s is strictly concave on $\text{dom}\, s$, then $s(u) - \gamma u^2$ is also strictly concave on this set for any $\gamma \geqslant 0$. We now consider the case in which s is not strictly concave on $\text{dom}\, s$. If $g(u) = \gamma u^2$, then $s - g$ is continuous on $\text{dom}\, s$. If, in addition, we choose $\gamma > \gamma_0$ in accordance with (5.1), then for all $u \in \text{int}(\text{dom}\, s)$

$$(s - g)''(u) = s''(u) - 2\gamma < 0.$$

A straightforward extension of the proof of Theorem 4.4 in ref. 47, in which the inequalities in the first two displays are replaced by strict inequalities, shows that $-(s - g)$ is strictly convex on $\text{int}(\text{dom}\, s)$ and thus that $s - g$ is strictly concave on $\text{int}(\text{dom}\, s)$. If $s - g$ is not strictly concave on $\text{dom}\, s$, then $s - g$ must be affine on an interval. Since this violates the strict concavity on $\text{int}(\text{dom}\, s)$, part (a) is proved.

(b) The first assertion follows from part (a) of the present theorem, part (a) of Theorem 3.6, and Proposition 5.1. Concerning the second assertion about boundary points, the reader is referred to the discussion before Theorem 3.3.

(c) The universal equivalence of the two ensembles is a consequence of part (a) of the present theorem and part (b) of Theorem 3.6. The full equivalence of the ensembles at all $u \in \text{int}(\text{dom}\, s)$ is equivalent to the existence of a strictly supporting hyperplane at all $u \in \text{int}(\text{dom}\, s)$ with supergradient β (Theorem 3.4(a)). Since $s(u) - \gamma u^2$ is differentiable at all $u \in \text{int}(\text{dom}\, s)$, part (b) of Theorem A.1 implies that β is unique and $\beta = (s(u) - \gamma u^2)'$.

(d) The strict concavity of $s - g$ on $\text{dom}\, s$ proved in part (a) implies that $s - g$ is concave on $\mathbb{R}$. Part (b) of Theorem 4.1 allows us to conclude that for all $u \in \mathbb{R}$, $s^{\sharp\sharp}(g, u) = s(u)$ or equivalently $(s - g)^{**}(u) = (s - g)(u)$.

(e) This follows from part (c) of Theorem 4.1. ∎

We now consider the analogue of Theorem 5.2 for arbitrary dimension $\sigma \geqslant 2$. In contrast to the case $\sigma = 1$, in which $s - g$ could always be extended to a strictly concave function on all of $\text{dom}\, s$, in the case $\sigma \geqslant 2$ there exists a quadratic g such that $s-g$ is strictly concave on the interior of $\text{dom}\, s$, but in general $s-g$ cannot be extended to a strictly concave function on all of $\text{dom}\, s$. One can easily find examples in which the boundary of $\text{dom}\, s$ has flat portions and $s-g$ is strictly concave on the interior of $\text{dom}\, s$ and constant on these flat portions. As a result, unless $\text{dom}\, s$ is open, we cannot apply part (c) of Theorem 4.1 to conclude that the generalized canonical free energy $\varphi_g = (s-g)^*$ is differentiable on $\mathbb{R}^\sigma$.

Theorem 5.3. Assume that the dimension $\sigma \geqslant 2$ and that $\text{dom}\, s$ is convex and has nonempty interior. Assume also that s is continuous on $\text{dom}\, s$, s is twice continuously differentiable on $\text{int}(\text{dom}\, s)$, and all second-order partial derivatives of s are bounded above on $\text{int}(\text{dom}\, s)$. Then for all sufficiently large $\gamma \geqslant 0$ and $g(u) = \gamma \|u\|^2$, conclusions (a)–(e) hold. Specifically, if s is strictly concave on $\text{int}(\text{dom}\, s)$, then we choose any $\gamma \geqslant 0$, and otherwise we choose

$$\gamma > \gamma_0 = \frac{1}{2} \cdot \sup_{u \in \text{int}(\text{dom}\, s)} \kappa(u), \tag{5.2}$$

where $\kappa(u)$ denotes the largest eigenvalue of the symmetric Hessian matrix of s at u.

(a) $s-g$ is strictly concave on int $(\text{dom}\, s)$ and concave and continuous on $\text{dom}\, s$.

(b) $s-g$ has a strictly supporting hyperplane, and s has a strictly supporting paraboloid, at all $u \in \text{dom}\, s$ except possibly boundary points.

(c) The microcanonical and Gaussian ensembles defined in terms of this g are universally equivalent; i.e., fully equivalent at all $u \in \text{dom}\, s$ except possibly boundary points. For all $u \in \text{int}(\text{dom}\, s)$ the value of β defining the universally equivalent Gaussian ensemble is unique and is given by $\beta = \nabla s(u) - 2\gamma u$.

(d) For all $u \in \mathbb{R}^\sigma$, $s^{\sharp\sharp}(g, u) = s(u)$ or equivalently $(s-g)^{**}(u) = (s-g)(u)$.

(e) Assume that $\text{dom}\, s$ is open. Then the generalized canonical free energy $\varphi_g = (s-g)^*$ is essentially smooth; in particular, φ_g is differentiable on $\mathbb{R}^\sigma$.

Proof. (a) If s is strictly concave on $\text{int}(\text{dom}\, s)$, then $s - \gamma \|\cdot\|^2$ is also strictly concave on this set for any $\gamma \geqslant 0$. We now consider the case in which s is not strictly concave on $\text{int}(\text{dom}\, s)$. If $g(u) = \gamma \|u\|^2$, then $s-g$ is continuous on $\text{dom}\, s$. For $u \in \text{int}(\text{dom}\, s)$, let $Q_u = \{\partial^2 s(u)/\partial u_i \partial u_j\}$ denote the Hessian matrix of s at u. We choose $\gamma > \gamma_0$ in accordance with (5.2), noting that

$$\gamma_0 = \frac{1}{2} \cdot \sup_{u \in \text{int}(\text{dom}\, s)} \kappa(u) \\ = \frac{1}{2} \cdot \sup_{u \in \text{int}(\text{dom}\, s)} \sup\big\{\langle Q_u \zeta, \zeta \rangle : \zeta \in \mathbb{R}^\sigma, \|\zeta\| = 1\big\}. \tag{5.3}$$

