ENSEMBLE EQUIVALENCE AND PHASE TRANSITIONS FOR GENERAL MODELS IN STATISTICAL MECHANICS AND FOR THE CURIE-WEISS-POTTS MODEL

A Dissertation Presented

by

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Submitted to the Graduate School of the
University of Massachusetts Amherst in partial fulfillment
of the requirements for the degree of

DOCTOR OF PHILOSOPHY

May 2005

Department of Mathematics and Statistics

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This dissertation is dedicated

to the memory of my father,

Professor Mircea Costeniuc.

ACKNOWLEDGMENTS

I would like to begin by thanking my advisor Richard S. Ellis, to whom I owe a deep debt of gratitude for his superb guidance, understanding, invaluable help, and great generosity and for teaching me not only about mathematics, but also about life. I would also like to thank him for his infinite kindness, for all his good advice inside and outside mathematics, and for doing so many nice things for me. Thank you for being so wonderful!

I would like to express my appreciation to Professors Bruce Turkington, Nathaniel Whitaker, and Jonathan Machta for their service on my dissertation committee. Thanks also to the Department of Mathematics and Statistics and the National Science Foundation (NSF-DMS-0202309) for providing the funding for this research. In addition, I would like to thank all the faculty, fellow graduate students, and staff who have made my time here at the University of Massachusetts so rewarding. Special thanks to Visweswaran Nageswaran for his invaluable friendship.

Lastly, I would like to express my gratitude to my family: my father Mircea, my mother Eugenia, and my sister Simona for their support, encouragement, and prayers. With all my love, I thank you.

ABSTRACT

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Using the theory of large deviations, we analyze in the first chapter the phase transition structure of the Curie-Weiss-Potts spin model, which is a mean-field approximation to the Potts model. This analysis is carried out both for the canonical ensemble and the microcanonical ensemble. Besides giving explicit formulas for the microcanonical entropy and for the equilibrium macrostates with respect to the two ensembles, we analyze ensemble equivalence and nonequivalence at the level of equilibrium macrostates, relating these to concavity and support properties of the microcanonical entropy.

In the second chapter we extend the results in [23] significantly by addressing the following motivational question. Given that the microcanonical ensemble is not equiv-

alent with the canonical ensemble, is it possible to replace the canonical ensemble with a generalized canonical ensemble that is equivalent with the microcanonical ensemble? The generalized canonical ensemble is obtained from the standard canonical ensemble 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.

As in [23], we analyze the equivalence of the two ensembles at both the level of equilibrium macrostates and the thermodynamic level. A neat but not quite precise statement of the main result in the second chapter 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 $s - g$ is concave. In order to carry out the analysis of ensemble equivalence, two forms of a generalized Legendre-Fenchel transform involving g are introduced and their properties are studied. The considerable freedom that one has in choosing g has the important consequence that even when the microcanonical and standard canonical ensembles are not equivalent, one can often find g with the property that the microcanonical and generalized canonical ensembles satisfy a strong form of equivalence which we call universal equivalence.

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CHAPTER 1

COMPLETE ANALYSIS OF PHASE TRANSITIONS AND ENSEMBLE EQUIVALENCE FOR THE CURIE-WEISS-POTTS MODEL

1.1 Introduction

The nearest-neighbor Potts model, introduced in [58], takes its place next to the Ising model as one of the most versatile models in equilibrium statistical mechanics [69]. Section I.C of [69] presents a mean-field approximation to the Potts model, defined in terms of a mean interaction averaged over all the sites in the model. We refer to this approximation as the Curie-Weiss-Potts model. Both the nearest-neighbor Potts model and the Curie-Weiss-Potts model are defined by sequences of probability distributions of n spin random variables that may occupy one of q different states $\theta^1, \ldots, \theta^q$, where $q \geq 3$. For $q = 2$ the Potts model reduces to the Ising model while the Curie-Weiss-Potts model reduces to the much simpler mean-field approximation to the Ising model known as the Curie-Weiss model [21].

Two ways in which the Curie-Weiss-Potts model approximates the Potts model, and in fact gives rigorous bounds on quantities in the Potts model, are discussed in [44] and [57]. Probabilistic limit theorems for the Curie-Weiss-Potts model are proved in

[28], including the law of large numbers and its breakdown as well as various types of central limit theorems. The model is also studied in [29], which focuses on a statistical estimation problem for two parameters defining the model.

In order to carry out the analysis of the model in [28, 29], detailed information about the structure of the set of canonical equilibrium macrostates is required, including the fact that it exhibits a discontinuous phase transition as the inverse temperature β increases through a critical value β_c. This information plays a central role in the present chapter, in which we use the theory of large deviations to study the equivalence and nonequivalence of the sets of equilibrium macrostates for the microcanonical and canonical ensembles. An important consequence of the discontinuous phase transition exhibited by the canonical ensemble in the Curie-Weiss-Potts model is the implication that the nearest-neighbor Potts model on $\mathbb{Z}^d$ also undergoes a discontinuous phase transition whenever d is sufficiently large [5, Thm. 2.1].

In [23] the problem of the equivalence of the microcanonical and canonical ensembles was completely solved for a general class of statistical mechanical models including short-range and long-range spin models and models of turbulence. This problem is fundamental in statistical mechanics because it focuses on the appropriate probabilistic description of statistical mechanical systems. While the theory developed in [23] is complete, our understanding is greatly enhanced by the insights obtained from studying specific models. In this regard the Curie-Weiss-Potts model is an excellent choice, lying at the boundary of the set of models for which a complete analysis involving explicit formulas is available.

For the Curie-Weiss-Potts model ensemble equivalence at the thermodynamic level is studied numerically in [42, §3–5]. This level of ensemble equivalence focuses on whether the microcanonical entropy is concave on its domain; equivalently, whether the microcanonical entropy and the canonical free energy, the basic thermodynamic functions in the two ensembles, can each be expressed as the Legendre-Fenchel transform of the other [23, pp. 1036–1037]. Nonconcave anomalies in the microcanonical entropy partially correspond to regions of negative specific heat and thus thermodynamic instability.

The present chapter significantly extends [42, §3–5] by analyzing rigorously ensemble equivalence at the thermodynamic level and by relating it to ensemble equivalence at the level of equilibrium macrostates via the results in [23]. As prescribed by the theory of large deviations, the set $\mathcal{E}^u$ of microcanonical equilibrium macrostates and the set $\mathcal{E}_\beta$ of canonical equilibrium macrostates are defined in (2.4) and (2.3). These macrostates are, respectively, the solutions of a constrained minimization problem involving probability vectors on $I\!R^q$ and a related, unconstrained minimization problem. The equilibrium macrostates for the two ensembles are probability vectors describing equilibrium configurations of the model in each ensemble in the thermodynamic limit $n \to \infty$. For each $i = 1, 2, \ldots, q$, the ith component of an equilibrium macrostate gives the asymptotic relative frequency of spins taking the spin-value θ^i.

Defined via conditioning on the energy per particle, the microcanonical ensemble expresses the conservation of physical quantities such as the energy. Among other reasons, the mathematically more tractable canonical ensemble was introduced by Gibbs [34] in the hope that in the $n \to \infty$ limit 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. Although most textbooks in statistical mechanics, including [1, 34, 40, 48, 59, 64], claim that the two ensembles always give the same predictions, in general this is not the case [68]. 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. Besides the

Curie-Weiss-Potts model, these models include the mean-field Blume-Emery-Griffiths model [2, 3, 27], the Hamiltonian mean-field model [16, 49], the mean-field X-Y model [15], models of turbulence [9, 24, 30, 46, 61], models of plasmas [47, 65], gravitational systems [35, 36, 37, 52, 67], and a model of the Lennard-Jones gas [7]. It is hoped that our detailed analysis of ensemble nonequivalence in the Curie-Weiss-Potts model will contribute to an understanding of this fascinating and fundamental phenomenon in a wide range of other settings.

In the present chapter, after summarizing the large deviation analysis of the Curie-Weiss-Potts model in Section 2, we give explicit formulas for the elements of $\mathcal{E}_\beta$ and the elements of $\mathcal{E}^u$ in Sections 3 and 4. This analysis shows that $\mathcal{E}_\beta$ exhibits a discontinuous phase transition at a critical inverse temperature β_c and that $\mathcal{E}^u$ exhibits a continuous phase transition at a critical energy u_c. The implications of these different phase transitions concerning ensemble nonequivalence are studied graphically in Section 5 and rigorously in Section 6, where we exhibit a range of values of the energy u for which the microcanonical equilibrium macrostates are not realized canonically; i.e., $\mathcal{E}^u$ is disjoint from $\mathcal{E}_\beta$ for all β. As described in the main theorem in [23] and summarized here in Theorem 1.5.1, this range of values of the energy is precisely the set on which the microcanonical entropy is not concave. The analysis of this bridge between ensemble nonequivalence at the thermodynamic level and ensemble nonequivalence at the level of equilibrium macrostates is one of the main contributions of [23] for general models and of the present chapter for the Curie-Weiss-Potts model. In a sequel to the present chapter [13], we will extend our analysis of the Curie-Weiss-Potts model to the so-called Gaussian ensemble [10, 11, 38, 39, 43, 66] to show, among other results, that for each value of the energy for which the microcanonical and canonical ensembles are nonequivalent, we can find a Gaussian ensemble that is fully equivalent with the microcanonical ensemble [14].

1.2 Sets of Equilibrium Macrostates for the Two Ensembles

Let $q \geq 3$ be a fixed integer and define $\Lambda = \{\theta^1, \theta^2, \ldots, \theta^q\}$, where the θ^i are any q distinct vectors in $I\!\!R^q$. In the definition of the Curie-Weiss-Potts model, the precise values of these vectors is immaterial. For each $n \in I\!\!N$ the model is defined by spin random variables $\omega_1, \omega_2, \ldots, \omega_n$ that take values in Λ. The canonical and microcanonical ensembles for the model are defined in terms of probability measures on the configuration spaces Λ^n, which consist of the microstates $\omega = (\omega_1, ..., \omega_n)$. We also introduce the n-fold product measure P_n on Λ^n with identical one-dimensional marginals

$$\bar{\rho} = \frac{1}{q} \sum_{i=1}^{q} \delta_{\theta^i}.$$

Thus for all $\omega \in \Lambda^n$, $P_n(\omega) = \frac{1}{q^n}$. For $n \in I\!\!N$ and $\omega \in \Lambda^n$ the Hamiltonian for the q-state Curie-Weiss-Potts model is defined by

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

where $\delta(\omega_j, \omega_k)$ equals 1 if $\omega_j = \omega_k$ and equals 0 otherwise. The energy per particle is defined by

$$h_n(\omega) = \frac{1}{n} H_n(\omega).$$

For inverse temperature $\beta \in I\!\!R$ and subsets B of Λ^n the canonical ensemble is the probability measure $P_{n,\beta}$ defined by

$$P_{n,\beta}\{B\} = \frac{1}{\sum_{\omega \in \Lambda^n} \exp[-n\beta h_n(\omega)]} \cdot \sum_{\omega \in B} \exp[-n\beta h_n(\omega)].$$

For energy $u \in I\!\!R$ and $r > 0$ the microcanonical ensemble is the conditioned probability measure $P_n^{u,r}$ defined by

$$P_n^{u,r}\{B\} = P_n\{B \,|\, h_n \in [u - r, u + r]\}.$$

The key to our analysis of the Curie-Weiss-Potts model is to express both the canonical and the microcanonical ensembles in terms of the empirical vector

$$L_n = L_n(\omega) = (L_{n,1}(\omega), L_{n,2}(\omega), \ldots, L_{n,q}(\omega)),$$

the ith component of which is defined by

$$L_{n,i}(\omega) = \frac{1}{n} \sum_{j=1}^{n} \delta(\omega_j, \theta^i).$$

This quantity equals the relative frequency with which $\omega_j, j \in \{1, \ldots, n\}$, equals θ^i. L_n takes values in the set of probability vectors

$$\mathcal{P} = \left\{ \nu \in I\!R^q : \nu = (\nu_1, \nu_2, \ldots, \nu_q), \text{ each } \nu_i \geq 0, \sum_{i=1}^{q} \nu_i = 1 \right\}.$$

As we will see, each probability vector in $\mathcal{P}$ represents a possible equilibrium macrostate for the model.

There is a one-to-one correspondence between $\mathcal{P}$ and the set $\mathcal{P}(\Lambda)$ of probability measures on Λ, $\nu \in \mathcal{P}$ corresponding to the probability measure $\sum_{i=1}^{q} \nu_i \delta_{\theta^i}$. The element $\rho \in \mathcal{P}$ corresponding to the one-dimensional marginal $\bar{\rho}$ of the prior measures P_n is the uniform vector having equal components $\frac{1}{q}$.

We denote by $\langle \cdot, \cdot \rangle$ the inner product on $I\!R^q$. Since

$$\sum_{i=1}^{q} \sum_{j=1}^{n} \delta(\omega_j, \xi^i) \cdot \sum_{k=1}^{n} \delta(\omega_k, \xi^i) = \sum_{j,k=1}^{n} \delta(\omega_j, \omega_k),$$

it follows that the energy per particle can be rewritten as

$$h_n(\omega) = -\frac{1}{2n^2} \sum_{j,k=1}^{n} \delta(\omega_j, \omega_k) = -\tfrac{1}{2} \langle L_n(\omega), L_n(\omega) \rangle,$$

i.e.,

$$h_n(\omega) = \tilde{H}(L_n(\omega)), \text{ where } \tilde{H}(\nu) = -\tfrac{1}{2} \langle \nu, \nu \rangle \text{ for } \nu \in \mathcal{P}. \tag{2.1}$$

We call $\tilde{H}$ the energy representation function.

We appeal to the theory of large deviations to define the sets of microcanonical equilibrium macrostates and canonical equilibrium macrostates. Sanov's Theorem states that with respect to the product measures P_n, the empirical vectors L_n satisfy the large deviation principle (LDP) on $\mathcal{P}$ with rate function given by the relative entropy $R(\cdot|\rho)$ [21, Thm. VIII.2.1]. For $\nu \in \mathcal{P}$ this is defined by

$$R(\nu|\rho) = \sum_{i=1}^{q} \nu_i \log(q\nu_i).$$

We express this LDP by the formal notation $P_n\{L_n \in d\nu\} \approx \exp[-nR(\nu|\rho)]$. The LDPs for L_n with respect to the two ensembles $P_{n,\beta}$ and $P_n^{u,r}$ in the thermodynamic limit $n \to \infty$, $r \to 0$ can be proved from the LDP for the P_n-distributions of L_n as in Theorems 2.4 and 3.2 in [23], in which minor notational changes have to be made. We express these LDPs by the formal notation

$$P_{n,\beta}\{L_n \in d\nu\} \approx \exp[-nI_\beta(\nu)] \text{ and } P_n^{u,r}\{L_n \in d\nu\} \approx \exp[-nI^u(\nu)], \qquad (2.2)$$

where for $\nu \in \mathcal{P}$

$$I_\beta(\nu) = R(\nu|\rho) - \tfrac{\beta}{2}\langle \nu, \nu \rangle - \text{const}$$

and

$$I^u(\nu) = \begin{cases} R(\nu|\rho) - \text{const} & \text{if } -\frac{1}{2}\langle \nu, \nu \rangle = u \\ \infty & \text{otherwise.} \end{cases}$$

The constants appearing in the definitions of I_β and I^u have the properties that $\inf_{\nu \in \mathcal{P}} I_\beta(\nu) = 0$ and $\inf_{\nu \in \mathcal{P}} I^u(\nu) = 0$. Thus I_β and I^u map $\mathcal{P}$ into $[0, \infty)$.

As the formulas in (2.2) suggest, if $I_\beta(\nu) > 0$ or $I^u(\nu) > 0$, then ν has an exponentially small probability of being observed in the corresponding ensemble in the thermodynamic limit. Hence it makes sense to define the corresponding sets of equilibrium macrostates to be

$$\mathcal{E}_\beta = \{\nu \in \mathcal{P} : I_\beta(\nu) = 0\} \text{ and } \mathcal{E}^u = \{\nu \in \mathcal{P} : I^u(\nu) = 0\}.$$

A rigorous justification for this is given in [23, Thm. 2.4(d)]. Using the formulas for I_β and I^u, we see that

$$\mathcal{E}_\beta = \left\{ \nu \in \mathcal{P} : \nu \text{ minimizes } R(\nu|\rho) - \tfrac{\beta}{2}\langle \nu, \nu \rangle \right\} \tag{2.3}$$

and

$$\mathcal{E}^u = \left\{ \nu \in \mathcal{P} : \nu \text{ minimizes } R(\nu|\rho) \text{ subject to } -\tfrac{1}{2}\langle \nu, \nu \rangle = u \right\}. \tag{2.4}$$

Each element ν in $\mathcal{E}_\beta$ and $\mathcal{E}^u$ describes an equilibrium configuration of the model in the corresponding ensemble in the thermodynamic limit. The ith component ν_i gives the asymptotic relative frequency of spins taking the value θ^i.

The set $\mathcal{E}^u$ is defined for all u for which the constraint in the definition of I^u is satisfied for some $\nu \in \mathcal{P}$. Otherwise, $\mathcal{E}^u$ is not defined. If $\mathcal{E}^u$ is defined, then $\mathcal{E}^u$ is nonempty; if $\mathcal{E}^u$ is not defined, then we shall set $\mathcal{E}^u = \emptyset$.

The question of equivalence of ensembles at the level of equilibrium macrostates focuses on the relationships between $\mathcal{E}^u$, defined in terms of the constrained minimization problem in (2.4), and $\mathcal{E}_\beta$, defined in terms of the related, unconstrained minimization problem in (2.3). We will focus on this question in Sections 5 and 6 after we determine the structures of $\mathcal{E}_\beta$ and $\mathcal{E}^u$ in the next two sections.

1.3 Form of $\mathcal{E}_\beta$ and Its Discontinuous Phase Transition

In this section we derive the form of the set $\mathcal{E}_\beta$ of canonical equilibrium macrostates for all $\beta \in I\!R$. This form is given in Theorem 1.3.1, which shows that with respect to the canonical ensemble the Curie-Weiss-Potts model undergoes a discontinuous phase transition at the critical inverse temperature

$$\beta_c = \frac{2(q-1)}{q-2} \log(q-1). \tag{3.1}$$

In order to describe the form of $\mathcal{E}_\beta$, we introduce the function ψ that maps $[0,1]$ into $\mathcal{P}$ and is defined by

$$\psi(w) = \left(\frac{1+(q-1)w}{q}, \frac{1-w}{q}, \ldots, \frac{1-w}{q}\right); \tag{3.2}$$

the last $q-1$ components all equal $\frac{1-w}{q}$. Recalling that ρ is the uniform vector in $\mathcal{P}$ having equal components $\frac{1}{q}$, we see that $\rho = \psi(0)$.

Theorem 1.3.1. *For $\beta > 0$ let $w(\beta)$ be the largest solution of the equation*

$$w = \frac{1-e^{-\beta w}}{1+(q-1)e^{-\beta w}}. \tag{3.3}$$

The following conclusions hold.

(a) *The quantity $w(\beta)$ is well defined and lies in $[0,1]$. It is positive, strictly increasing, and differentiable for $\beta \in (\beta_c, \infty)$ and satisfies $w(\beta_c) = \frac{q-2}{q-1}$ and $\lim_{\beta\to\infty} w(\beta) = 1$.*

(b) *For $\beta \geq \beta_c$, define $\nu^1(\beta) = \psi(w(\beta))$ and let $\nu^i(\beta)$, $i = 2, \ldots, q$, denote the points in $\mathbb{R}^q$ obtained by interchanging the first and ith components of $\nu^1(\beta)$. Then the set $\mathcal{E}_\beta$ defined in* (2.3) *has the form*

$$\mathcal{E}_\beta = \begin{cases} \{\rho\} & \text{for } \beta < \beta_c\,, \\ \{\rho, \nu^1(\beta_c), \nu^2(\beta_c), \ldots, \nu^q(\beta_c)\} & \text{for } \beta = \beta_c\,, \\ \{\nu^1(\beta), \nu^2(\beta), \ldots, \nu^q(\beta)\} & \text{for } \beta > \beta_c\,. \end{cases} \tag{3.4}$$

For $\beta \geq \beta_c$, the vectors in $\mathcal{E}_\beta$ are all distinct and each $\nu^i(\beta)$ is continuous. The vector $\nu^1(\beta_c)$ is given by

$$\nu^1(\beta_c) = \psi(w(\beta_c)) = \psi\left(\tfrac{q-2}{q-1}\right) = \left(1 - \tfrac{1}{q}, \tfrac{1}{q(q-1)}, \ldots, \tfrac{1}{q(q-1)}\right); \tag{3.5}$$

the last $q-1$ components all equal $\frac{1}{q(q-1)}$.

The form of $\mathcal{E}_\beta$ for $\beta > 0$ is proved in Section 1.8 from a new convex-duality theorem proved in Section 1.7 and from the complicated calculation of the global minimum points of a related function given in Theorem 2.1 in [28]. The form of $\mathcal{E}_\beta$ for $\beta \leq 0$ is also determined in Section 1.8. The assertions in part (b) of Theorem 1.3.1 appearing after (3.4) are proved in Theorem 2.1 in [28].

For $\beta > 0$ the form of $\mathcal{E}_\beta$ reflects a competition between disorder, as represented by the relative entropy $R(\nu|\rho)$, and order, as represented by the energy representation function $-\frac{1}{2}\langle \nu, \nu \rangle$. For small $\beta > 0$, $R(\nu|\rho)$ predominates. Since $R(\nu|\rho)$ attains its minimum of 0 at the unique vector ρ, we expect that for small β, $\mathcal{E}_\beta$ should contain a single vector. On the other hand, for large $\beta > 0$, $-\frac{1}{2}\langle \nu, \nu \rangle$ predominates. This function attains its minimum at $\nu^1 = (1, 0, \ldots, 0)$ and at the vectors ν^i, $i = 1, \ldots, q$, obtained by interchanging the first and ith components of ν^1. Hence we expect that for large β, $\mathcal{E}_\beta$ should contain q distinct vectors $\nu^i(\beta)$ having the property that $\nu^i(\beta) \to \nu^i$ as $\beta \to \infty$. The major surprise of the theorem is that for $\beta = \beta_c$, $\mathcal{E}_\beta$ consists of the $q + 1$ distinct vectors ρ and $\nu^i(\beta_c)$ for $i = 1, 2, \ldots, q$.

The discontinuous bifurcation in the composition of $\mathcal{E}_\beta$ from 1 vector for $\beta < \beta_c$ to $q + 1$ vectors for $\beta = \beta_c$ to q vectors for $\beta > \beta_c$ corresponds to a discontinuous phase transition exhibited by the canonical ensemble. In Figure 2 in Section 5 this phase transition is shown together with the continuous phase transition exhibited by the microcanonical ensemble. The latter phase transition and the form of the set of microcanonical equilibrium macrostates are the focus of the next section.

1.4 Form of $\mathcal{E}^u$ and Its Continuous Phase Transition

We now turn to the form of the set $\mathcal{E}^u$ for all $u \in [-\frac{1}{2}, -\frac{1}{2q}]$, which is the set of u for which $\mathcal{E}^u$ is nonempty. In the specific case $q = 3$ part (c) of Theorem 1.4.2 gives the form of $\mathcal{E}^u$, the calculation of which is much simpler than the calculation of the form of $\mathcal{E}_\beta$. The proof is based on the method of Lagrange multipliers, which also works for general $q \geq 4$ provided the next conjecture on the form of the elements in $\mathcal{E}^u$ is valid. The validity of this conjecture has been confirmed numerically for all $q \in \{4, 5, \ldots, 10^4\}$ and all $u \in (-\frac{1}{2}, -\frac{1}{2q})$ of the form $u = -\frac{1}{2} + 0.02k$, where k is a positive integer.

Conjecture 1.4.1. *For any $q \geq 4$ and all $u \in (-\frac{1}{2}, -\frac{1}{2q})$, there exist $a \neq b \in (0, 1)$ such that modulo permutations, any $\nu \in \mathcal{E}^u$ has the form $(a, b, \ldots, b)$, the last $q - 1$ components of which all equal b.*

Parts (a) and (b) of Theorem 1.4.2 are proved for general $q \geq 3$. Part (c) shows that modulo permutations, for $q = 3$, $\nu \in \mathcal{E}^u$ has the form $(a(u), b(u), b(u))$ and determines the precise formulas for $a(u)$ and $b(u)$. As specified in part (d), for $q \geq 4$ we can also determine the precise formula for $\nu \in \mathcal{E}^u$ provided Conjecture 1.4.1 is valid.

Theorem 1.4.2 shows that with respect to the microcanonical ensemble the Curie-Weiss-Potts model undergoes a continuous phase transition as u decreases from the critical energy value $u_c = -\frac{1}{2q}$. This contrast with the discontinuous phase transition exhibited by the canonical ensemble is closely related to the nonequivalence of the microcanonical and canonical ensembles for a range of u. Ensemble equivalence and nonequivalence will be explored in the next section, where we will see that it is reflected by support and concavity properties of the microcanonical entropy. An explicit formula for the microcanonical entropy is given in Theorem 1.4.3.

Theorem 1.4.2. *For $u \in I\!R$ we define $\mathcal{E}^u$ by* (2.4). *The following conclusions hold.*

(a) *For any $q \geq 3$, $\mathcal{E}^u$ is nonempty if and only if $u \in [-\frac{1}{2}, -\frac{1}{2q}]$. This interval coincides with the range of the energy representation function $\tilde{H}(\nu) = -\frac{1}{2}\langle \nu, \nu \rangle$ on $\mathcal{P}$.*

(b) *For any $q \geq 3$, $\mathcal{E}^{-\frac{1}{2q}} = \{\rho\} = \{(\frac{1}{q}, \frac{1}{q}, \ldots \frac{1}{q})\}$ and*

$$\mathcal{E}^{-\frac{1}{2}} = \{(1, 0, \ldots, 0), (0, 1, \ldots, 0), \ldots, (0, 0, \ldots, 1)\}.$$

(c) *Let $q = 3$. For $u \in (-\frac{1}{2}, -\frac{1}{2q})$, $\mathcal{E}^u$ consists of the 3 distinct vectors $\{\mu^1(u), \mu^2(u), \mu^3(u)\}$, where $\mu^1(u) = (a(u), b(u), b(u))$,*

$$a(u) = \frac{1 + \sqrt{2(-6u - 1)}}{3} \quad \textit{and} \quad b(u) = \frac{2 - \sqrt{2(-6u - 1)}}{6}. \tag{4.1}$$

The vectors $\mu^i(u)$, $i = 2, 3$, denote the points in $I\!R^3$ obtained by interchanging the first and the ith components of $\mu^1(u)$.

(d) *Let $q \geq 4$ and assume that Conjecture* 1.4.1 *is valid. Then for $u \in (-\frac{1}{2}, -\frac{1}{2q})$, $\mathcal{E}^u$ consists of the q distinct vectors $\{\mu^1(u), \ldots, \mu^q(u)\}$, where $\mu^1(u) = (a(u), b(u), \ldots, b(u))$,*

$$a(u) = \frac{1 + \sqrt{(q-1)(-2qu - 1)}}{q} \quad \textit{and} \quad b(u) = \frac{q - 1 - \sqrt{(q-1)(-2qu - 1)}}{(q-1)q}.$$

The last $q - 1$ components of $\mu^1(u)$ all equal $b(u)$, and the vectors $\mu^i(u), i = 2, \ldots, q$, denote the points in $I\!R^q$ obtained by interchanging the first and the ith components of $\mu^1(u)$.

We return to part (b) of Theorem 1.4.2 in order to discuss the nature of the phase transition exhibited by the microcanonical ensemble. The functions $a(u)$ and $b(u)$ given in (4.1) are both continuous for $u \in [-\frac{1}{2}, -\frac{1}{2q}]$ and satisfy

$$\lim_{u \to (-\frac{1}{2q})^-} a(u) = \lim_{u \to (-\frac{1}{2q})^-} b(u) = \tfrac{1}{q} = a(-\tfrac{1}{2q}) = b(-\tfrac{1}{2q}).$$

Therefore, for $i = 1, \ldots, q$, $\lim_{u \to (-\frac{1}{2q})^-} \mu^i(u) = \rho$. It follows that the microcanonical ensemble exhibits a continuous phase transition as u decreases from $u_c = -\frac{1}{2q}$, the unique equilibrium macrostate ρ for $u = u_c$ bifurcating continuously into the q distinct macrostates $\mu^i(u)$ as u decreases from its maximum value. This is rigorously true for $q = 3$. Provided Conjecture 1.4.1 is true, it is also true for $q \geq 4$, as one easily checks using part (d) of Theorem 1.4.2.

Before proving Theorem 1.4.2, we introduce the microcanonical entropy

$$s(u) = -\inf\Big\{R(\nu|\rho) : \nu \in \mathcal{P}, -\tfrac{1}{2}\langle \nu, \nu \rangle = u\Big\}. \tag{4.2}$$

As we will see in the next section, this function plays a crucial role in the analysis of ensemble equivalence and nonequivalence for the Curie-Weiss-Potts model. The domain of s is the set $\operatorname{dom} s = \{u \in I\!R : s(u) > -\infty\}$; for $u \not\in \operatorname{dom} s$, we set $s(u) = -\infty$. Since $R(\nu|\rho) < \infty$ for all $\nu \in \mathcal{P}$, $\operatorname{dom} s$ equals the range of $\tilde{H}(\nu) = -\frac{1}{2}\langle \nu, \nu\rangle$ on $\mathcal{P}$, which is the interval $[-\frac{1}{2}, -\frac{1}{2q}]$ [Thm. 1.4.2(a)].

Since $0 \leq R(\nu|\rho)$ for all $\nu \in \mathcal{P}$, $s(u) \in [-\infty, 0]$ for all u. The continuity of $R(\nu|\rho)$ on $\mathcal{P}$ and the compactness of the constraint set in (4.2) guarantee that for $u \in \operatorname{dom} s$ the infimum in the definition of $s(u)$ is attained for some $\nu \in \mathcal{P}$. Since $R(\nu|\rho) > R(\rho|\rho) = 0$ for all $\nu \neq \rho$, it follows that s attains its maximum of 0 at the unique value $-\frac{1}{2q} = -\frac{1}{2}\langle \rho, \rho\rangle$.

As we have just seen, $s(-\frac{1}{2q}) = 0$. For $u \in (-\frac{1}{2}, -\frac{1}{2q})$, according to parts (c)–(d) of Theorem 1.4.2 $\mathcal{E}^u$ consists of the unique vector $\mu^1(u)$ modulo permutations. Since for $i = 2, 3, \ldots, q$, $R(\mu^i(u)|\rho) = R(\mu^1(u)|\rho)$, we conclude that

$$s(u) = -R(\mu^1(u)|\rho) = -a(u)\log(q\,a(u)) - (q-1)b(u)\log(q\,b(u)).$$

Finally, for $u = -\frac{1}{2}$, modulo permutations $\mathcal{E}^u$ consists of the unique vector $(1, 0, \ldots, 0)$ [see (4.7)], and so $s(-\frac{1}{2}) = -R((1, 0, \ldots, 0)|\rho) = -\log q$. The resulting formulas for $s(u)$ are recorded in the next theorem, where we distinguish between $q = 3$ and $q \geq 4$.