Let I be the identity matrix. It follows that for any $u \in \text{int}(\text{dom}\, s)$ and all nonzero $z \in \mathbb{R}^\sigma$

$$\langle (Q_u - 2\gamma I)z, z \rangle < 0.$$

By analogy with the proof of Theorem 4.5 in ref. 47, the strict concavity of $s - g$ on $\text{int}(\text{dom}\, s)$ is equivalent to the strict concavity of $s - g$ on each line segment in $\text{int}(\text{dom}\, s)$. This, in turn, is equivalent to the strict concavity, for each $v \in \text{int}(\text{dom}\, s)$ and nonzero $z \in \mathbb{R}^\sigma$, of $\psi(\lambda) = (s - g)(v + \lambda z)$ on the open interval $G(v, z) = \{\lambda \in \mathbb{R} : v + \lambda z \in \text{int}(\text{dom}\, s)\}$. Since

$$\psi''(\lambda) = \langle (Q_{v+\lambda z} - 2\gamma I)z, z \rangle < 0,$$

ψ' is strictly decreasing on $G(v, z)$. A straightforward extension of the proof of Theorem 4.4 in ref. 47, in which the inequalities in the first two displays are replaced by strict inequalities, shows that $-\psi$ is strictly convex on $G(v, z)$ and thus that ψ is strictly concave on $G(v, z)$. It follows that $s - g$ is strictly concave on $\text{int}(\text{dom}\, s)$. By Proposition A.3 the continuity of $s - g$ on $\text{dom}\, s$ allows us to extend the strict concavity of $s - g$ on $\text{int}(\text{dom}\, s)$ to the concavity of $s - g$ on $\text{dom}\, s$. This completes the proof of part (a).

(b)–(d) These are proved as in Theorem 5.2.

(e) If $\text{dom}\, s$ is open, then part (a) implies that $s - g$ is strictly concave on $\text{dom}\, s$. The essential smoothness of $(s - g)^*$, and thus its differentiability, are consequences of part (c) of Theorem 4.1. ∎

In the next theorem we give other conditions on s guaranteeing conclusions similar to those in Theorems 5.2 and 5.3.

Theorem 5.4. Assume that $\text{dom}\, s$ is convex, closed, and bounded and that s is bounded and continuous on $\text{dom}\, s$. Then there exists a continuous function g mapping $\mathbb{R}^\sigma$ into $\mathbb{R}$ such that the following conclusions hold.

(a) $s-g$ is strictly concave and continuous on $\operatorname{dom} s$, and the generalized canonical free energy $\varphi_g = (s-g)^*$ is essentially smooth; in particular, φ_g is differentiable on $\mathbb{R}^\sigma$.

(b) $s-g$ has a strictly supporting hyperplane at all $u \in \operatorname{dom} s$ except possibly relative boundary points.

(c) The microcanonical and generalized canonical ensembles defined in terms of this g are universally equivalent; i.e., fully equivalent at all $u \in \operatorname{dom} s$ except possibly relative boundary points.

(d) For all $u \in \mathbb{R}^\sigma$, $s^{\sharp\sharp}(g,u) = s(u)$ or equivalently $(s-g)^{**}(u) = (s-g)(u)$.

Proof. (a) Let h be any strictly concave function on $\mathbb{R}^\sigma$. Since h is continuous on $\mathbb{R}^\sigma$ (ref. 47, Corollary 10.1.1), h is also bounded and continuous on $\operatorname{dom} s$. For $u \in \operatorname{dom} s$ define $g(u) = s(u) - h(u)$. Since g is bounded and continuous on the closed set $\operatorname{dom} s$, the Tietze Extension Theorem guarantees that g can be extended to a bounded, continuous function on $\mathbb{R}^\sigma$ (ref. 26, Theorem 4.16). Then $s-g$ has the properties in part (a). The strict concavity of $s-g$ on $\operatorname{dom} s$ implies the essential smoothness of $(s-g)^*$ and thus its differentiability (Theorem 4.1(c)).

(b) This follows from part (a) of the present theorem and part (a) of Theorem 3.6.

(c) The universal equivalence of the two ensembles is a consequence of part (a) of the present theorem and part (b) of Theorem 3.6.

(d) The function g constructed in the proof of part (a) is bounded and continuous on $\mathbb{R}^\sigma$. In addition, $s-g$ is strictly concave on $\operatorname{dom} s$ and thus concave on $\mathbb{R}^\sigma$. Since $s-g$ is continuous on the closed set $\operatorname{dom} s$, $s-g$ is also upper semicontinuous on $\mathbb{R}^\sigma$. Part (b) of Theorem 4.1 implies that for all $u \in \mathbb{R}^\sigma$, $s^{\sharp\sharp}(g,u) = s(u)$ or equivalently $(s-g)^{**}(u) = (s-g)(u)$. ∎

Suppose that s is C^2 on the interior of $\operatorname{dom} s$ but the second-order partial derivatives of s are not bounded above. This arises, for example, in the Curie–Weiss–Potts model, in which $\operatorname{dom} s$ is a closed, bounded interval of $\mathbb{R}$ and $s''(u) \to \infty$ as u approaches the right hand endpoint of $\operatorname{dom} s$.[11] In such cases one cannot expect that the conclusions of Theorems 5.2 and 5.3 will be satisfied; in particular, that there exists a quadratic function g such that $s-g$ has a strictly supporting hyperplane at each point of the interior of $\operatorname{dom} s$ and thus that the ensembles are universally equivalent.

In order to overcome this difficulty, we introduce Theorem 5.5, a local version of Theorems 5.2 and 5.3. Theorem 5.5 handles the case in which s is C^2 on an open set K but either K is not all of int(dom s) or $K = \text{int}(\text{dom}\, s)$ and the second-order partial derivatives of s are not all bounded above on K. In neither of these situations are the hypotheses of Theorem 5.2 or 5.3 satisfied. In Theorem 5.5 additional conditions are given guaranteeing that for each $u \in K$ there exists γ depending on u such that $s - \gamma\|\cdot\|^2$ has a strictly supporting hyperplane at u. Our strategy is first to choose a paraboloid that is strictly supporting in a neighborhood of u and then to adjust γ so that the paraboloid becomes strictly supporting on all $\mathbb{R}^\sigma$. Proposition 5.1 then guarantees that $s - \gamma\|\cdot\|^2$ has a strictly supporting hyperplane at u.