Theorem 1.4.3. *We define the microcanonical entropy* $s(u)$ *in* (4.2). *The following conclusions hold.*

(a) $\operatorname{dom} s = [-\frac{1}{2}, -\frac{1}{2q}]$; *for any* $u \in \operatorname{dom} s$, $u \neq -\frac{1}{2q}$, $s(u) < s(-\frac{1}{2q}) = 0$; *and* $s(-\frac{1}{2}) = -\log q$.

(b) *Let* $q = 3$. *Then for* $u \in (-\frac{1}{2}, -\frac{1}{2q}) = (-\frac{1}{2}, -\frac{1}{6})$

$$\begin{aligned} s(u) \;&=\; -\frac{1+\sqrt{2(-6u-1)}}{3}\,\log\Big(1+\sqrt{2(-6u-1)}\Big) \\ &\quad\; -\frac{2-\sqrt{2(-6u-1)}}{3}\,\log\left(\frac{2-\sqrt{2(-6u-1)}}{2}\right). \end{aligned} \tag{4.3}$$

(c) *Let* $q \geq 4$ *and assume that Conjecture* 1.4.1 *is valid. Then for* $u \in (-\frac{1}{2}, -\frac{1}{2q})$

$$\begin{aligned} s(u) \;\; = \;\; & -\frac{1+\sqrt{(q-1)(-2qu-1)}}{q}\,\log\Big(1+\sqrt{(q-1)(-2qu-1)}\Big) \\ & -\frac{q-1-\sqrt{(q-1)(-2qu-1)}}{q}\,\log\left(\frac{q-1-\sqrt{(q-1)(-2qu-1)}}{q-1}\right). \end{aligned} \tag{4.4}$$

We now turn to the proof of Theorem 1.4.2, which gives the form of $\mathcal{E}^u$. We start by proving part (a). The set $\mathcal{E}^u$ of microcanonical equilibrium macrostates consists of all $\nu \in \mathcal{P}$ that minimize the relative entropy $R(\nu|\rho)$ subject to the constraint that

$$\tilde{H}(\nu) = -\tfrac{1}{2}\langle \nu, \nu \rangle = u.$$

Let $u = -\frac{1}{2}r^2$. Since $\mathcal{P}$ consists of all nonnegative vectors in $I\!R^q$ satisfying $\nu_1 + \cdots + \nu_q = 1$, the constraint set in the minimization problem defining $\mathcal{E}^u$ is given by

$$C(u) = C(-\tfrac{1}{2}r^2) = \left\{ \nu \in I\!R^q : \nu_1 \geq 0, \ldots, \nu_q \geq 0,\ \sum_{j=1}^{q} \nu_j = 1,\ \sum_{j=1}^{q} \nu_j^2 = r^2 \right\}. \tag{4.5}$$

Geometrically, $C(-\frac{1}{2}r^2)$ is the intersection of the nonnegative orthant of $I\!R^q$, the hyperplane consisting of $\nu \in I\!R^\sigma$ that satisfy $\nu_1 + \cdots + \nu_q = 1$, and the hypersphere in $I\!R^q$ with center 0 and radius r. Clearly, $C(u) \neq \emptyset$ if and only if u lies in the range of the energy representation function $\tilde{H}(\nu) = -\frac{1}{2}\langle \nu, \nu \rangle$ on $\mathcal{P}$. Because $0 \leq R(\nu|\rho) < \infty$ for all $\nu \in C(u)$, the range of $\tilde{H}$ on $\mathcal{P}$ also equals the set of u for which $\mathcal{E}^u \neq \emptyset$.

The geometric description of $C(u)$ makes it straightforward to determine those values of u for which this constraint set is nonempty. The smallest value of r for which $C(-\frac{1}{2}r^2) \neq \emptyset$ is obtained when the hypersphere of radius r is tangent to the hyperplane, the point of tangency being $\rho = (\frac{1}{q}, \frac{1}{q}, \ldots, \frac{1}{q})$, the closest probability vector to the origin. The hypersphere and the hyperplane are tangent when $r = \frac{1}{\sqrt{q}}$, which coincides with the distance from the center of the hypersphere to the hyperplane. It follows that the largest value of u for which $C(u) \neq \emptyset$, and thus $\mathcal{E}^u \neq \emptyset$, is $u = -\frac{1}{2}r^2 = -\frac{1}{2q}$. In this case

$$C(-\tfrac{1}{2q}) = \{\rho\} = \{(\tfrac{1}{q}, \tfrac{1}{q}, \ldots, \tfrac{1}{q})\} = \mathcal{E}^{-\frac{1}{2q}}. \tag{4.6}$$

For all sufficiently large r, $C(-\frac{1}{2}r^2)$ is empty because the hypersphere of radius r has empty intersection with the intersection of the hyperplane and the nonnegative orthant of $\mathbb{R}^q$. The largest value for r for which this does not occur is found by subtracting the two equations defining the hyperplane and the hypersphere. Since each $\nu_i \in [0, 1]$, it follows that

$$0 \leq \sum_{i=1}^{q} \nu_i(1 - \nu_i) = 1 - r^2,$$

and this in turn implies that $r^2 \leq 1$. Thus $r = 1$ is the largest value for r for which $C(-\frac{1}{2}r^2) \neq \emptyset$. We conclude that the smallest value of u for which $C(u) \neq \emptyset$, and thus $\mathcal{E}^u \neq \emptyset$, is $u = -\frac{1}{2}r^2 = -\frac{1}{2}$. The set $\mathcal{E}^{-\frac{1}{2}}$ consists of the points at which the hyperplane intersects each of the positive coordinate axes; i.e.,

$$\mathcal{E}^{-\frac{1}{2}} = \{(1, 0, \ldots, 0), (0, 1, \ldots, 0), \ldots, (0, 0, \ldots, 1)\}. \tag{4.7}$$

This completes the proof of part (a) of Theorem 1.4.2.

For $u \in [-\frac{1}{2}, -\frac{1}{2q}]$, we now determine the form $\mathcal{E}^u$ as specified in parts (b)–(d) of Theorem 1.4.2. Part (b) considers any $q \geq 3$ and the values $u = -\frac{1}{2q}$ and $u = -\frac{1}{2}$, part (c) $q = 3$ and $u \in (-\frac{1}{2}, -\frac{1}{2q})$, and part (d) $q \geq 4$ and $u \in (-\frac{1}{2}, -\frac{1}{2q})$. Part (b) has already been proved; for $u = -\frac{1}{2q}$ and $u = -\frac{1}{2}$, the sets $\mathcal{E}^u$ are given in (4.6) and (4.7).

We now consider $q \geq 3$ and $u \in (-\frac{1}{2}, -\frac{1}{2q})$. For $\nu \in \mathcal{P}$ define

$$K(\nu) = \sum_{j=1}^{q} \nu_j \ \text{ and } \ \tilde{H}(\nu) = -\tfrac{1}{2}\langle \nu, \nu \rangle.$$

By definition $\nu = (\nu_1, \ldots, \nu_q) \in \mathcal{E}^u$ if and only if ν minimizes $R(\nu|\rho) = \sum_{j=1}^{q} \nu_j \log(q\nu_j)$ subject to the constraints $K(\nu) = 1$, $\tilde{H}(\nu) = u$, and $\nu_1 \geq 0, \ldots, \nu_q \geq 0$. For $u \in (-\frac{1}{2}, -\frac{1}{2q})$ we divide into two parts the calculation of the form of $\nu \in \mathcal{E}^u$. First we use Lagrange multipliers to solve the constrained minimization problem when $\nu_1 > 0, \ldots, \nu_1 > 0$. Then we argue that the vectors ν found via Lagrange multipliers solve the original constrained minimization problem when $\nu_1 \geq 0, \ldots, \nu_q \geq 0$.

We introduce Lagrange multipliers γ and λ. Any critical point of $R(\nu|\rho)$ subject to the constraints $K(\nu) = 1$, $\tilde{H}(\nu) = u$, and $\nu_1 > 0, \nu_2 > 0, \ldots, \nu_q > 0$ satisfies

$$\begin{cases} \nabla R(\nu|\rho) = \gamma \nabla K(\nu) + \lambda \nabla \tilde{H}(\nu) \\ K(\nu) = 1 \\ \tilde{H}(\nu) = u \\ \nu_j > 0 \ \text{ for } j = 1, 2, \ldots, q. \end{cases}$$

This system of equations is equivalent to

$$\begin{cases} 1 + \log(q\nu_j) = \gamma - \lambda \nu_j \ \text{ for } j = 1, 2, \ldots, q \\ \sum_{j=1}^q \nu_j = 1 \\ -\frac{1}{2} \sum_{j=1}^q \nu_j^2 = u \\ \nu_j > 0 \ \text{ for } j = 1, 2, \ldots, q. \end{cases} \tag{4.8}$$

By the strict concavity of the logarithm, the first equation can have at most two solutions. Hence modulo permutations, there exists $n \in \{0, 1, \ldots, q\}$ and distinct numbers $a, b \in (0, 1)$ such that the first n components of any critical point ν all equal a and the last $q - n$ components of ν all equal b. The second and third equations in (4.8) take the form

$$na + (q - n)b = 1 \ \text{ and } \ na^2 + (q - n)b^2 = -2u. \tag{4.9}$$

If $n = 0$, then $b = \frac{1}{q}$, while if $n = q$, then $a = \frac{1}{q}$. Both cases correspond to $\nu = (\frac{1}{q}, \ldots, \frac{1}{q}) = \rho$ and $u = -\frac{1}{2q}$, which does not lie in the open interval $(-\frac{1}{2}, -\frac{1}{2q})$ currently under consideration.

We now focus on $n \in \{1, \ldots, q-1\}$. In this case the two solutions of (4.9) are

$$a_1(n) = \frac{n - \sqrt{n(q-n)(-2qu-1)}}{nq}, \ \ b_1(n) = \frac{q - n + \sqrt{n(q-n)(-2qu-1)}}{(q-n)q}, \tag{4.10}$$

and

$$a_2(n) = \frac{n + \sqrt{n(q-n)(-2qu-1)}}{nq}, \ \ b_2(n) = \frac{q - n - \sqrt{n(q-n)(-2qu-1)}}{(q-n)q}. \tag{4.11}$$

Since $u \in (-\frac{1}{2}, -\frac{1}{2q})$, these quantities are all well defined and $a_j(n) \neq b_j(n)$ for $j = 1, 2$. In addition,

$$a_1(q-n) = b_2(n) \text{ and } b_1(q-n) = a_2(n).$$

This means that the point having the first n components $a_2(n)$ and the last $q-n$ components $b_2(n)$ equals, modulo permutations, the point having the first $q-n$ components $a_1(q-n)$ and the last n components $b_1(q-n)$.

Thus, without loss of generality, we can seek solutions of the system (4.8) having the first n components $a_2(n)$ and the last $q-n$ components $b_2(n)$. While $a_2(1)$ and $b_2(1)$ are always positive for all $u \in (-\frac{1}{2}, -\frac{1}{2q})$, $b_2(n)$ might be negative for some $n \in \{2, \ldots, q-1\}$ and some $u \in (-\frac{1}{2}, -\frac{1}{2q})$. In this case the positivity constraint in the last line of (4.8) excludes such values of n and u.

We give full details when $q = 3$, the case considered in part (c) of Theorem 1.4.2. When $q = 3$, the interval $(-\frac{1}{2}, -\frac{1}{2q})$ equals $(-\frac{1}{2}, -\frac{1}{6})$ and we have $n \in \{1, 2\}$. For $n = 1$ and $n = 2$ (4.11) takes the form

$$a_2(1) = \frac{1 + \sqrt{2(-6u-1)}}{3}, \quad b_2(1) = \frac{2 - \sqrt{2(-6u-1)}}{6}$$

and

$$a_2(2) = \frac{2 + \sqrt{2(-6u-1)}}{6}, \quad b_2(2) = \frac{1 - \sqrt{2(-6u-1)}}{3}.$$

For $u \in (-\frac{1}{2}, -\frac{1}{4})$, $b_2(2)$ is negative and hence a solution of (4.8) cannot have the form $(a_2(2), a_2(2), b_2(2))$. We conclude that when $u \in (-\frac{1}{2}, -\frac{1}{4})$, $\nu = (a_2(1), b_2(1), b_2(1))$ is, modulo permutations, the unique solution of (4.8) and thus the unique minimizer of $R(\nu|\rho)$ subject to the constraints in the last three lines of (4.8). For $u \in [-\frac{1}{4}, -\frac{1}{6})$, a straightforward calculation shows that

$$R(\,(a_2(1), b_2(1), b_2(1))\,|\,\rho) < R(\,(a_2(2), a_2(2), b_2(2)))\,|\,\rho).$$

It follows again that $\nu = (a_2(1), b_2(1), b_2(1))$ is, modulo permutations, the unique minimizer of $R(\nu|\rho)$ subject to the constraints in the last three lines of (4.8). This completes the proof that for $q = 3$ and any $u \in (-\frac{1}{2}, -\frac{1}{6})$, $\nu = (a_2(1), b_2(1), b_2(1))$ is, modulo permutations, the unique minimizer of $R(\mu|\rho)$ subject to the constraints $K(\nu) = 1$, $\tilde{H}(\nu) = u$, and $\nu_1 > 0, \nu_2 > 0, \nu_3 > 0$.

We now prove for $q = 3$ that the minimizers found via Lagrange multipliers when $K(\nu) = 1$, $\tilde{H}(\nu) = u$, and $\nu_1 > 0, \nu_2 > 0, \nu_3 > 0$ also minimize $R(\nu|\rho)$ subject to the constraints $K(\nu) = 1$, $\tilde{H}(\nu) = u$, and $\nu_1 \geq 0, \nu_2 \geq 0, \nu_3 \geq 0$. If $\nu = (\nu_1, \nu_2, \nu_3)$ satisfies the latter constraints and has two components equal to zero, then modulo permutations $\nu = (1, 0, 0)$ and $\tilde{H}(\nu) = u = -\frac{1}{2}$, which does not lie in the open interval $(-\frac{1}{2}, -\frac{1}{6})$ currently under consideration. Thus we only have to consider the case where ν has one component equal to zero; i.e, $\nu = (0, a_0, b_0)$ with $a_0 \geq b_0$. In this case the second and third equations in (4.8) have the solution

$$a_0 = \frac{1 + \sqrt{-4u - 1}}{2}, \;\; b_0 = \frac{1 - \sqrt{-4u - 1}}{2}.$$

We now claim that modulo permutations the unique minimizer of $R(\nu|\rho)$ subject to the constraints $K(\nu) = 1$, $\tilde{H}(\nu) = u$, and $\nu_1 \geq 0, \nu_2 \geq 0, \nu_3 \geq 0$ has the form $(a_2(1), b_2(1), b_2(1))$ found in the preceding paragraph. The claim follows from the calculation

$$R(\,(a_2(1), b_2(1), b_2(1))\,|\,\rho) < R(\,(0, a_0, b_0)\,|\,\rho),$$

which is valid for all $u \in (-\frac{1}{2}, -\frac{1}{6})$. This completes the proof of part (c) of Theorem 1.4.2, which gives the form of $\nu \in \mathcal{E}^u$ for $q = 3$ and $u \in (-\frac{1}{2}, -\frac{1}{6})$.

We now turn to part (d) of Theorem 1.4.2, which gives the form of $\mathcal{E}^u$ for $q \geq 4$ and $u \in (-\frac{1}{2}, -\frac{1}{2q})$. If, as in the case $q = 3$, we knew that modulo permutations, the minimizers have the form $(a, b, \ldots, b)$ as specified in Conjecture 1.4.1, then as in the case $q = 3$ we would be able to derive explicit formulas for these minimizers. If

Conjecture 1.4.1 is true, then it is easily verified that modulo permutations, $\mathcal{E}^u$ consists of the unique point $\nu = (a_2(1), b_2(1), \ldots, b_2(1))$, where $a_2(1)$ and $b_2(1)$ are defined in (4.11) for $u \in (-\frac{1}{2}, -\frac{1}{2q})$. This gives part (d) of Theorem 1.4.2. The proof of the theorem is complete.

At the end of Section 6 we will see that there exists an explicit value of $u_0 \in (-\frac{1}{2}, -\frac{1}{2q})$ such that Conjecture 1.4.1 is valid for any $q \geq 4$ and all $u \in (-\frac{1}{2}, u_0]$. Hence for these values of u the form of $\nu \in \mathcal{E}^u$ given in part (d) of Theorem 1.4.2 and the formula for $s(u)$ given in part (c) of Theorem 1.4.3 are both rigorously true.

1.5 Equivalence and Nonequivalence of Ensembles

As we saw in Section 3, the set $\mathcal{E}_\beta$ of canonical equilibrium macrostates undergoes a discontinuous phase transition as β increases through $\beta_c = \frac{2(q-1)}{q-2}\log(q-1)$, the unique macrostate ρ bifurcating discontinuously into the q distinct macrostates $\nu^{(i)}(\beta)$. By contrast, as we saw in Section 4, the set $\mathcal{E}^u$ of microcanonical equilibrium macrostates undergoes a continuous phase transition as u decreases from $u_c = -\frac{1}{2q}$, the unique macrostate ρ bifurcating continuously into the q distinct macrostates $\mu^i(u)$. The different continuity properties of these phase transitions shows already that the canonical and microcanonical ensembles are nonequivalent. In this section we study this nonequivalence in detail and relate the equivalence and nonequivalence of these two sets of equilibrium macrostates to concavity and support properties of the microcanonical entropy s defined in (4.2). This is done with the help of Figure 2, which is based on the form of s in Figure 1 and on the results on ensemble equivalence and nonequivalence in Theorem 1.5.1. In Figures 3 and 4 at the end of the section we give, for $q = 3$, a beautiful geometric representation of $\mathcal{E}_\beta$ and $\mathcal{E}^u$ that also shows the ensemble nonequivalence for a range of u.

We start by stating in Theorem 1.5.1 results on ensemble equivalence and nonequivalence for the Curie-Weiss-Potts model. Theorem 5.1 summarizes Theorems 4.4, 4.6, and 4.8 in [23], which apply to a wide range of statistical mechanical models. The Curie-Weiss-Potts model is a special case. In this special case, we will show that the values of u and β in part (a)(i) of the next theorem are related by the thermodynamic formula $s'(u) = \beta$ [Thm. 1.6.2(b)]. For $u \in \text{dom}\, s$ the possible relationships between $\mathcal{E}^u$ and $\mathcal{E}_\beta$, given in part (a) of Theorem 1.5.1, are that either the ensembles are fully equivalent, partially equivalent, or nonequivalent. According to part (b) of the theorem, canonical equilibrium macrostates are always realized microcanonically — i.e., lie in $\mathcal{E}^u$ for some u — while according to part (a)(iii), microcanonical equilibrium macrostates are in general not realized canonically — i.e., do not lie in $\mathcal{E}_\beta$ for any β. It follows that the microcanonical ensemble is the richer of the two ensembles.

Theorem 1.5.1. *We define* s *by* (4.2) *and* $\mathcal{E}_\beta$ *and* $\mathcal{E}^u$ *by* (2.3) *and* (2.4). *The following conclusions hold.*

(a) *For fixed* $u \in \text{dom}\, s$ *one of the following three possibilities occurs.*

(i) **Full equivalence.** *There exists* $\beta \in I\!R$ *such that* $\mathcal{E}^u = \mathcal{E}_\beta$. *This is the case if and only if* s *has a strictly supporting line at* u *with slope* β*; i.e.,*

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

(ii) **Partial equivalence.** *There exists* $\beta \in I\!R$ *such that* $\mathcal{E}^u \subset \mathcal{E}_\beta$ *but* $\mathcal{E}^u \neq \mathcal{E}_\beta$. *This is the case if and only if* s *has a nonstrictly supporting line at* u *with slope* β*; i.e.,*

$$s(v) \leq s(u) + \beta(v-u) \text{ for all } v \in I\!R \text{ with equality for some } v \neq u.$$

(iii) **Nonequivalence.** *For all* $\beta \in I\!R$, $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$. *This is the case if and only if* s *has no supporting line at* u*; i.e., for any* $\beta \in I\!R$ *there exists* v *such that* $s(v) > s(u) + \beta(v-u)$.

(b) **Canonical is always realized microcanonically.** *For $\nu \in \mathcal{P}$ we define $\tilde{H}(\nu) = -\frac{1}{2}\langle \nu, \nu \rangle$. Then for any $\beta \in I\!R$*

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

We next relate ensemble equivalence and nonequivalence with concavity and support properties of s in the Curie-Weiss-Potts model. For $q = 3$ an explicit formula for s is given in part (b) of Theorem 1.4.3. If Conjecture 1.4.1 is true, then the formula for s given in part (c) of Theorem 1.4.3 is also valid for $q \geq 4$. Figure 1 exhibits all the concavity and support features of s. However, Figure 1 is not the actual graph of s but a schematic graph that accentuates the shape of s together with the intervals of strict concavity and nonconcavity of s. For arbitrary $q \geq 3$, as discussed in the second paragraph after Theorem 1.6.2, the concavity and support features of s exhibited in Figure 1 follow from Theorems 1.5.1 and 1.6.2.

Concavity properties of s are defined in reference to the double-Legendre-Fenchel transform s^{**}, which can be characterized as the smallest concave, upper semicontinuous function that satisfies $s^{**}(u) \geq s(u)$ for all $u \in I\!R$ [14, Prop. A.2]. For $u \in \text{dom}\, s$ we say that s is concave at u if $s(u) = s^{**}(u)$ and that s is not concave at u if $s(u) < s^{**}(u)$. Also, we say that s is strictly concave at $u \in \text{dom}\, s$ if s has a strictly supporting line at u and that s is strictly concave on a convex subset A of $\text{dom}\, s$ if s is strictly concave at each $u \in A$. If s is strictly concave at u, then a straightforward argument shows that s is concave at u, as one expects [14, Lem. 4.1(a)].

According to Figure 1 and Theorem 1.5.1, there exists $u_0 \in (-\frac{1}{2}, -\frac{1}{2q})$ with the following properties.

- s is strictly concave on the interval $(-\frac{1}{2}, u_0)$ and at the point $-\frac{1}{2q}$. Hence for $u \in F = (-\frac{1}{2}, u_0) \cup \{-\frac{1}{2q}\}$ the ensembles are fully equivalent [Thm. 1.5.1(a)(i)].

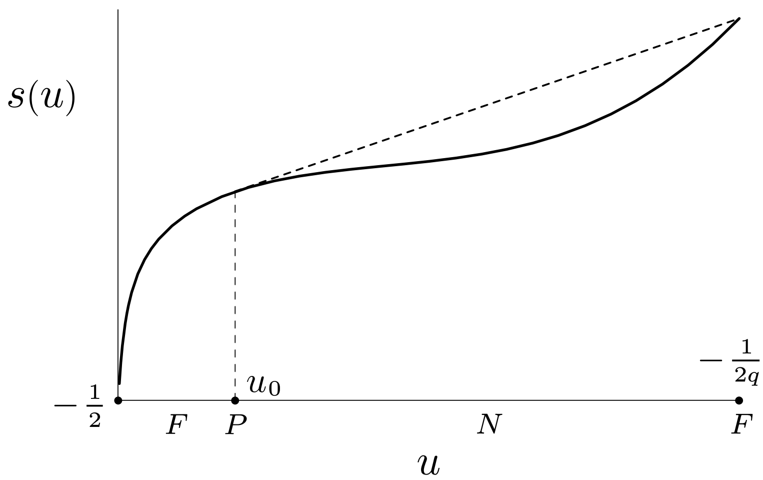

Figure 1. **Schematic graph of $s(u)$, showing the set $F = (-\frac{1}{2}, u_0) \cup \{-\frac{1}{2q}\}$ of full ensemble equivalence, the singleton set $P = \{u_0\}$ of partial equivalence, and the set $N = (u_0, -\frac{1}{2q})$ of nonequivalence. For $u \in F \cup P = (-\frac{1}{2}, u_0] \cup \{-\frac{1}{2q}\}$, $s(u) = s^{**}(u)$; for $u \in N$, $s(u) < s^{**}(u)$ and the graph of s^{**} consists of the dotted line segment with slope β_c. The slope of s at $-\frac{1}{2}$ is ∞.**

In fact, for $u \in \operatorname{int} F = (-\frac{1}{2}, u_0)$, $\mathcal{E}^u = \mathcal{E}_\beta$ with β given by the thermodynamic formula $\beta = s'(u)$ [Thm. 1.6.2(b)].

- s is concave but not strictly concave at u_0 and has a nonstrictly supporting line at u_0 that also touches the graph of s over the right hand endpoint $-\frac{1}{2q}$. Hence for $u = u_0$ the ensembles are partially equivalent in the sense that there exists $\beta \in I\!R$ such that $\mathcal{E}^u \subset \mathcal{E}_\beta$ but $\mathcal{E}^u \neq \mathcal{E}_\beta$ [Thm. 1.5.1(a)(ii)]. In fact, β equals the critical inverse temperature β_c defined in (3.1).

- s is not concave on the interval $N = (u_0, -\frac{1}{2q})$ and has no supporting line at any $u \in N$ [14, Thm. A.4(c)]. Hence for $u \in N$ the ensembles are nonequivalent in the sense that for all $\beta \in I\!R$, $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ [Thm. 1.5.1(a)(iii)].

As we have just seen, u_0 can be characterized in terms of concavity and support properties of s. The quantity u_0 can also be characterized in terms of mapping properties of $\tilde{H}(\nu) = -\frac{1}{2}\langle\nu,\nu\rangle$. Using this characterization, we give an explicit formula for u_0 in (6.2).

We point out two additional features of Figure 1. First, although $\mathcal{E}^u \neq \emptyset$ for u equal to the left hand endpoint $-\frac{1}{2}$ of $\operatorname{dom} s$, we do not include this point in the set F of full ensemble equivalence. Indeed, s is not strictly concave at $-\frac{1}{2}$ because there is no strictly supporting line at $-\frac{1}{2}$; as one can see in (5.1), the slope of s at $-\frac{1}{2}$ is ∞. Nevertheless, by introducing the limiting set

$$\mathcal{E}_\infty = \{(1,0,\ldots,0),(0,1,\ldots,0),\ldots,(0,0,\ldots,1)\} = \lim_{\beta\to\infty} \mathcal{E}_\beta,$$

we can extend full ensemble equivalence to $u = -\frac{1}{2}$ since $\mathcal{E}^{-\frac{1}{2}} = \mathcal{E}_\infty$.

Second, for u in the interval N of ensemble nonequivalence, the graph of s^{**} is affine; this is depicted by the dotted line segment in Figure 1. The slope of the affine portion of the graph of s^{**} equals the critical inverse temperature β_c defined in (3.1). This can be proved using concave-duality relationships involving s^{**} and the canonical free energy. The quantity β_c also satisfies an equal-area property, first observed by Maxwell [40, p. 45] and explained in the context of another spin model in [27, p. 535].

The relationships stated in the three bulleted items above give valuable insight into equivalence and nonequivalence of ensembles in the Curie-Weiss-Potts model. These relationships are illustrated in Figure 2. In this figure we exhibit the graph of s' and the sets $\mathcal{E}_\beta$ and $\mathcal{E}^u$ in order to compare the phase transitions in the two ensembles and to understand the implications for ensemble equivalence and nonequivalence. In order to accentuate properties of s', $\mathcal{E}_\beta$, and $\mathcal{E}^u$ that are related to ensemble equivalence and nonequivalence, we focus on $q = 8$. In presenting the graph of s' and the form of $\mathcal{E}^u$, we assume that for $q = 8$ Conjecture 1.4.1 is valid. We then appeal to part (c) of Theorem 1.4.3, which gives an explicit formula for s, and to part (d) of Theorem 1.4.2, which gives an explicit formula for the elements of $\mathcal{E}^u$. The derivative s', graphed in the top left plot in Figure 2, is given by

$$s'(u) = \sqrt{\frac{q-1}{-2qu-1}} \left[\log\left(1 + \sqrt{(q-1)(-2qu-1)}\ \right) - \log\left(1 - \sqrt{\frac{-2qu-1}{q-1}}\right)\right]. \tag{5.1}$$

The canonical phase diagram, given in the top right plot in Figure 2, summarizes the description of $\mathcal{E}_\beta$ given in Theorem 1.3.1 and shows the discontinuous phase transition exhibited by this ensemble at $\beta_c = \frac{2(q-1)}{q-2}\log(q-1) = \frac{7}{3}\log 7$. The solid line in this plot for $\beta < \beta_c$ represents the common value $\frac{1}{8}$ of each of the components of ρ, which is the unique phase for $\beta < \beta_c$. For $\beta > \beta_c$ there are eight phases given by $\nu^1(\beta)$ together with the vectors $\nu^i(\beta)$ obtained by interchanging the first and ith components of $\nu^1(\beta)$. Finally, for $\beta = \beta_c$ there are nine phases consisting of ρ and the vectors $\nu^i(\beta_c)$ for $i = 1, 2, \ldots, 8$. The solid and dashed curves in the top right plot in Figure 2 show the first component and the last seven, equal components of $\nu^1(\beta)$ for $\beta \in [\beta_c, \infty)$. The first component is a strictly increasing function equal to $\frac{7}{8}$ for $\beta = \beta_c$ and increasing to 1 as $\beta \to \infty$ while the last seven, equal components are strictly decreasing functions equal to $\frac{1}{56}$ for $\beta = \beta_c$ and decreasing to 0 as $\beta \to \infty$.

The microcanonical phase diagram, given in the bottom left plot in Figure 2, summarizes the description of $\mathcal{E}^u$ given in Theorem 1.4.2 and shows the continuous phase transition exhibited by this ensemble as u decreases from the maximum value $u_c = -\frac{1}{2q} = -\frac{1}{16}$. The single phase ρ for $u = -\frac{1}{16}$ is represented by the point lying over this value of u. For $u \in [-\frac{1}{2}, -\frac{1}{16})$ there are eight phases given by $\mu^1(u)$ together with the vectors $\mu^i(u)$ obtained by interchanging the first and ith components of $\mu^1(u)$. The solid and dashed curves in the bottom left plot in Figure 2 show the first component $a(u)$ and the last seven, equal components $b(u)$ of $\mu^1(u)$ for $u \in [-\frac{1}{2}, -\frac{1}{16})$. The first component is a strictly increasing function of $-u$ equal to $\frac{1}{8}$ for $u = -\frac{1}{16}$ and increasing to 1 as $u \to (-\frac{1}{2})^+$, while the last seven, equal components are strictly decreasing functions of

$-u$ equal to $\frac{1}{8}$ for $u = -\frac{1}{16}$ and decreasing to 0 as $u \to (-\frac{1}{2})^+$.