This construction for each $u \in K$ implies a form of universal equivalence of ensembles that is weaker than that in Theorems 5.2 and 5.3 but is still useful. In contrast to those theorems, which state that $s^{\sharp\sharp}(g,u) = s(u)$ for all $u \in \mathbb{R}^\sigma$, in Theorem 5.5 we prove the alternative representation $\inf_{\gamma \geqslant 0} s^{\sharp\sharp}(g_\gamma, u) = s(u)$ for all u in K, where $g_\gamma = \gamma\|\cdot\|^2$ for $\gamma \geqslant 0$. This alternative representation is necessitated by the fact that the quadratic depends on u.

For each fixed $u \in K$ the value of γ for which $s - \gamma\|\cdot\|^2$ has a strictly supporting hyperplane at u depends on u. However, with the same γ one might also have a strictly supporting hyperplane at other values of u. In general, as one increases γ, the set of u at which $s - \gamma\|\cdot\|^2$ has a strictly supporting hyperplane cannot decrease. Because of part (a) of Theorem 3.4, this can be restated in terms of ensemble equivalence involving the Gaussian ensemble and the corresponding set $\mathcal{E}(\gamma)_\beta$ of equilibrium macrostates defined in (1.2.5). Defining

$$U_\gamma = \{u \in K : \text{there exists } \beta \text{ such that } \mathcal{E}(\gamma)_\beta = \mathcal{E}^u\},$$

we have $U_{\gamma_1} \subset U_{\gamma_2}$ whenever $\gamma_2 > \gamma_1$ and because of Theorem 5.5, $\bigcup_{\gamma>0} U_\gamma = K$. This phenomenon is investigated in detail in ref. 12 for the Curie-Weiss-Potts model.

In order to state Theorem 5.5, we define for $u \in K$ and $\lambda \geqslant 0$

$$D(u, \nabla s(u), \lambda) = \left\{ v \in \text{dom}\, s : s(v) \geqslant s(u) + \langle \nabla s(u), v - u \rangle + \lambda \|v - u\|^2 \right\}.$$

Geometrically, this set contains all points for which the paraboloid with parameters $(\nabla s(u), \lambda)$ passing through $(u, s(u))$ lies below the graph of s. Clearly, since $\lambda \geqslant 0$, we have $D(u, \nabla s(u), \lambda) \subset D(u, \nabla s(u), 0)$; the set $D(u, \nabla s(u), 0)$ contains all points for which the graph of the hyperplane with normal vector $[\nabla s(u), -1]$ passing through $(u, s(u))$ lies below the graph of s. Thus, in the next theorem the hypothesis that for each $u \in K$

the set $D(u, \nabla s(u), \lambda)$ is bounded for some $\lambda \geqslant 0$ is satisfied if $\operatorname{dom} s$ is bounded or, more generally, if $D(s, \nabla s(u), 0)$ is bounded. The latter set is bounded if, for example, $-s$ is superlinear; i.e.,

$$\lim_{\|v\| \to \infty} s(v)/\|v\| = -\infty.$$

As we have remarked, the next theorem can often be applied when the hypotheses of Theorem 5.2 or 5.3 are not satisfied.

Theorem 5.5. Let K an open subset of $\operatorname{dom} s$ and assume that s is twice continuously differentiable on K. Assume also that $\operatorname{dom} s$ is bounded or, more generally, that for every $u \in \operatorname{int} K$ there exists $\lambda \geqslant 0$ such that $D(u, \nabla s(u), \lambda)$ is bounded. The following conclusions hold.

(a) For each $u \in K$, define $\gamma_0(u) \geqslant 0$ by (5.7). Then for any $\gamma > \gamma_0(u)$, s has a strictly supporting paraboloid at u with parameters $(\nabla s(u), \gamma)$.

(b) For each $u \in K$ we choose $\gamma > \gamma_0(u)$ as in part (a) and define $g_\gamma = \gamma \|\cdot\|^2$. Then $s - g_\gamma$ has a strictly supporting hyperplane at u with normal vector $[\nabla s(u) - 2\gamma u, -1]$.

(c) For each $u \in K$

$$\inf_{\gamma \geqslant 0} s^{\sharp\sharp}(g_\gamma, u) = \inf_{\gamma \geqslant 0} \{g_\gamma(u) + (s - g_\gamma)^{**}(u)\} = s(u).$$

(d) For each $u \in K$ choose $g = \gamma \|\cdot\|^2$ such that, in accordance with part (b), $s - g$ has a strictly supporting hyperplane at u. Then the microcanonical and Gaussian ensembles defined in terms of this g are fully equivalent at u. The value of β defining the Gaussian ensemble is unique and is given by $\beta = \nabla s(u) - 2\gamma u$.

Proof. (a) Given $u \in K$, let $B(u, r) \subset K$ be an open ball with center u and positive radius r whose closure is contained in K. If the dimension $\sigma = 1$, then s'' is bounded above on $B(u, r)$, while if $\sigma \geqslant 2$, then all second-order partial derivatives of s are bounded above on $B(u, r)$. We now apply, to the restriction of s to $B(u, r)$, part (a) of Theorem 5.2 when $\sigma = 1$ and part (a) of Theorem 5.3 when $\sigma \geqslant 2$. We conclude that there exists a sufficiently large $A \geqslant 0$ such that $s - A\|\cdot\|^2$ is strictly concave on $B(u, r)$. Part (c) of Theorem A.4 implies that when restricted to $B(u, r)$, $s - A\|\cdot\|^2$ has a strictly supporting hyperplane at u; that is, there exists $\theta \in \mathbb{R}^\sigma$ such that

$$s(v) - A\|v\|^2 < s(u) - A\|u\|^2 + \langle \theta, v - u \rangle \quad \text{for all } v \in B(u, r), v \neq u. \tag{5.4}$$

In fact, $\theta = \nabla s(u) - 2Au$ because $s - A\|\cdot\|^2$ is concave and differentiable on $B(u,r)$ (Theorem A.1(b)). We rewrite the inequality in the last display as

$$s(v) < s(u) + \langle \nabla s(u), v-u \rangle + A\|v-u\|^2 \quad \text{for all } v \in B(u,r), v \neq u. \tag{5.5}$$