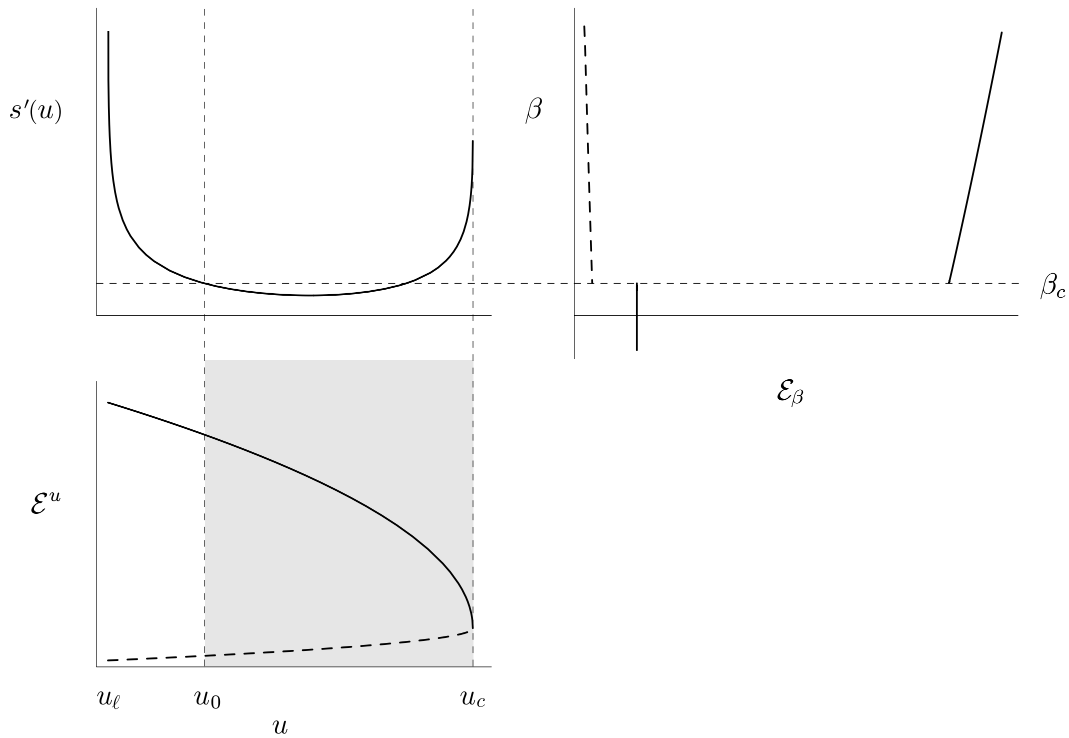

Figure 2. For $q = 8$ the top right plot shows $\mathcal{E}_\beta$, the top left plot the graph of $s'(u)$ for $u \in$ dom $s = [u_\ell, u_c] = [-\frac{1}{2}, -\frac{1}{2q}]$, and the bottom left plot $\mathcal{E}^u$. The discontinuous phase transition at β_c in the top right plot and the continuous phase transition at u_c in the bottom left plot imply that the ensembles are nonequivalent for all $u \in N = (u_0, u_c)$. On this interval s is not concave and s^{**} is affine with slope β_c. The shaded area in the bottom left plot corresponds to the region of nonequivalence of ensembles delineated by $u \in N$.

The different nature of the two phase transitions — discontinuous in the canonical ensemble versus continuous in the microcanonical ensemble — implies that the two ensembles are not fully equivalent for all values of u. By necessity, the set $\mathcal{E}_\beta$ of canonical equilibrium macrostates must omit a set of microcanonical equilibrium macrostates. Further details concerning ensemble equivalence and nonequivalence can be seen by examining the graph of s', given in the top left plot of Figure 2. This graph, which is the bridge between the canonical and microcanonical phase diagrams, shows that s' is strictly decreasing on the interval $\operatorname{int} F = (-\frac{1}{2}, u_0)$, which is the interior of the set F of full ensemble equivalence. The critical value β_c equals the slope of the affine portion of the graph of s^{**} over the interval $N = (u_0, -\frac{1}{2q})$ of ensemble nonequivalence. This affine portion is represented in the top left plot of Figure 2 by the horizontal dashed line at β_c.

Figure 2 exhibits the full equivalence of ensembles that holds for $u \in \operatorname{int} F = (-\frac{1}{2}, u_0)$ [Thm. 1.6.2(a)]. For u in this interval the solid and dashed curves representing the components of $\mu^1(u) \in \mathcal{E}^u$ can be put in one-to-one correspondence with the solid and dashed curves representing the same two components of $\nu^1(\beta) \in \mathcal{E}_\beta$ for $\beta \in (\beta_c, \infty)$. As we remarked earlier, the values of u and β are related by the thermodynamic formula $s'(u) = \beta$ [Thm. 1.6.2(b)]. Full equivalence of ensembles also holds for $u = -\frac{1}{2q} \in F$, the right-hand endpoint of the interval on which s is finite. The solid vertical line in the top right plot for $\beta < \beta_c$, which represents the unique canonical phase ρ, is collapsed in the bottom left plot to the single energy value $u = -\frac{1}{2q}$, which corresponds to the unique microcanonical phase ρ. This collapse shows that the canonical notion of temperature is somewhat ill-defined at $u = -\frac{1}{2q}$ since there are infinitely many values of β associated with this energy value. This feature of the Curie-Weiss-Potts model is not present, for example, in the mean-field Blume-Emery-Griffiths spin model, which also exhibits nonequivalence of ensembles [27].

By comparing the top right and bottom left plots, we see that the elements of $\mathcal{E}^u$ cease to be related to those of $\mathcal{E}_\beta$ for $u \in N = (u_0, -\frac{1}{2q})$, which is the interval on which s is not concave. For any energy value u in this interval no $\nu \in \mathcal{E}_\beta$ exists that can be put in correspondence with an equivalent equilibrium empirical vector contained in $\mathcal{E}^u$. Thus, although the equilibrium macrostates corresponding to $u \in N$ are characterized by a well defined value of the energy, it is impossible to assign an inverse temperature β to those macrostates from the viewpoint of the canonical ensemble. In other words, the canonical ensemble is blind to all energy values u contained in the interval N of nonconcavity of s. This is closely related to the presence of the discontinuous phase transition seen in the canonical ensemble.

The quantity u_0 defined in (6.2) plays a central role in the analysis of phase transitions and ensemble equivalence in the Curie-Weiss-Potts model. First, as we saw in our discussion of Figure 1, u_0 separates the interval $(-\frac{1}{2}, u_0)$ of strict concavity of s and of full ensemble equivalence from the interval $(u_0, -\frac{1}{2q})$ of nonconcavity of s and of ensemble nonequivalence. Second, part (a) of Lemma 1.6.1 shows that u_0 equals the limiting mean energy $\tilde{H}(\nu^1(\beta_c))$ in the canonical equilibrium macrostate $\nu^1(\beta)$ as $\beta \to (\beta_c)^+$. In Figures 3 and 4 we present for $q = 3$ a third, geometric interpretation of u_0 that is also related to ensemble nonequivalence.

Before explaining this third, geometric interpretation of u_0, we recall that according to part (a) of Theorem 1.4.2 specialized to $q = 3$, $\mathcal{E}^u$ is nonempty, or equivalently the constraint set in (4.5) is nonempty, if and only if $u \in [-\frac{1}{2}, -\frac{1}{2q}] = [-\frac{1}{2}, -\frac{1}{6}]$. Geometrically, the energy constraint $\tilde{H}(\nu) = -\frac{1}{2}\langle \nu, \nu \rangle = u$ corresponds to the sphere in $I\!R^3$ with center 0 and radius $\sqrt{-2u}$. This sphere intersects the set $\mathcal{P}$ of probability vectors if and only if $u \in [-\frac{1}{2}, -\frac{1}{6}]$. For $u = -\frac{1}{6}$, the sphere is tangent to $\mathcal{P}$ at the unique point ρ while for $u = -\frac{1}{2}$, the hypersphere intersects $\mathcal{P}$ at the q unit-coordinate vectors. The intersection of the sphere and $\mathcal{P}$ undergoes a phase transition at u_0 in the following sense. For $u \in [u_0, -\frac{1}{6})$ the sphere intersects $\mathcal{P}$ in a circle while for $u \in [-\frac{1}{2}, u_0)$, the sphere intersects $\mathcal{P}$ in a proper subset of a circle; the complement of this subset lies outside the nonnegative octant of $I\!R^3$. For $u = u_0 = -\frac{1}{4}$, the circle of intersection is maximal and is tangent to the boundary of $\mathcal{P}$.

The set $\mathcal{E}_\beta$ of canonical equilibrium macrostates for $q = 3$ is represented in Figure 3. In this figure the maximal circle of intersection corresponding to $u = u_0 = -\frac{1}{4}$ is shown together with the vector ρ at its center; the points A, B, and C representing the respective unit-coordinate vectors $(1,0,0)$, $(0,1,0)$, and $(0,0,1)$; and the points A_c, B_c, and C_c representing the respective equilibrium macrostates $\nu^1(\beta_c)$, $\nu^2(\beta_c)$, and $\nu^3(\beta_c)$. These three macrostates lie on the maximal circle of intersection since $\tilde{H}(\nu^1(\beta_c)) = u_0$ [Lem. 1.6.1(b)]. For $\beta > \beta_c$ all $\nu \in \mathcal{E}_\beta$ have two equal components, and as $\beta \to \infty$ these vectors converge to the unit-coordinate vectors A, B, and C. Hence for $\beta > \beta_c$ the equilibrium macrostates $\nu^1(\beta)$, $\nu^2(\beta)$, and $\nu^3(\beta)$ are represented by the open line segments $\overline{A_cA}$, $\overline{B_cB}$, and $\overline{C_cC}$.

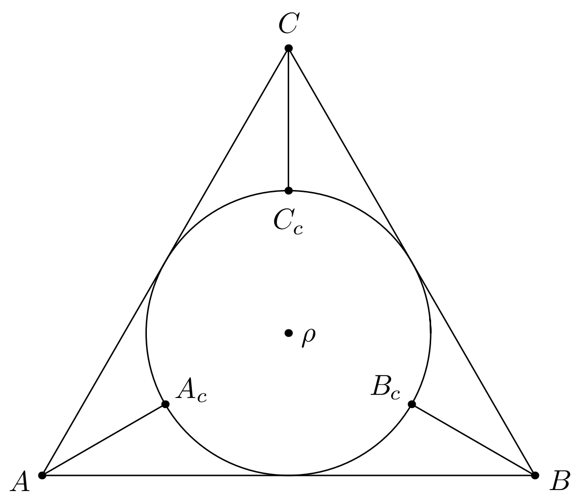

Figure 3. Graphical representation of the set $\mathcal{E}_\beta$ of canonical equilibrium macrostates for $q = 3$ showing the maximal circle of intersection corresponding to $u = u_0$; the vector ρ; the unit-coordinate vectors A, B, and C; and the macrostates $A_c = \nu^1(\beta_c)$, $B_c = \nu^2(\beta_c)$, and $C_c = \nu^3(\beta_c)$. The line segments $\overline{A_cA}$, $\overline{B_cB}$, and $\overline{C_cC}$ represent the elements of $\mathcal{E}_\beta$ for $\beta > \beta_c$.

The set $\mathcal{E}^u$ of microcanonical equilibrium macrostates for $q = 3$ is represented in Figure 4. In this figure the maximal circle of intersection corresponding to $u = u_0 = -\frac{1}{4}$ is shown together with the vector ρ at its center; the points A, B, and C representing the unit-coordinate vectors; and the points A_0, B_0, and C_0 representing the respective equilibrium macrostates $\mu^1(u_0)$, $\mu^2(u_0)$, and $\mu^3(u_0)$. For $u \in (-\frac{1}{2}, -\frac{1}{6})$ all $\nu \in \mathcal{E}^u$ have two equal components, and as $u \to -\frac{1}{2}$ they converge to the unit coordinate vectors

A, B, and C. Hence for $u \in (-\frac{1}{2}, -\frac{1}{6})$ the equilibrium macrostates $\mu^1(u)$, $\mu^2(u)$, and $\mu^3(u)$ are represented by the open line segments $\overline{\rho A}$, $\overline{\rho B}$, and $\overline{\rho C}$. As we saw in the preceding section, for each $u \in (-\frac{1}{2}, -\frac{1}{6})$ the macrostates $\mu^1(u)$, $\mu^2(u)$, and $\mu^3(u)$ lie on the intersection of the sphere of radius $\sqrt{-2u}$ with $\mathcal{P}$. In particular, $A_0 = \mu^1(u_0)$, $B_0 = \mu^2(u_0)$, and $C_0 = \mu^3(u_0)$ lie on the maximal circle of intersection.

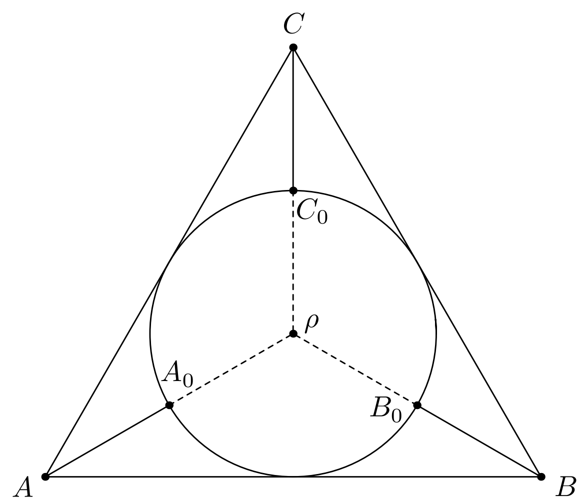

Figure 4. Graphical representation of the set $\mathcal{E}^u$ of microcanonical equilibrium macrostates for $q = 3$ showing the maximal circle of intersection corresponding to $u = u_0$; the vector ρ; the unit-coordinate vectors A, B, and C; and the macrostates $A_0 = \mu^1(u_0)$, $B_0 = \mu^2(u_0)$, and $C_0 = \mu^3(u_0)$. The solid-line segments $\overline{A_0 A}$, $\overline{B_0 B}$, and $\overline{C_0 C}$ represent the elements of $\mathcal{E}^u$ that are realized canonically. The dashed-line segments $\overline{\rho A_0}$, $\overline{\rho B_0}$, and $\overline{\rho C_0}$ represent the elements of $\mathcal{E}^u$ that are not realized canonically.

The distinguishing feature of Figure 4 is the three open dashed-line segments $\overline{\rho A_0}$, $\overline{\rho B_0}$, and $\overline{\rho C_0}$ representing the elements of $\mathcal{E}^u$ that are not realized canonically; namely, $\mu^1(u)$, $\mu^2(u)$, and $\mu^3(u)$ for $u \in (u_0, -\frac{1}{6})$. The three half open solid-line segments $\overline{A_0 A}$, $\overline{B_0 B}$, and $\overline{C_0 C}$ represent the elements of $\mathcal{E}^u$ that are realized canonically; namely, $\mu^1(u)$, $\mu^2(u)$, and $\mu^3(u)$ for $u \in (-\frac{1}{2}, u_0]$. For each such u the value of β for which $\mathcal{E}^u = \mathcal{E}_\beta$ is determined by the equation $\tilde{H}(\nu^1(\beta)) = u$ [Thm. 1.6.2(a)]. Thus in Figure 3 the corresponding elements of $\mathcal{E}_\beta$ lie on the intersection of the sphere of radius $\sqrt{-2u}$ and

$\mathcal{P}$.

This completes our discussion of equivalence and nonequivalence of ensembles. In the next section we will prove a number of statements concerning ensemble equivalence and nonequivalence that have been determined graphically.

1.6 Proofs of Equivalence and Nonequivalence of Ensembles

Using the general results of [23], we stated in the preceding section the equivalence and nonequivalence relationships that exist between $\mathcal{E}^u$ and $\mathcal{E}_\beta$ and verified these relationships using the plots of these sets for $q = 8$ given in Figure 2. Our purpose in the present section is to prove these relationships using mapping properties of the mean energy function $u(\beta)$ defined for $\beta \neq \beta_c$ by

$$u(\beta) = \begin{cases} \tilde{H}(\rho) = -\frac{1}{2q} & \text{for } \beta < \beta_c, \\ \tilde{H}(\nu^1(\beta)) = -\frac{1}{2}\langle \nu^1(\beta), \nu^1(\beta) \rangle & \text{for } \beta > \beta_c. \end{cases} \tag{6.1}$$

Here $\nu^1(\beta)$ is the unique canonical equilibrium macrostate modulo permutations for $\beta > \beta_c$ [Thm. 1.3.1]. According to the next lemma, for $\beta > \beta_c$, $u(\beta)$ is continuous and strictly decreasing and $u(\beta) < -\frac{1}{2q}$, which equals the mean energy for $\beta < \beta_c$. It follows that as β increases through β_c, $u(\beta)$ is discontinuous, jumping down from $-\frac{1}{2q}$ to $\tilde{H}(\nu^1(\beta))$. This discontinuity in $u(\beta)$ mirrors in a natural way the discontinuity in $\mathcal{E}_\beta$ as β increases through β_c.