This inequality continues to hold if we take larger values of A, and so without loss of generality we can assume that $A > \lambda$. Because $s(v) = -\infty$ for $v \notin \operatorname{dom} s$, the set where the inequality in the last display does not hold is $D(u, \nabla s(u), A)$. Since $A > \lambda$, we have $D(u, \nabla s(u), A) \subset D(u, \nabla s(u), \lambda)$, and since the latter set is assumed to be bounded, there exists $b \in (0, \infty)$ such that

$$D(u, \nabla s(u), A) \subset \{v \in \mathbb{R}^\sigma : \|v-u\| < b\}. \tag{5.6}$$

Let γ be any number satisfying

$$\gamma > \gamma_0(u) = \max\left\{A, \frac{-s(u) + \|\nabla s(u)\|b}{r^2}\right\}. \tag{5.7}$$

Since $A \geqslant 0$, it follows that $\gamma_0(u) \geqslant 0$. We now prove that s has a strictly supporting paraboloid at u with parameters $(\nabla s(u), \gamma)$; i.e.,

$$s(v) < s(u) + \langle \nabla s(u), v-u \rangle + \gamma\|v-u\|^2 \quad \text{for all } v \in \mathbb{R}^\sigma, v \neq u. \tag{5.8}$$

It suffices to prove (5.8) for all $v \in \operatorname{dom} s$. Since $\gamma > A$ and since (5.5) is valid for all $v \in B(u,r)$, $v \neq u$, (5.8) is also valid for all $v \in B(u,r)$, $v \neq u$. In addition, for all $v \in \operatorname{dom} s \setminus D(u, \nabla s(u), A)$

$$\begin{aligned} s(v) &< s(u) + \langle \nabla s(u), v-u \rangle + A\|v-u\|^2 \\ &\leqslant s(u) + \langle \nabla s(u), v-u \rangle + \gamma\|v-u\|^2 \end{aligned}$$

and so (5.8) is also valid for all such v. We finally show that (5.8) is valid for all $v \in D(u, \nabla s(u), A) \setminus B(u,r)$. This follows from the string of inequalities:

$$\begin{aligned} & s(u) + \langle \nabla s(u), v-u \rangle + \gamma\|v-u\|^2 \\ &\quad > s(u) + \langle \nabla s(u), v-u \rangle + \gamma r^2 \\ &\quad > s(u) - \|\nabla s(u)\|b - s(u) + \|\nabla s(u)\|b \\ &\quad = 0 \\ &\quad \geqslant s(v). \end{aligned}$$

By proving that (5.8) is valid for all $v \in \mathbb{R}^\sigma$, we have completed the proof of part (a).

(b) This follows from part (a) of the present theorem and Proposition 5.1.

(c) By part (b), for each $u \in K$ and any $\tilde{\gamma} > \gamma_0$, $s - g_{\tilde{\gamma}}$ has a strictly supporting hyperplane, and thus a supporting hyperplane, at u. We now apply to $s - g_{\tilde{\gamma}}$ part (a) of Theorem A.4, obtaining $(s - g_{\tilde{\gamma}})^{**}(u) = (s - g_{\tilde{\gamma}})(u)$ or

$$s(u) = g_{\tilde{\gamma}}(u) + (s - g_{\tilde{\gamma}})^{**}(u).$$

Since for any $\gamma \geqslant 0$, $(s - g_\gamma)^{**}(u) \geqslant (s - g_\gamma)(u)$ (Proposition A.2), it follows from (4.2) that

$$s(u) = \inf_{\gamma \geqslant 0} \{g_\gamma(u) + (s - g_\gamma)^{**}(u)\} = \inf_{\gamma \geqslant 0} s^{\sharp\sharp}(g_\gamma, u).$$

(d) Fix $u \in K$ and let $B(u, r)$ be an open ball with center u and radius r whose closure is contained in K. The full equivalence of the ensembles follows from part (b) of the present theorem and part (a) of Theorem 3.4. The value of β defining the fully equivalent Gaussian ensemble is characterized by the property that $[\beta, -1]$ is the normal vector to a strictly supporting hyperplane for $s - \gamma \|\cdot\|^2$ at u. In order to identify β, we consider the convex function h that equals $s - \gamma \|\cdot\|^2$ on the open ball $B(u, r)$ and equals $-\infty$ on the complement. Since h is differentiable at u, part (b) of Theorem A.1 implies that β is unique and equals $\nabla h(u) = \nabla(s - \gamma \|\cdot\|^2)(u)$. This completes the proof. ∎

Theorem 5.5 suggests an extended form of the notion of universal equivalence of ensembles. In Theorems 5.2–5.4 we are able to achieve full equivalence of ensembles for all $u \in \operatorname{dom} s$ except possibly relative boundary points by choosing an appropriate g that is valid for all u. This leads to the observation in each theorem that the microcanonical and generalized canonical ensembles defined in terms of this g are universally equivalent. In Theorem 5.5 we can also achieve full equivalence of ensembles for all $u \in K$. However, in contrast to Theorems 5.2–5.4, the choice of g for which the two ensembles are fully equivalent depends on u. We summarize the ensemble equivalence property articulated in part (d) of Theorem 5.5 by saying that relative to the set of quadratic functions, the microcanonical and Gaussian ensembles are universally equivalent on the open set K of energy values.

We complete our discussion of the generalized canonical ensemble and its equivalence with the microcanonical ensemble by noting that the smoothness hypothesis on s in Theorem 5.5 is essentially satisfied whenever the microcanonical ensemble exhibits no phase transition at any $u \in K$. In order to see this, we recall that a point u_c at which s is not differentiable represents a first-order, microcanonical phase transition (ref. 23, Fig. 3). In addition, a point u_c at which s is differentiable but not twice differentiable represents a second-order, microcanonical phase transition (ref. 23, Fig. 4). It follows that s is smooth on any open set K not containing such phase-transition points. Hence, if the other conditions in Theorem 5.5 are valid, then the microcanonical and Gaussian ensembles are universally equivalent on K relative to the set of quadratic functions. In particular, if the microcanonical ensemble exhibits no phase transitions, then s is smooth on all of int(dom s). This implies the universal equivalence of the two ensembles provided that the other conditions are valid in Theorem 5.2 if $\sigma = 1$ or in Theorem 5.3 if $\sigma \geqslant 2$.