We use the same notation u_0 for the quantity defined in (6.2) as for the quantity u_0 appearing in Figure 1 in Section 5 because these two quantities coincide. Indeed, with u_0 defined in (6.2), we prove in Theorem 1.6.2 that the largest open interval on which full equivalence of ensembles holds is int $F = (-\frac{1}{2}, u_0)$. This coincides with the interior of the interval F shown in Figure 1. As that figure exhibits, int F is the largest open interval on which s is strictly concave; by Theorem 1.5.1, that open interval coincides with the largest open interval on which full equivalence of ensembles holds.

Lemma 1.6.1. *For* $\beta \in [\beta_c, \infty)$ *we define* $\nu^1(\beta)$ *as in part* (b) *of Theorem* 1.3.1 *and we define*

$$u_0 = \frac{-q^2+3q-3}{2q(q-1)}, \tag{6.2}$$

The following conclusions hold.

(a) $-\frac{1}{2} < u_0 < -\frac{1}{2q}$ *and* $\lim_{\beta \to (\beta_c)^+} u(\beta) = \tilde{H}(\nu^1(\beta_c)) = u_0$.

(b) *The function mapping*

$$\beta \in (\beta_c, \infty) \mapsto u(\beta) = \tilde{H}(\nu^1(\beta)) = -\tfrac{1}{2}\langle \nu^1(\beta), \nu^1(\beta)\rangle$$

is a strictly decreasing, differentiable bijection onto the interval $(-\frac{1}{2}, u_0)$.

Proof. (a) The inequalities involving u_0 follow immediately from the inequality $q \geq 3$. The relationship $\tilde{H}(\nu^1(\beta_c)) = u_0$ is easily determined using the explicit form of $\nu^1(\beta_c)$ given in (3.5). That $\lim_{\beta \to (\beta_c)^+} u(\beta) = \tilde{H}(\nu^1(\beta_c))$ follows from the definition of $u(\beta)$ and the continuity of $\nu^1(\beta)$ for $\beta \geq \beta_c$.

(b) For $w \in I\!\!R$ define

$$f(w) = -\frac{1}{2}\left(\frac{[1+(q-1)w]^2}{q^2} + (q-1)\frac{[1-w]^2}{q^2}\right).$$

For $\beta \in (\beta_c, \infty)$ we use the formula for $\nu^1(\beta)$ given in part (b) of Theorem 1.3.1 to write $u(\beta) = -f(w(\beta))$. The quantity $w(\beta)$ is positive and strictly increasing, and for all $w > 0$,

$$f'(w) = \frac{(q-1)w}{q} > 0.$$

As the composition of two strictly increasing functions, for $\beta \in (\beta_c, \infty)$, $-u(\beta)$ is strictly increasing and thus $u(\beta)$ is strictly decreasing. In addition, since $\lim_{\beta \to \infty} w(\beta) =$

1 [Thm. 1.3.1(a)], we have $\lim_{\beta\to\infty} u(\beta) = -\frac{1}{2}$, and by part (a) of this lemma

$$\lim_{\beta\to(\beta_c)^+} u(\beta) = \tilde{H}(\nu(\beta_c)) = u_0.$$

It follows that the function mapping $\beta \in (\beta_c, \infty) \mapsto u(\beta)$ is a strictly decreasing, differentiable bijection onto the interval $(-\frac{1}{2}, u_0)$. This completes the proof of part (b). ■

Mapping properties of $u(\beta)$ play an important role in the next theorem, in which we prove that the sets F, P, and N defined in (6.3) correspond to full equivalence, partial equivalence, and nonequivalence of ensembles. For $u \in F$ we consider three subcases in order to indicate the value of β for which $\mathcal{E}^u = \mathcal{E}_\beta$; for $u \in \operatorname{int} F = (-\frac{1}{2}, u_0)$, β and u are related by $\beta = s'(u)$ and $u = u(\beta)$. Part (c) shows an interesting degeneracy in the equivalence-of-ensemble picture, the set $\mathcal{E}^u$ for $u = -\frac{1}{2q}$ corresponding to all $\mathcal{E}_\beta$ for $\beta < \beta_c$. This is related to the fact that for all such values of β, $\mathcal{E}_\beta = \{\rho\}$ and thus the mean energy $u(\beta)$ equals $-\frac{1}{2q}$.

Theorem 1.6.2. *We define $s(u)$ in* (4.2)*, $u(\beta)$ in* (6.1)*, $\mathcal{E}_\beta$ in* (2.3)*, and $\mathcal{E}^u$ in* (2.4)*. We also define β_c in* (3.1) *and u_0 in* (6.2)*. The sets*

$$F = (-\tfrac{1}{2}, u_0) \cup \{-\tfrac{1}{2q}\},\ P = \{u_0\},\ \text{ and } N = (u_0, -\tfrac{1}{2q}) \qquad (6.3)$$

have the following properties.

(a) **Full equivalence on int $\boldsymbol{F}$.** *For $u \in \operatorname{int} F = (-\frac{1}{2}, u_0)$, there exists a unique $\beta \in (\beta_c, \infty)$ such that $\mathcal{E}^u = \mathcal{E}_\beta$; β satisfies $u(\beta) = \tilde{H}(\nu^1(\beta)) = u$.*

(b) *For $u \in \operatorname{int} F = (-\frac{1}{2}, u_0)$, s is differentiable. The values u and β for which $\mathcal{E}^u = \mathcal{E}_\beta$ in part* (a) *are also related by the thermodynamic formula $s'(u) = \beta$.*

(c) **Full equivalence at $\boldsymbol{-\frac{1}{2q}}$.** *For $u = -\frac{1}{2q} \in F$, $\mathcal{E}^{-\frac{1}{2q}} = \mathcal{E}_\beta$ for any $\beta < \beta_c$.*

(d) **Partial equivalence on $\boldsymbol{P}$.** *For $u \in P = \{u_0\}$, $\mathcal{E}^{u_0} \subset \mathcal{E}_{\beta_c}$ but $\mathcal{E}^{u_0} \neq \mathcal{E}_{\beta_c}$. In fact, $\mathcal{E}_{\beta_c} = \mathcal{E}^{u_0} \cup \mathcal{E}^{-\frac{1}{2q}}$.*

(e) **Nonequivalence on $\boldsymbol{N}$.** *For any $u \in N = (u_0, -\frac{1}{2q})$, $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ for all $\beta \in I\!\!R$.*

In reference to the properties of s given in part (b), one can show that the function mapping $u \in (-\frac{1}{2}, u_0) \mapsto s'(u)$ is a strictly decreasing, differentiable bijection onto the interval (β_c, ∞) and that this bijection is the inverse of the bijection mapping $\beta \in (\beta_c, \infty) \mapsto u(\beta)$.

Before we prove the theorem, it is instructive to compare its assertions with those in Theorem 1.5.1, which formulates ensemble equivalence and nonequivalence in terms of support properties of s. These support properties can be seen in the schematic plot of the the graph of s in Figure 1. We start with part (a) of Theorem 1.6.2, which states that for any $u \in \operatorname{int} F = (-\frac{1}{2}, u_0)$ there exists a unique $\beta \in (\beta_c, \infty)$ such that $\mathcal{E}^u = \mathcal{E}_\beta$. As promised in part (a)(i) of Theorem 1.5.1, this β is the slope of a strictly supporting line to the graph of s at u, and so s is strictly concave on $\operatorname{int} F$. The situation that holds when $u = -\frac{1}{2q}$ [Thm. 1.6.2(c)] is also consistent with part (a)(i) of Theorem 1.5.1. For this value of u, which is the isolated point of the set F of full equivalence, there exist infinitely many strictly supporting lines to the graph of s, the possible slopes of which are all $\beta \in (-\infty, \beta_c)$. On the other hand, when $u = u_0$, which is the only value lying in the set P of partial equivalence, we have $\mathcal{E}^{u_0} \subset \mathcal{E}_{\beta_c}$ but $\mathcal{E}^{u_0} \neq \mathcal{E}_{\beta_c}$ [Thm. 1.6.2(d)]. In combination with part (a)(ii) of Theorem 1.5.1, it follows that there exists a nonstrictly supporting line at u_0 with slope β_c and that s is concave at u_0 but not strictly concave. Finally, for $u \in N = (u_0, -\frac{1}{2q})$, we have $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ for all $\beta \in I\!\!R$ [Thm. 1.6.2(e)]. In accordance with part (a)(iii) of Theorem 1.5.1, s has no supporting line at any $u \in N$, and by Theorem A.4 in [14] s is not concave at any $u \in N$.

Proof of Theorem 1.6.2. (a) For $\beta > \beta_c$ part (b) of Theorem 1.3.1 and part (b) of Theorem 1.5.1 imply that

$$\mathcal{E}_\beta = \{\nu^1(\beta), \ldots, \nu^q(\beta)\} = \bigcup_{u \in \tilde{H}(\mathcal{E}_\beta)} \mathcal{E}^u.$$

The symmetry of $\tilde{H}$ with respect to permutations implies that $\tilde{H}(\mathcal{E}_\beta) = \{\tilde{H}(\nu^1(\beta))\}$. Thus for any $\beta > \beta_c$

$$\mathcal{E}_\beta = \mathcal{E}^{\tilde{H}(\nu^1(\beta))}. \tag{6.4}$$

Since for any $u \in \text{int}\, F = (-\frac{1}{2}, u_0)$ there exists a unique $\beta \in (\beta_c, \infty)$ satisfying $u(\beta) = \tilde{H}(\nu^1(\beta)) = u$ [Lem. 1.6.1(b)], it follows that $\mathcal{E}^u = \mathcal{E}_\beta$.

(b) The differentiability of s on $\text{int}\, F$ is proved in part (b) of Theorem 1.6.3, which depends only on part (a) of the present theorem. By part (a) of the present theorem and part (a) of Theorem 1.5.1, s has a strictly supporting line at each $u \in \text{int}\, F$. It follows that s is strictly concave on $\text{int}\, F$ and thus concave on $\text{int}\, F$ [14, Lem. 4.1(a)]; i.e., $s(u) = s^{**}(u)$ for all $u \in \text{int}\, F$. The differentiability of s on $\text{int}\, F$ [Thm. 1.6.3(b)] combined with part (a) of Theorem A.3 in [14] implies that $s'(u) = \beta$.

(c) By (4.6) and part (b) of Theorem 1.3.1

$$\mathcal{E}^{-\frac{1}{2q}} = \{\rho\} = \mathcal{E}_\beta \text{ for any } \beta < \beta_c. \tag{6.5}$$

(d) By part (b) of Theorem 1.3.1, symmetry, and part (a) of Lemma 1.6.1

$$\tilde{H}(\mathcal{E}_{\beta_c}) = \{\tilde{H}(\rho), \tilde{H}(\nu^1(\beta_c))\} = \{-\tfrac{1}{2q}, u_0\}.$$

Hence by (6.4) and (6.5)

$$\mathcal{E}_{\beta_c} = \bigcup_{u \in \tilde{H}(\mathcal{E}_{\beta_c})} \mathcal{E}^u = \mathcal{E}^{-\frac{1}{2q}} \cup \mathcal{E}^{u_0} = \{\rho\} \cup \mathcal{E}^{u_0}.$$

However, $\rho \notin \mathcal{E}^{u_0}$ since ρ does not satisfy the constraint $\tilde{H}(\rho) = u_0$. It follows that $\mathcal{E}^{u_0} \subset \mathcal{E}_{\beta_c}$ but that $\mathcal{E}^{u_0} \neq \mathcal{E}_{\beta_c}$.

(e) If $u \in N$, then $u \notin (-\frac{1}{2}, u_0)$, and so by part (b) of Lemma 1.6.1 $u \neq \tilde{H}(\nu^1(\beta))$ for any $\beta \in (\beta_c, \infty)$. Since by (6.4) $\mathcal{E}_\beta = \mathcal{E}^{\tilde{H}(\nu^1(\beta))}$ for all $\beta > \beta_c$, it follows that for all $\beta > \beta_c$

$$\mathcal{E}^u \cap \mathcal{E}^{\tilde{H}(\nu^1(\beta))} = \emptyset$$

and thus that $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$. For any $\beta < \beta_c$ (6.5) states that $\mathcal{E}_\beta = \mathcal{E}^{-\frac{1}{2q}} = \{\rho\}$. Since $u \in N$, we have $u \neq -\frac{1}{2q}$ and thus $\mathcal{E}^{-\frac{1}{2q}} \cap \mathcal{E}^u = \emptyset$. It follows that $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ for any $\beta < \beta_c$. Finally, for $\beta = \beta_c$ part (b) of Theorem 1.3.1 states that $\mathcal{E}_{\beta_c} = \{\rho, \nu^1(\beta_c), \ldots, \nu^q(\beta_c)\}$. However, since $\tilde{H}(\rho) = -\frac{1}{2q} \notin N$ and $\tilde{H}(\nu^i(\beta_c)) = u_0 \notin N$, none of the vectors in $\mathcal{E}_{\beta_c}$ satisfies the constraint $\tilde{H}(\nu) = u$. Thus $\mathcal{E}^u \cap \mathcal{E}_{\beta_c} = \emptyset$. We have proved $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ for all $\beta \in I\!R$. The proof of the theorem is complete. ■

We end this section by showing that for arbitrary $q \geq 4$ and u in the equivalence sets $F \cup P = (-\frac{1}{2}, u_0] \cup \{-\frac{1}{2q}\}$ the formulas for $\mathcal{E}^u$ and $s(u)$ given in part (d) of Theorem 1.4.2 and part (c) of Theorem 1.4.3 are rigorously true. Our strategy is to use the equivalence of the microcanonical and canonical ensembles for $u \in F \cup P$ and the fact that the form of $\mathcal{E}_\beta$ is known exactly for all β. Thus, we translate the form of $\nu \in \mathcal{E}_\beta$, as given in part (b) of Theorem 1.3.1, into the form of $\nu \in \mathcal{E}^u$ for $u \in F \cup P$. For $\beta \in [\beta_c, \infty)$, the last $q - 1$ components of $\nu^1(\beta) \in \mathcal{E}_\beta$ are given by

$$\nu_j^1(\beta) = \frac{1 - w(\beta)}{q}, \tag{6.6}$$

and these components are not equal to the first component. Since for each $u \in F \cup P$ there exists $\beta \in [\beta_c, \infty]$ such that either $\mathcal{E}^u = \mathcal{E}_\beta$ or $\mathcal{E}^u \subset \mathcal{E}_\beta$, it follows that modulo permutations all $\nu \in \mathcal{E}^u$ have their last $q - 1$ components equal to each other. That is, modulo permutations there exist numbers a and b in $[0, 1]$ such that $\nu = (a, b, \ldots, b)$. The possible values of a and b are easily determined by considering the constraints satisfied by $\nu \in \mathcal{E}^u$. These constraints are

$$a + (q-1)b = 1 \text{ and } a^2 + (q-1)b^2 = -2u.$$

The two solutions of these equations are

$$a_1 = \frac{1 - \sqrt{(q-1)(-2qu-1)}}{q}, \quad b_1 = \frac{q - 1 + \sqrt{(q-1)(-2qu-1)}}{(q-1)q}$$

and

$$a_2 = \frac{1 + \sqrt{(q-1)(-2qu-1)}}{q}, \quad b_2 = \frac{q - 1 - \sqrt{(q-1)(-2qu-1)}}{(q-1)q}.$$

Of the two values b_1 and b_2, only b_2 has the form given in (6.6) with

$$w(\beta) = \frac{\sqrt{(q-1)(-2qu-1)}}{q-1} \in [0,1].$$

We conclude that modulo permutations each $\nu \in \mathcal{E}^u$ has the form $(a_2, b_2, \ldots, b_2)$, in which the last $q-1$ components all equal b_2. This coincides with the formula for $\mu^1(u)$ given in part (d) of Theorem 1.4.2, which in turn gives the explicit formula for $s(u)$ in part (c) of Theorem 1.4.3. This information is summarized in part (a) of the next theorem. The differentiability of s on int F, which is stated in part (b), is an immediate consequence of the explicit formula for $s(u)$.