APPENDIX A: MATERIAL ON CONCAVE FUNCTIONS

This appendix contains a number of technical results on concave functions needed in the main body of the paper. The theory of concave functions, rather than that of convex functions, is the natural setting for statistical mechanics. This is convincingly illustrated by the main theme of this paper, which is that concavity and strict concavity properties of the microcanonical entropy are closely related to the equivalence and nonequivalence of the microcanonical and canonical ensembles.

Let σ be a positive integer. A function f on $\mathbb{R}^\sigma$ is said to be concave on $\mathbb{R}^\sigma$, or concave, if $-f$ is a proper convex function in the sense of ref. 47, p. 24; that is, f maps $\mathbb{R}^\sigma$ into $\mathbb{R} \cup \{-\infty\}$, $f \not\equiv -\infty$, and for all u and v in $\mathbb{R}^\sigma$ and all $\lambda \in (0, 1)$

$$f(\lambda u + (1-\lambda)v) \geqslant \lambda f(u) + (1-\lambda) f(v).$$

Given $f \not\equiv -\infty$ a function mapping $\mathbb{R}^\sigma$ into $\mathbb{R} \cup \{-\infty\}$, we define dom f to be the set of $u \in \mathbb{R}^\sigma$ for which $f(u) > -\infty$. Let β be a point in $\mathbb{R}^\sigma$. The function f is said to have a supporting hyperplane at $u \in \mathrm{dom}\, f$ with normal vector $[\beta, -1]$ if

$$f(v) \leqslant f(u) + \langle \beta, v - u \rangle \quad \text{for all } v \in \mathbb{R}^\sigma.$$

It follows from this inequality that $u \in \mathrm{dom}\, f$. In addition, f is said to have a strictly supporting hyperplane at $u \in \mathrm{dom}\, f$ with normal vector $[\beta, -1]$ if the inequality in the last display is strict for all $v \neq u$.

Two useful facts for concave functions on $\mathbb{R}^\sigma$ are given in the next theorem. They are proved in Theorems 23.4 and 25.1 in ref. 47. The quantities appearing in Theorem A.1 are defined after Corollary 3.2.

Theorem A.1. Let f be a concave function on $\mathbb{R}^\sigma$. The following conclusions hold.

(a) $\mathrm{ri}(\mathrm{dom}\, f) \subset \mathrm{dom}\, \partial f \subset \mathrm{dom}\, f$.

(b) If f is differentiable at $u \in \mathrm{dom}\, f$, then $\nabla f(u)$ is the unique supergradient of f at u.

Let $f \not\equiv -\infty$ be a function mapping $\mathbb{R}^\sigma$ into $\mathbb{R} \cup \{-\infty\}$. For β and u in $\mathbb{R}^\sigma$ the Legendre-Fenchel transforms f^* and f^{**} are defined in ref. 47, p. 308 by the formulas

$$f^*(\beta) = \inf_{u \in \mathbb{R}^\sigma} \{\langle \beta, u\rangle - f(u)\} \quad \text{and} \quad f^{**}(u) = \inf_{\beta \in \mathbb{R}^\sigma} \{\langle \beta, u\rangle - f^*(\beta)\}.$$

As in the case of convex functions (ref. 17, Theorem VI.5.3), f^* is concave and upper semicontinuous on $\mathbb{R}^\sigma$ and for all $u \in \mathbb{R}^\sigma$ we have $f^{**}(u) = f(u)$ if and only if f is concave and upper semicontinuous on $\mathbb{R}^\sigma$. When f is not concave and upper semicontinuous, the relationship between f and f^{**} is given in the next proposition.

Proposition A.2. Let $f \not\equiv -\infty$ be a function mapping $\mathbb{R}^\sigma$ into $\mathbb{R} \cup \{-\infty\}$. If f is not concave and upper semicontinuous on $\mathbb{R}^\sigma$, then f^{**} is the smallest concave, upper semicontinuous function on $\mathbb{R}^\sigma$ that satisfies $f^{**}(u) \geqslant f(u)$ for all $u \in \mathbb{R}^\sigma$. In particular, if for some u, $f(u) \neq f^{**}(u)$, then $f(u) < f^{**}(u)$.

Proof. For any u and β in $\mathbb{R}^\sigma$ we have $f(u) \leqslant \langle \beta, u\rangle - f^*(\beta)$ and thus

$$f(u) \leqslant \inf_{\beta \in \mathbb{R}^\sigma} \{\langle \beta, u\rangle - f^*(\beta)\} = f^{**}(u).$$

If φ is any concave, upper semicontinuous function satisfying $\varphi(u) \geqslant f(u)$ for all u, then $\varphi^*(\beta) \leqslant f^*(\beta)$ for all β, and so $\varphi^{**}(u) = \varphi(u) \geqslant f^{**}(u)$ for all u. ∎

Let $f \not\equiv -\infty$ be a function mapping $\mathbb{R}^\sigma$ into $\mathbb{R} \cup \{-\infty\}$, u a point in $\mathrm{dom}\, f$, and K a convex subset of $\mathrm{dom}\, f$. Since f^{**} is concave on $\mathbb{R}^\sigma$, the first three of the following four definitions are consistent with Proposition A.2: f is concave at u if $f(u) = f^{**}(u)$; f is not concave at u if

$f(u) < f^{**}(u)$; f is concave on K if f is concave at all $u \in K$; and f is strictly concave on K if for all $u \neq v$ in K and all $\lambda \in (0,1)$

$$f(\lambda u + (1-\lambda)v) > \lambda f(u) + (1-\lambda) f(v).$$

The next proposition gives a useful extension property of strictly concave functions.

Proposition A.3. Assume that $\operatorname{dom} f$ is convex and that f is strictly concave on $\operatorname{ri}(\operatorname{dom} f)$ and continuous on $\operatorname{dom} f$. Then f is concave on $\operatorname{dom} f$ and on $\mathbb{R}^\sigma$.