Theorem 1.6.3. *We define u_0 in* (6.2). *The following conclusions hold.*

(a) *For arbitrary $q \geq 4$ and u in the equivalence sets $F \cup P = (-\frac{1}{2}, u_0] \cup \{-\frac{1}{2q}\}$ the formulas for $\mathcal{E}^u$ and $s(u)$ given in part* (d) *of Theorem* 1.4.2 *and part* (c) *of Theorem* 1.4.3 *are rigorously true.*

(b) *For arbitrary $q \geq 4$, s is differentiable on the interval* int $F = (-\frac{1}{2}, u_0)$ *and $s'(u)$ is given by* (5.1).

1.7 Two Related Maximization Problems

Theorem 1.7.1 is a new result on the maximum points of certain functions related by convex duality. It is formulated for a finite, differentiable, convex function F on $I\!R^\sigma$ and its Legendre-Fenchel transform

$$F^*(z) = \sup_{x \in I\!R^\sigma} \{\langle x, z\rangle - F(x)\}.$$

The domain of F^* is the set $\text{dom}\, F^* = \{z \in I\!R^\sigma : F^*(z) < \infty\}$. With only minor changes in notation the theorem is also valid for a finite, Gateaux-differentiable, convex function on a Hilbert space.

Theorem 1.7.1 will be applied in Section 1.8 to prove that for $\beta > 0$, $\mathcal{E}_\beta$ has the form given in part (b) of Theorem 1.3.1. Another application of Theorem 1.7.1 is given in Proposition 3.4 in [26]. It is used there to determine the form of the set of canonical equilibrium macrostates for another important spin system known as the mean-field Blume-Emery-Griffiths model.

Theorem 1.7.1. *Let σ be a positive integer and F a finite, differentiable, convex function mapping $I\!R^\sigma$ into $I\!R$. Assume that $\sup_{z\in I\!R^\sigma}\{F(z) - \frac{1}{2}\|z\|^2\} < \infty$ and that $F(z) - \frac{1}{2}\|z\|^2$ attains its supremum. The following conclusions hold.*

(a) $\sup_{z \in I\!R^\sigma}\{F(z) - \frac{1}{2}\|z\|^2\} = \sup_{z \in \text{dom}\, F^*}\{\frac{1}{2}\|z\|^2 - F^*(z)\}$.

(b) $\frac{1}{2}\|z\|^2 - F^*(z)$ *attains its supremum on* $\text{dom}\, F^*$.

(c) *The global maximum points of $F(z) - \frac{1}{2}\|z\|^2$ coincide with the global maximum points of $\frac{1}{2}\|z\|^2 - F^*(z)$.*

Proof. We define the subdifferential of F^* at $z_0 \in I\!R^\sigma$ by

$$\partial F^*(z_0) = \{y \in I\!R^\sigma : F^*(z) \geq F^*(z_0) + \langle y, z - z_0\rangle \text{ for all } z \in I\!R^\sigma\}.$$

We also define the domain of ∂F^* to be the set of $z_0 \in I\!R^\sigma$ for which $\partial F^*(z_0) \neq \emptyset$. The proof of the theorem uses three properties of Legendre-Fenchel transforms.

1. F^* is a convex, lower semicontinuous function mapping $\mathbb{R}^\sigma$ into $\mathbb{R} \cup \{\infty\}$, and for all $z \in \mathbb{R}^\sigma$, $F^{**}(z) = (F^*)^*(z)$ equals $F(z)$ [21, Thm. VI.5.3(a),(e)].

2. If for some $z_0 \in \mathbb{R}^\sigma$ and $z \in \mathbb{R}^\sigma$ we have $z = \nabla F(z_0)$, then $F(z_0) + F^*(z) = \langle z_0, z\rangle$ [21, Thms. VI.3.5(d), VI.5.3(c)], and so $z \in \operatorname{dom} F^*$. In particular, if $z = z_0$, then $z_0 \in \operatorname{dom} F^*$ and $F(z_0) + F^*(z_0) = \|z_0\|^2$.

3. For $z_0 \in \operatorname{dom} F^*$ and $y \in \partial F^*(z_0)$ we have $F(y) + F^*(z_0) = \langle y, z_0\rangle$ [21, Thm. VI.5.3(c),(d)]. In particular, if $y = z_0$, then $F(z_0) + F^*(z_0) = \|z_0\|^2$.

We first prove part (a), which is a special case of Theorem C.1 in [20]. Let $M = \sup_{z\in\mathbb{R}^\sigma}\{F(z) - \|z\|^2/2\}$. Since for any $z \in \operatorname{dom} F^*$ and x in $\mathbb{R}^\sigma$

$$F^*(z) + M \geq \langle x, z\rangle - F(x) + M \geq \langle x, z\rangle - \|x\|^2/2,$$

we have

$$F^*(z) + M \geq \sup_{x\in\mathbb{R}^\sigma}\{\langle x, z\rangle - \|x\|^2/2\} = \|z\|^2/2.$$

It follows that $M \geq \|z\|^2/2 - F^*(z)$ and thus that $M \geq \sup_{z\in\operatorname{dom} F^*}\{\|z\|^2/2 - F^*(z)\}$. To prove the reverse inequality, let $N = \sup_{z\in\operatorname{dom} F^*}\{\|z\|^2/2 - F^*(z)\}$. Then for any $z \in \mathbb{R}^\sigma$ and $x \in \operatorname{dom} F^*$

$$\|z\|^2/2 + N \geq \langle x, z\rangle - \|x\|^2/2 + N \geq \langle x, z\rangle - F^*(x).$$

Since $F^*(x) = \infty$ for $x \notin \operatorname{dom} F^*$, it follows from property 1 that

$$\|z\|^2/2 + N \geq \sup_{x\in\operatorname{dom} F^*}\{\langle x, z\rangle - F^*(x)\} = F(z)$$

and thus that $N \geq \sup_{z\in\mathbb{R}^\sigma}\{F(z) - \|z\|^2/2\}$.

In order to prove parts (b) and (c) of Theorem 1.7.1, let z_0 be any point in $\mathbb{R}^\sigma$ at which $F(z) - \frac{1}{2}\|z\|^2$ attains its supremum. Then $z_0 = \nabla F(z_0)$, and so by the last line of property 2, $z_0 \in \text{dom}\, F^*$ and $F(z_0) + F^*(z_0) = \|z_0\|^2$. Part (a) now implies that

$$\begin{aligned}\sup_{z \in I\!\!R^\sigma} \{F(z) - \tfrac{1}{2}\|z\|^2\} &= F(z_0) - \tfrac{1}{2}\|z_0\|^2 \\ &= \tfrac{1}{2}\|z_0\|^2 - F^*(z_0) = \sup_{z \in \text{dom}\, F^*} \{\tfrac{1}{2}\|z\|^2 - F^*(z)\}.\end{aligned}$$

We conclude that $\frac{1}{2}\|z\|^2 - F^*(z)$ attains its supremum on dom F^* at z_0. Not only have we proved part (b), but also we have proved half of part (c); namely, any global maximizer of $F(z) - \frac{1}{2}\|z\|^2$ is a global maximizer of $\frac{1}{2}\|z\|^2 - F^*(z)$.

Now let z_0 be any point at which $\frac{1}{2}\|z\|^2 - F^*(z)$ attains its supremum. Then for any $z \in I\!\!R^\sigma$

$$\tfrac{1}{2}\langle z_0, z_0\rangle - F^*(z_0) \geq \tfrac{1}{2}\langle z, z\rangle - F^*(z).$$

It follows that for any $z \in I\!\!R^\sigma$

$$F^*(z) \geq F^*(z_0) + \tfrac{1}{2}(\langle z, z\rangle - \langle z_0, z_0\rangle) \geq F^*(z_0) + \langle z_0, z - z_0\rangle$$

and thus that $z_0 \in \partial F^*(z_0)$. By the last line of property 3 this implies that $F(z_0) + F^*(z_0) = \|z_0\|^2$. In conjunction with part (a) this in turn implies that

$$\begin{aligned}\sup_{z \in \text{dom}\, F^*} \{\tfrac{1}{2}\|z\|^2 - F^*(z)\} &= \tfrac{1}{2}\|z_0\|^2 - F^*(z_0) \\ &= F(z_0) - \tfrac{1}{2}\|z_0\|^2 = \sup_{z \in I\!\!R^\sigma} \{F(z) - \tfrac{1}{2}\|z\|^2\}.\end{aligned}$$

We conclude that $F(z) - \frac{1}{2}\|z\|^2$ attains its supremum at z_0. This completes the proof of the theorem. ■

1.8 Form of $\mathcal{E}_\beta$

We first derive the form of $\mathcal{E}_\beta$ for $\beta > 0$ as given in part (b) of Theorem 1.3.1. We then prove that $\mathcal{E}_\beta = \{\rho\}$ for all $\beta \leq 0$.

$\mathcal{E}_\beta$ is defined as the set of $\nu \in \mathcal{P}$ that minimize $R(\nu|\rho) - \frac{\beta}{2}\langle \nu, \nu \rangle$. Since $\beta > 0$, this is equivalent to

$$\mathcal{E}_\beta = \left\{ \nu \in \mathcal{P} : \nu \text{ maximizes } \tfrac{1}{2}\langle \nu, \nu \rangle - \tfrac{1}{\beta} R(\nu|\rho) \right\}. \tag{8.1}$$

This maximization problem has the form of the right hand side of part (a) of Theorem 1.7.1; viz.,

$$\sup_{\nu \in \mathcal{P}} \left\{ \tfrac{1}{2}\langle \nu, \nu \rangle - \tfrac{1}{\beta} R(\nu|\rho) \right\} = \sup_{\nu \in \text{dom } F^*} \{ \tfrac{1}{2}\|\nu\|^2 - F^*(\nu) \}$$

with $F^*(\nu) = \frac{1}{\beta} R(\nu|\rho)$.

In order to determine the function F having this Legendre-Fenchel transform, for $z \in I\!\!R^q$ we define the finite, differentiable, convex function

$$\Gamma(z) = \log \left(\textstyle\sum_{i=1}^q e^{z_i} \, \frac{1}{q} \right) \tag{8.2}$$

and set $\Gamma_\beta(z) = \frac{1}{\beta}\Gamma(\beta z)$. Since for $\nu \in I\!\!R^q$ [21, Thm. VIII.2.2]

$$\Gamma^*(\nu) = \begin{cases} R(\nu|\rho) & \text{for } \nu \in \mathcal{P} \\ \infty & \text{otherwise}, \end{cases}$$

it follows that for $\nu \in I\!\!R^q$

$$\begin{aligned} (\Gamma_\beta)^*(\nu) &= \sup_{z \in I\!\!R^q} \left\{ \langle z, \nu \rangle - \tfrac{1}{\beta}\Gamma(\beta z) \right\} \\ &= \tfrac{1}{\beta}\Gamma^*(\nu) = \begin{cases} \frac{1}{\beta} R(\nu|\rho) & \text{for } \nu \in \mathcal{P} \\ \infty & \text{otherwise}. \end{cases} \end{aligned}$$

Thus $F(z) = \frac{1}{\beta}\Gamma(\beta z)$. By part (a) of Theorem 1.7.1

$$\sup_{z \in I\!\!R^q} \left\{ \tfrac{1}{\beta}\Gamma(\beta z) - \tfrac{1}{2}\|z\|^2 \right\} = \sup_{\nu \in \mathcal{P}} \left\{ \tfrac{1}{2}\langle \nu, \nu \rangle - \tfrac{1}{\beta} R(\nu|\rho) \right\},$$

and by part (b) of the theorem the global maximum points of $\Gamma(\beta z) - \frac{1}{2}\|z\|^2$ and $\frac{1}{2}\langle \nu, \nu \rangle - \frac{1}{\beta} R(\nu|\rho)$ coincide.

Equation (8.1) now implies that

$$\begin{aligned}\mathcal{E}_\beta &= \left\{z \in I\!R^q : z \text{ maximizes } \tfrac{1}{\beta}\Gamma(\beta z) - \tfrac{1}{2}\|z\|^2\right\} \\ &= \left\{z \in I\!R^q : z \text{ minimizes } \tfrac{\beta}{2}\|z\|^2 - \Gamma(\beta z)\right\}.\end{aligned}$$

We summarize this discussion in the following corollary. Part (b) of the corollary is proved in part (b) of Theorem 2.1 in [28].

Corollary 1.8.1. *We define the finite, convex, continuous function* Γ *in* (8.2). *The following conclusions hold.*

(a) $\mathcal{E}_\beta$ *coincides with the set of global minimum points of*

$$G_\beta(z) = \tfrac{\beta}{2}\|z\|^2 - \log \sum_{i=1}^{q} e^{\beta z_i} = \tfrac{\beta}{2}\|z\|^2 - \Gamma(\beta z) - \log q.$$

(b) *For* $0 < \beta < \beta_c$, $\beta = \beta_c$, *and* $\beta > \beta_c$ *the set of global minimum points of* G_β *has the form given by the right hand side of* (3.4) [*Thm.* 1.3.1(b)].

Corollary 1.8.1 completes the proof of Theorem 1.3.1. Michael Kiessling's proof of this corollary based on Lagrange multipliers is given in Appendix B of [29]. Continuous analogues of the corollary are mentioned in [45], [46], and [53], but are not proved there.

We now show that for all $\beta \leq 0$, $\mathcal{E}_\beta = \{\rho\}$. This is obvious for $\beta = 0$ since $\nu = \rho$ is the unique vector in $\mathcal{P}$ that minimizes $R(\nu|\rho)$. Our goal is to prove that for $\beta < 0$, $\nu = \rho$ is also the unique vector in $\mathcal{P}$ that minimizes $R(\nu|\rho) - \frac{\beta}{2}\langle\nu,\nu\rangle$. Let $\bar{\nu}$ be a point in $\mathcal{P}$ at which $R(\nu|\rho) - \frac{\beta}{2}\langle\nu,\nu\rangle$ attains its infimum. For any $i = 1, 2, \ldots, q$,

$$\frac{\partial(R(\nu|\rho) - \frac{\beta}{2}\langle\nu,\nu\rangle)}{\partial\nu_i} = \log\nu_i + 1 - \beta\nu_i,$$

which is negative for all sufficiently small $\nu_i > 0$. It follows that $\bar{\nu}$ does not lie on the relative boundary of $\mathcal{P}$; i.e., $\bar{\nu}_j > 0$ for all $i = 1, 2, \ldots, q$. We complete the proof by showing that for any $1 \leq j < k \leq q$, $\bar{\nu}_j = \bar{\nu}_k$. Since ρ is the only point in $\mathcal{P}$ satisfying these equalities, we will be done.