Proof. Any point in $\operatorname{dom} f \setminus \operatorname{int}(\operatorname{dom} f)$ is the limit of a sequence of points in $\operatorname{ri}(\operatorname{dom} f)$ (ref. 47, Theorem 6.1). Hence by the continuity of f on $\operatorname{dom} f$, the strict concavity inequality for all $u \neq v$ in $\operatorname{ri}(\operatorname{dom} f)$ can be extended to a nonstrict inequality for all u and v in $\operatorname{dom} f$. Hence f is convex on $\operatorname{dom} f$. Since f equals $-\infty$ on the complement of $\operatorname{dom} f$, it also follows that f is convex on $\mathbb{R}^\sigma$. ∎

Parts (a) and (c) of the next theorem are fundamental in this paper because they relate concavity and support properties of functions f on $\mathbb{R}^\sigma$. When applied to the microcanonical entropy s and to $s-g$, where g is a continuous function defining the generalized canonical ensemble, part (c) of Theorem A.4 allows us to deduce, from strict concavity properties of s and $s-g$, universal equivalence properties involving the canonical ensemble and the generalized canonical ensemble.

Theorem A.4. Let $f \not\equiv -\infty$ be a function mapping $\mathbb{R}^\sigma$ into $\mathbb{R} \cup \{-\infty\}$. The following conclusions hold:

(a) f has a supporting hyperplane at $u \in \operatorname{dom} f$ with normal vector $[\beta, -1]$ if and only if $f(u) = f^{**}(u)$ and $\beta \in \partial f^{**}(u)$.

(b) Assume that f has a supporting hyperplane at $u \in \operatorname{dom} f$ with normal vector $[\beta, -1]$. If f is differentiable at u and $f = f^{**}$ in a neighborhood of u, then β is unique and $\beta = \nabla f(u)$.

(c) Assume that $\operatorname{dom} f$ is convex and that f is strictly concave on $\operatorname{ri}(\operatorname{dom} f)$ and continuous on $\operatorname{dom} f$. Then f has a strictly supporting hyperplane at all $u \in \operatorname{dom} f$ except possibly relative boundary points. In particular, if $\operatorname{dom} f$ is relatively open, then f has a strictly supporting hyperplane at all $u \in \operatorname{dom} f$.

Proof. (a) This is proved in part (a) of Lemma 4.1 in ref. 18 when $f = s$. The same proof applies to general f.

(b) If f has a supporting hyperplane at $u \in \text{dom}\, f$ with normal vector $[\beta, -1]$, then by part (a), $\beta \in \partial f^{**}(u)$. If in addition f is differentiable at u and $f = f^{**}$ in a neighborhood of u, then f^{**} is also differentiable at u and $\nabla f^{**}(u) = \nabla f(u)$. The conclusion that β is unique and $\beta = \nabla f(u)$ then follows from part (b) of Theorem A.1 applied to f^{**}.

(c) By Proposition A.3 the assumptions on f guarantee that f is concave on $\mathbb{R}^\sigma$. Since ri(dom f) $\subset \text{dom}\, \partial f$ (Theorem A.1(a)), for any $u \in$ ri(dom f) and any $\beta \in \partial f(u)$, f has a supporting hyperplane at u with normal vector $[\beta, -1]$; i.e.,

$$f(v) \leqslant f(u) + \langle \beta, v - u \rangle \quad \text{for all } v \in \mathbb{R}^\sigma. \tag{A.1}$$

If this hyperplane is not a strictly supporting hyperplane, then there exists $v_0 \neq u$ such that

$$f(v_0) = f(u) + \langle \beta, v_0 - u \rangle. \tag{A.2}$$

Thus $v_0 \in \text{dom}\, f$. We claim that f is strictly concave on ri(dom f) $\cup \{v_0\}$. If not, then f must be affine on a line segment containing v_0. Since this violates the strict concavity of f on ri(dom f), the claim is proved. Hence for all $\lambda \in (0, 1)$

$$\lambda f(u) + (1 - \lambda) f(v_0) < f(\lambda u + (1 - \lambda) v_0).$$

Substituting (A.2) gives

$$f(u) + (1 - \lambda)\langle \beta, v_0 - u \rangle < f(\lambda u + (1 - \lambda) v_0). \tag{A.3}$$

On the other hand, applying (A.1) to $v = \lambda u + (1 - \lambda) v_0$, we obtain

$$\begin{aligned} f(\lambda u + (1 - \lambda) v_0) &\leqslant f(u) + \langle \beta, \lambda u + (1 - \lambda) v_0 - u \rangle \\ &= f(u) + (1 - \lambda)\langle \beta, v_0 - u \rangle. \end{aligned}$$

This contradicts (A.3), proving that the supporting hyperplane at u with normal vector $[\beta, -1]$ is a strictly supporting hyperplane. We have proved that f has a strictly supporting hyperplane at all $u \in$ ri(dom f) except possibly for relative boundary points.

If in addition dom f is relatively open, then ri(dom f) = dom f. It follows that in this case f has a strictly supporting hyperplane at all $u \in$ dom f. This completes the proof of part (b). ∎

The next result is applied in Theorem 4.2, which relates ensemble equivalence at the thermodynamic level and at the level of equilibrium macrostates. Given $f \not\equiv -\infty$ a function mapping $\mathbb{R}^\sigma$ into $\mathbb{R} \cup \{-\infty\}$, we define

$$C(f) = \{u \in \mathbb{R}^\sigma : \exists \beta \in \mathbb{R}^\sigma \ni f(v) \leqslant f(u) + \langle \beta, v - u\rangle \; \forall v \in \mathbb{R}^\sigma\} \tag{A.4}$$

and

$$\Gamma(f) = \{u \in \mathbb{R}^\sigma : f(u) = f^{**}(u)\}. \tag{A.5}$$

$C(f)$ consists of all $u \in \mathbb{R}^\sigma$ such that f has a supporting hyperplane at u, and so if $u \in C(f)$, then $\text{dom}\, \partial f(u) \neq \emptyset$. In addition, $u \in \Gamma(f) \cap \text{dom}\, f$ if and only if f is concave at u.

Theorem A.5. Let $f \not\equiv -\infty$ be a function mapping $\mathbb{R}^\sigma$ into $\mathbb{R} \cup \{-\infty\}$. The following conclusions hold.

(a) $C(f) = \Gamma(f) \cap \text{dom}\, \partial f^{**}$. In particular, if f is concave on $\mathbb{R}^\sigma$, then $C(f) = \text{dom}\, \partial f$, and so f has a supporting hyperplane at all $u \in \text{dom}\, f$ except possibly relative boundary points.

(b) $\Gamma(f) \cap \text{ri}(\text{dom}\, f) \subset C(f) \subset \Gamma(f) \cap \text{dom}\, f$.

(c) Except possibly for relative boundary points of $\text{dom}\, f$, f has no supporting hyperplane at $u \in \text{dom}\, f$ if and only if f is not concave at u.

Proof. (a) The assertion that $C(f) = \Gamma(f) \cap \text{dom}\, \partial f^{**}$ is a consequence of part (a) of Theorem A.4. Now assume that f is concave on $\mathbb{R}^\sigma$. Then, since $f = f^{**}$, it follows that $\Gamma(f) = \mathbb{R}^\sigma$, $\text{dom}\, \partial f^{**} = \text{dom}\, \partial f$, and thus $C(f) = \text{dom}\, \partial f$. Part (a) of Theorem A.1 implies that f has a supporting hyperplane at all points in $\text{dom}\, f$ except possibly relative boundary points.

(b) If $u \in \Gamma(f) \cap \text{ri}(\text{dom}\, f)$, then $f(u) = f^{**}(u)$ and $u \in \text{ri}(\text{dom}\, f^{**})$, which in turn is a subset of $\text{dom}\, \partial f^{**}$ (Theorem A.1(a)). Hence $\Gamma(f) \cap \text{ri}(\text{dom}\, f) \subset \Gamma(f) \cap \text{dom}\, \partial f^{**}$, which by part (a) equals $C(f)$. This proves the first inclusion in part (b). To prove the second inclusion, we note that by part (a) $C(f) \subset \Gamma(f)$ and that for all $u \in C$, $f(u) > -\infty$. Thus $C(f) \subset \Gamma(f) \cap \text{dom}\, f$.

(c) If f has no supporting hyperplane at $u \in \text{ri}(\text{dom}\, f)$, then $u \notin C(f)$, and so by the first inclusion in part (b) $u \notin \Gamma(f)$; i.e., f is not concave at u. Conversely, if f is not concave at $u \in \text{dom}\, f$, then $u \notin \Gamma(f)$, and so by the second inclusion in part (b) $u \notin C(f)$; i.e., f has no supporting hyperplane at u. ∎

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REFERENCES

1. J. Barré, D. Mukamel, and S. Ruffo. Ensemble inequivalence in mean-field models of magnetism, in *Dynamics and Thermodynamics of Systems with Long Interactions*, T. Dauxois, S. Ruffo, E. Arimondo, and M. Wilkens (eds). Volume 602 of Lecture Notes in Physics (Springer-Verlag, New York, 2002). pp. 45–67.
2. J. Barré, D. Mukamel, and S. Ruffo, Inequivalence of ensembles in a system with long-range interactions, *Phys. Rev. Lett.* **87**:030601 (2001).
3. D. P. Bertsekas, *Constrained Optimization and Lagrange Multiplier Methods*, (Academic Press, New York, 1982).
4. M. Blume, V. J. Emery, and R. B. Griffiths, Ising model for the λ transition and phase separation in He^3-He^4 mixtures, *Phys. Rev. A* **4**:1071–1077 (1971).
5. E. P. Borges and C. Tsallis, Negative specific heat in a Lennard–Jones–like gas with long-range interactions, *Physica A* **305**:148–151 (2002).
6. C. Boucher, R. S. Ellis, and B. Turkington, Derivation of maximum entropy principles in two-dimensional turbulence via large deviations, *J. Statist. Phys.* **98**:1235–1278 (2000).
7. E. Caglioti, P. L. Lions, C. Marchioro, and M. Pulvirenti, A special class of stationary flows for two-dimensional Euler equations: a statistical mechanical description, *Commun. Math. Phys.* **143**:501–525 (1992).
8. M. S. S. Challa and J. H. Hetherington, Gaussian ensemble: an alternate Monte-Carlo scheme, *Phys. Rev. A* **38**:6324–6337 (1988).
9. M. S. S. Challa and J. H. Hetherington, Gaussian ensemble as an interpolating ensemble, *Phys. Rev. Lett.* **60**:77–80 (1988).
10. M. Costeniuc, *Ensemble Equivalence and Phase Transitions for General Models in Statistical Mechanics and for the Curie-Weiss-Potts Model*, PhD thesis, Univ. of Mass. Amherst, 2005.
11. M. Costeniuc, R. S. Ellis, and H. Touchette, Complete analysis of phase transitions and ensemble equivalence for the Curie-Weiss-Potts model. Accepted for publication, *J. Math. Phys.* 2005.
12. M. Costeniuc, R. S. Ellis, and H. Touchette, The Gaussian ensemble and universal ensemble equivalence for the Curie-Weiss-Potts model. In preparation, 2005.
13. T. Dauxois, V. Latora, A. Rapisarda, S. Ruffo, and A. Torcini, The Hamiltonian mean field model: from dynamics to statistical mechanics and back, in *Dynamics and Thermodynamics of Systems with Long Interactions*, T. Dauxois, S. Ruffo, E. Arimondo, and M. Wilkens (eds). Volume 602 of Lecture Notes in Physics (Springer-Verlag, New York, 2002). pp. 458–487.
14. T. Dauxois, P. Holdsworth, and S. Ruffo, Violation of ensemble equivalence in the antiferromagnetic mean-field XY model, *Eur. Phys. J. B* **16**:659 (2000).

15. J.-D. Deuschel, D. W. Stroock, and H. Zessin, Microcanonical distributions for lattice gases, *Commun. Math. Phys.* **139**:83–101 (1991).
16. P. Dupuis and R. S. Ellis, *A Weak Convergence Approach to the Theory of Large Deviations* (Wiley, New York, 1997).
17. R. S. Ellis, *Entropy, Large Deviations, and Statistical Mechanics* (Springer-Verlag, New York, 1985).
18. R. S. Ellis, K. Haven, and B. Turkington, Analysis of statistical equilibrium models of geostrophic turbulence, *J. Appl. Math. Stoch. Anal.* **15**:341–361 (2002).
19. R. S. Ellis, K. Haven, and B. Turkington, Large deviation principles and complete equivalence and nonequivalence results for pure and mixed ensembles, *J. Statist. Phys.* **101**:999–1064 (2000).
20. R. S. Ellis, K. Haven, and B. Turkington, Nonequivalent statistical equilibrium ensembles and refined stability theorems for most probable flows, *Nonlinearity* **15**:239–255 (2002).
21. R. S. Ellis, R. Jordan, P. Otto, and B. Turkington, A statistical approach to the asymptotic behavior of a generalized class of nonlinear Schrödinger equations, *Commun. Math. Phys.* **244**:187–208 (2004).
22. R. S. Ellis, P. Otto, and H. Touchette, Analysis of phase transitions in the mean-field Blume-Emery-Griffiths model, Accepted for publication in *Annals of Applied Probability*, 2005.
23. R. S. Ellis, H. Touchette, and B. Turkington, Thermodynamic versus statistical nonequivalence of ensembles for the mean-field Blume-Emery-Griffiths model, *Physica A* **335**:518–538 (2004).
24. G. L. Eyink and H. Spohn, Negative-temperature states and large-scale, long-lived vortices in two-dimensional turbulence, *J. Statist. Phys.* **70**:833–886 (1993).
25. H. Föllmer and S. Orey, Large deviations for the empirical field of a Gibbs measure, *Ann. Prob.* **16**:961–977 (1987).
26. G. B. Folland, *Real Analysis: Modern Techniques and Their Applications*, 2nd edn. (Wiley, New York, 1999).
27. H.-O. Georgii, Large deviations and maximum entropy principle for interacting random fields on $\mathbb{Z}^d$, *Ann. Probab.* **21**:1845–1875 (1993).
28. J. W. Gibbs, *Elementary Principles in Statistical Mechanics with Especial Reference to the Rational Foundation of Thermodynamics* (Yale University Press, New Haven, 1902). Reprinted by Dover, New York, 1960.
29. D. H. E. Gross, Microcanonical thermodynamics and statistical fragmentation of dissipative systems: the topological structure of the n-body phase space, *Phys. Rep.* **279**:119–202 (1997).
30. P. Hertel and W. Thirring, A soluble model for a system with negative specific heat, *Ann. Phys. (NY)* **63**:520 (1971).
31. J. H. Hetherington, Solid ^{3}He magnetism in the classical approximation, *J. Low Temp. Phys.* **66**:145–154 (1987).
32. J. H. Hetherington and D. R. Stump, Sampling a Gaussian energy distribution to study phase transitions of the Z(2) and U(1) lattice gauge theories, *Phys. Rev. D* **35**:1972–1978 (1987).
33. R. S. Johal, A. Planes, and E. Vives, Statistical mechanics in the extended Gaussian ensemble, *Phys. Rev. E* **68**:056113 (2003).
34. R. Jordan, B. Turkington, and C. L. Zirbel, A mean-field statistical theory for the nonlinear Schrödinger equation, *Physica D* **137**:353–378 (2000).
35. M. K.-H. Kiessling and J. L. Lebowitz, The micro-canonical point vortex ensemble: beyond equivalence, *Lett. Math. Phys.* **42**:43–56 (1997).

36. M. K.-H. Kiessling and T. Neukirch, Negative specific heat of a magnetically self-confined plasma torus, *Proc. Natl. Acad. Sci. USA* **100**:1510–1514 (2003).
37. V. Latora, A. Rapisarda, and C. Tsallis, Non-Gaussian equilibrium in a long-range Hamiltonian system, *Phys. Rev. E* **64**:056134 (2001).
38. J. L. Lebowitz, H. A. Rose, and E. R. Speer, Statistical mechanics of a nonlinear Schrödinger equation. II. Mean field approximation, *J. Statist. Phys.* **54**:17–56 (1989).
39. J. T. Lewis, C.-E. Pfister, and W. G. Sullivan, The equivalence of ensembles for lattice systems: some examples and a counterexample, *J. Statist. Phys.* **77**:397–419 (1994).
40. J. T. Lewis, C.-E. Pfister, and W. G. Sullivan, Entropy, concentration of probability and conditional limit theorems, *Markov Proc. Related Fields* **1**:319–386 (1995).
41. D. Lynden-Bell and R. Wood, The gravo-thermal catastrophe in isothermal spheres and the onset of red-giant structure for stellar systems, *Mon. Notic. Roy. Astron. Soc.* **138**:495 (1968).
42. J. Miller, Statistical mechanics of Euler equations in two dimensions, *Phys. Rev. Lett.* **65**:2137–2140 (1990).
43. M. Minoux, *Mathematical Programming: Theory and Algorithms* (Wiley-Interscience, Wiley, Chichester, 1986).
44. S. Olla, Large deviations for Gibbs random fields, *Probab. Th. Rel. Fields* **77**:343–359 (1988).
45. R. Robert, A maximum-entropy principle for two-dimensional perfect fluid dynamics, *J. Statist. Phys.* **65**:531–553 (1991).
46. R. Robert and J. Sommeria, Statistical equilibrium states for two-dimensional flows, *J. Fluid Mech.* **229**:291–310 (1991).
47. R. T. Rockafellar, *Convex Analysis* (Princeton University Press, Princeton, NJ, 1970).
48. S. Roelly and H. Zessin, The equivalence of equilibrium principles in statistical mechanics and some applications to large particle systems, *Expositiones Mathematicae* **11**:384–405 (1993).
49. R. A. Smith and T. M. O'Neil, Nonaxisymmetric thermal equilibria of a cylindrically bounded guiding center plasma or discrete vortex system, *Phys. Fluids B* **2**:2961–2975 (1990).
50. D. R. Stump and J. H. Hetherington, Remarks on the use of a microcanonical ensemble to study phase transitions in the lattice gauge theory, *Phys. Lett. B* **188**:359–363 (1987).
51. W. Thirring, Systems with negative specific heat, *Z. Physik* **235**:339–352 (1970).
52. H. Touchette, R. S. Ellis, and B. Turkington, An introduction to the thermodynamic and macrostate levels of nonequivalent ensembles, *Physica A* **340**:138–146 (2004).
53. F. Y. Wu, The Potts model, *Rev. Mod. Phys.* **54**:235–268 (1982).