Given $a \in (0,1)$, we consider the reduced two-variable problem of minimizing $R(\nu|\rho) - \frac{\beta}{2}\langle \nu, \nu \rangle$ over $\nu_j > 0$ and $\nu_k > 0$ under the constraint $\nu_j + \nu_k = a$; all the other components ν_i are fixed and equal $\bar{\nu}_i$. Setting $\nu_k = a - \nu_j$, we define

$$F(\nu_j) = R(\nu|\rho) - \tfrac{\beta}{2}\langle \nu, \nu \rangle.$$

Differentiating with respect to ν_j shows that any global minimizer ν_j must satisfy

$$F'(\nu_j) = \log \nu_j - \log(a - \nu_j) - \beta(2\nu_j - a) = 0.$$

Since

$$F''(\nu_j) = \tfrac{1}{\nu_j} + \tfrac{1}{a - \nu_j} - 2\beta > 0,$$

$F'(\nu_j)$ is strictly increasing from negative values for all ν_j near 0 to positive values for all ν_j near a. It follows that the only root of $F'(\nu_j) = 0$ is $\nu_j = \frac{a}{2}$ and thus that $\nu_k = \frac{a}{2} = \nu_j$. Being a global minimizer of $R(\nu|\rho) - \frac{\beta}{2}\langle \nu, \nu \rangle$ over $\mathcal{P}$, $\bar{\nu}$ is also a global minimizer of the reduced two-variable problem. Since $a \in (0,1)$ is arbitrary, it follows that for any distinct pair of indices $\bar{\nu}_j = \bar{\nu}_k$. This completes the proof.

CHAPTER 2

THE GENERALIZED CANONICAL ENSEMBLE AND ITS UNIVERSAL EQUIVALENCE WITH THE MICROCANONICAL ENSEMBLE

2.1 Introduction

The problem of ensemble equivalence is a fundamental one lying at the foundations of equilibrium statistical mechanics. When formulated in mathematical terms, it is apparent that this problem also addresses a fundamental issue in global optimization. Given a constrained minimization problem, under what conditions does there exist a related, unconstrained minimization problem having the same minimum points?

In order to explain the connection between ensemble equivalence and global optimization and in order to outline the contributions of this chapter, 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 $I\!R^\sigma$, where σ is a positive integer. For $u \in I\!R^\sigma$ we consider the following constrained minimization problem:

$$\text{minimize } I(x) \text{ over } x \in \mathcal{X} \text{ subject to the constraint } \tilde{H}(x) = u. \tag{1.1}$$

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 $\beta \in I\!\!R^\sigma$:

$$\text{minimize } I(x) + \langle \beta, \tilde{H}(x) \rangle \text{ over } x \in \mathcal{X}, \tag{1.2}$$

where $\langle \cdot, \cdot \rangle$ denotes the Euclidean inner product on $I\!\!R^\sigma$. The theory of Lagrange multipliers outlines suitable conditions under which the solutions of the constrained problem (1.1) lie among the critical points of $I + \langle \beta, \tilde{H} \rangle$. However, it does not indicate when the solutions of (1.1) lie among the minimum points of the unconstrained problem (1.2).

These two minimization problems arise in a natural way in the context of equilibrium statistical mechanics [23], 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 minimization problem (1.1) and the unconstrained minimization problem (1.2); i.e.,

$$\mathcal{E}^u = \{x \in X : I(x) \text{ is minimized subject to } \tilde{H}(x) = u\} \tag{1.3}$$

and

$$\mathcal{E}_\beta = \{x \in X : I(x) + \langle \beta, \tilde{H}(x) \rangle \text{ is minimized}\}. \tag{1.4}$$

For a given statistical mechanical model $\mathcal{X}$ represents the set of all possible equilibrium macrostates. As we outline in the next few paragraphs, 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.

The two ensembles are defined in terms of a number of quantities that specify the model: a sequence of prior measures P_n on configuration spaces Ω_n, a sequence of positive scaling constants $a_n \to \infty$; functions H_n mapping Ω_n into $I\!\!R^\sigma$, where σ is a positive integer; and the functions $h_n = H_n/a_n$. 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. The components of H_n include the Hamiltonian and, if $\sigma > 1$, other dynamical invariants appropriate to the system under investigation.

For $u \in I\!\!R^\sigma$, $r > 0$, and subsets B of Ω_n, the microcanonical ensemble is the conditioned measure

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

where $\{u\}^{(r)}$ denotes the hypercube in $I\!\!R^\sigma$ with center u and side length $2r$. A mathematically more tractable probability measure is the canonical ensemble, defined for $\beta \in I\!\!R^\sigma$ and subsets B of Ω_n by

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

In this formula $Z_n(\beta)$ is a normalization constant that makes $P_{n,\beta}$ a probability measure.

In order to identify the set of equilibrium macrostates for each ensemble, we assume that there exist macroscopic variables Y_n mapping the configuration spaces Ω_n into $\mathcal{X}$ and satisfying two basic properties:

1. With respect to P_n, Y_n satisfies the large deviation principle (LDP) on $\mathcal{X}$ with scaling constants a_n and rate function I. This is summarized by the formal notation

$$P_n\{Y_n \approx x\} \asymp e^{-a_n I(x)}. \tag{1.5}$$

2. There exists a bounded, continuous function $\tilde{H}$ mapping $\mathcal{X}$ into $I\!\!R^\sigma$ such that as $n \to \infty$

$$h_n(Y_n(\omega)) = \tilde{H}(Y_n(\omega)) + \mathrm{o}(1) \text{ uniformly over } \omega \in \Omega_n. \tag{1.6}$$

   We call $\tilde{H}$ the interaction representation function.

A number of models for which these properties are valid, including long-range and short-range spin models and models of coherent structures in turbulence, are discussed in Example 2.5.1. In the case of the long-range spin models discussed in items 1 and 2 in

Example 2.5.1, $a_n = n$ denotes the number of spin random variables, which take values in a finite set Λ; P_n denotes product measure with uniform one-dimensional marginals ρ on the configuration spaces $\Omega_n = \Lambda^n$; and Y_n denotes the empirical measure associated with the spin random variables, which takes values in the set $\mathcal{X}$ of probability measures on Λ. In this case, the LDP summarized in (1.5) is Sanov's Theorem, the rate function I is the relative entropy with respect to ρ, and the interaction representation function $\tilde{H}$ is a quadratic function of Y_n.

Using properties 1 and 2, the authors prove in [23] that with respect to $P_n^{u,r}$, in the double limit $n \to \infty$ and $r \to 0$, Y_n satisfies the LDP on $\mathcal{X}$ with rate function

$$I^u(x) = \begin{cases} I(x) - \text{const} & \text{if } \tilde{H}(x) = u \\ \infty & \text{otherwise.} \end{cases} \tag{1.7}$$

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

$$I_\beta(x) = I(x) + \langle \beta, \tilde{H}(x) \rangle - \text{const.} \tag{1.8}$$

These LDPs are summarized by the formal notations

$$P_n^{u,r}\{Y_n \approx x\} \asymp \exp[-a_n I^u(x)] \text{ and } P_{n,\beta}\{Y_n \approx x\} \asymp \exp[-a_n I_\beta(x)]. \tag{1.9}$$

The constants in (1.7) and (1.8) have the property that the infimums of I^u and I_β over $\mathcal{X}$ are both 0. Thus I^u and I_β are nonnegative on $\mathcal{X}$. If $I^u(x) > 0$ or $I_\beta(x) > 0$, then the corresponding probability in the last display converges exponentially fast to 0 as $n \to \infty$. Hence it makes sense to identify the equilibrium macrostates for each ensemble with the 0-sets of the associated rate function. This procedure gives rise to the set $\mathcal{E}^u$ defined in (1.3) and the set $\mathcal{E}_\beta$ defined in (1.4).

Defined via conditioning on h_n, 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 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 discussed near the end of this introduction 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 [23] 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

$$s(u) = -\inf\{I(x) : x \in \mathcal{X}, \tilde{H}(x) = u\}. \tag{1.10}$$

Since I maps $\mathcal{X}$ into $[0, \infty]$, s maps $I\!R^\sigma$ into $[-\infty, 0]$; the domain of s is the set dom $s = \{u \in I\!R^\sigma : s(u) > -\infty\}$. The main results in [23] are summarized in Theorem 2.1.1, which we now discuss under the simplifying assumption that dom s is an open subset of $I\!R^\sigma$.

We focus on $u \in$ dom s. Part (a) of Theorem 2.1.1 shows 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 dom s is convex and open and s is strictly concave at all u, then s has a strictly supporting hyperplane at all u [Prop. 2.2.9(b)] and thus full equivalence of ensembles holds at all u. In this case we say that the microcanonical and canonical ensembles are **universally equivalent**. Part (b) of the theorem treats a variation of part (a) involving partial equivalence.

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 $\beta \in I\!R^\sigma$. 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 shows 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.

Parts (a)–(c) of the next theorem are proved in Theorems 4.4 and 4.8 of [23]. Part (d) gives an alternative version of Theorem 4.6 in [23] proved in Corollary 2.5.3 in the present chapter. In order to state the theorem, we introduce some notation. For $\beta \in I\!R^\sigma$ we define $[\beta, -1]$ to be the vector in $I\!R^{\sigma+1}$ whose first σ components agree with those of β and whose last component equals -1.

Theorem 2.1.1. *For fixed u, the conclusions given in parts* (a)–(d) *hold.*

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

(b) **Partial equivalence.** *There exists $\beta \in I\!R^\sigma$ 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 $[\beta, -1]$.*

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

(d) **Canonical is always realized microcanonically.** *For $\beta \in I\!R^\sigma$ we define A_β to be the set of u such that s has a supporting hyperplane at u with normal vector $[\beta, -1]$. Then*

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

The starting point of the present chapter is the following natural question suggested by Theorem 2.1.1.

Motivational question. Given that the microcanonical ensemble is not equivalent with the canonical ensemble on a subset of values of u, 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 is a natural perturbation of the standard canonical ensemble, obtained from it by adding an exponential factor involving a continuous function g of h_n. 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 [10, 11, 43]. Although not referred to by name, the Gaussian ensemble also plays a key role in [46], 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. For $n \in I\!N$, $\beta \in I\!R^\sigma$, $\gamma \geq 0$, u in $I\!R^\sigma$, and subsets B of Ω_n, the Gaussian ensemble is defined by

$$P^u_{n,\beta,\gamma}\{B\} = \frac{1}{Z_n(\beta,\gamma,u)} \cdot \int_B \exp\Big[-a_n\langle\beta, h_n\rangle - a_n\gamma\|h_n - u\|^2\Big]\, dP_n,$$

where $Z_n(\beta,\gamma,u)$ is a normalization constant and $\|\cdot\|$ denotes the Euclidean norm on $I\!R^\sigma$. By modifying the proof of the LDP with respect to $P_{n,\beta}$ summarized in (1.9), one shows that with respect to $P^u_{n,\beta,\gamma}$, Y_n satisfies the LDP on $\mathcal{X}$ with rate function

$$I_{\beta,\gamma,u}(x) = I(x) + \langle\beta, \tilde{H}(x)\rangle + \gamma\|\tilde{H}(x) - u\|^2 - \text{const.}$$

We denote the 0-set of this rate function by

$$\mathcal{E}(\gamma)^u_\beta = \Big\{x \in \mathcal{X} : I(x) + \langle\beta, \tilde{H}(x)\rangle + \gamma\|\tilde{H}(x) - u\|^2 \text{ is minimized}\Big\}.$$

As before, we identify $\mathcal{E}(\gamma)^u_\beta$ with the subset of $\mathcal{X}$ consisting of equilibrium macrostates for the Gaussian ensemble.

The Gaussian ensemble can be viewed as an approximation to the microcanonical ensemble. In fact, since

$$\lim_{\gamma \to \infty} \exp\Big[-a_n \gamma \|h_n - u\|^2\Big] = \begin{cases} 1 & \text{if } h_n = u \\ 0 & \text{otherwise,} \end{cases}$$

the factor $\exp[-a_n \gamma \|h_n - u\|^2]$ in the definition of $P^u_{n,\beta,\gamma}$ acts as a penalty function. It follows that

$$\lim_{\gamma \to \infty} P^u_{n,\beta,\gamma}\{B\} = P_n\{B \mid h_n = u\}, \tag{1.11}$$

which except for the slightly different form of the conditioning equals the microcanonical probability $P^{u,r}_n\{B\}$. In a similar way, $\mathcal{E}(\gamma)^u_\beta$ can be viewed as an approximation to the set $\mathcal{E}^u$ of equilibrium macrostates for the microcanonical ensemble. This follows from the calculation

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

These observations make it plausible that for a given u there exist a β and a sufficiently large γ such that $\mathcal{E}^u$ equals $\mathcal{E}(\gamma)^u_\beta$; i.e., the microcanonical ensemble and the Gaussian ensemble are fully equivalent. In order to explore the possibility of universal equivalence between the two ensembles, we rewrite the Gaussian ensemble and the associated set of equilibrium macrostates without the parameter u. By expanding $\gamma\|h_n - u\|^2$ in the definition of $P^u_{n,\beta,\gamma}$ and absorbing the linear term in the term $\langle \beta, h_n\rangle$, we see that for subsets B of Ω_n, $P^u_{n,\beta,\gamma}$ equals

$$P_{n,\beta,\gamma}\{B\} = \frac{1}{Z_n(\beta,\gamma,0)} \cdot \int_B \exp\Big[-a_n \langle \beta, h_n\rangle - a_n \gamma \|h_n\|^2\Big]\, dP_n, \tag{1.12}$$

with a different choice of β if $u \neq 0$. With respect to $P_{n,\beta,\gamma}$, Y_n satisfies the LDP on $\mathcal{X}$ with rate function

$$I_{\beta,\gamma}(x) = I(x) + \langle \beta, \tilde{H}(x)\rangle + \gamma \|\tilde{H}(x)\|^2 - \text{const},$$

the 0-set of which is identified with the set of associated equilibrium macrostates. This set is given by

$$\mathcal{E}(\gamma)_\beta = \left\{ x \in \mathcal{X} : I(x) + \langle \beta, \tilde{H}(x) \rangle + \gamma \|\tilde{H}(x)\|^2 \text{ is minimized} \right\}. \tag{1.13}$$

$\mathcal{E}(\gamma)_\beta$ equals $\mathcal{E}(\gamma)^u_\beta$ with a different choice of β if $u \neq 0$.

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 $I\!R^\sigma$ into $I\!R$, the generalized canonical ensemble $P_{n,\beta,g}$ is defined like $P_{n,\beta,\gamma}$ with the term $\gamma \|h_n\|^2$ replaced by $g(h_n)$; thus,

$$P_{n,\beta,g}\{B\} = \frac{1}{Z_n(\beta, g)} \cdot \int_B \exp[-a_n \langle \beta, h_n \rangle - a_n g(h_n)]\, dP_n. \tag{1.14}$$

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

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

The associated set of equilibrium macrostates is identified with the 0-set of $I_{\beta,g}$, which is given by

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

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 [23] concerning ensemble equivalence, including Theorem 2.1.1, generalize to the setting of the generalized canonical ensemble by replacing the microcanonical entropy s by $s - g$. The generalization of Theorem 2.1.1 is stated in Theorem 2.1.2, 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 properties of $s - g$. Since g takes values in $I\!R$, the domain of $s - g$ equals the domain of s.

Theorem 2.1.2. *Let g be a continuous function mapping $\mathbb{R}^\sigma$ into $\mathbb{R}$, in terms of which the generalized canonical ensemble* (1.14) *is defined. For fixed u, the conclusions given in parts* (a)–(d) *hold.*

(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 $\mathcal{E}^u \neq \mathcal{E}(g)_\beta$ 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.*

(d) **Generalized canonical is always realized microcanonically.** *For $\beta \in \mathbb{R}^\sigma$ we define $A(g)_\beta$ to be the set of u 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 relationships between $\mathcal{E}^u$ and $\mathcal{E}(g)_\beta$ are expressed in Theorem 2.1.2 in terms of support properties of $s - g$. As we explain in a moment, because of the considerable freedom that one has in choosing g, this theorem is a significant extension of Theorem 2.1.1 that greatly increases the possibility of obtaining universal equivalence of ensembles. However, it is important to make Theorem 2.1.2 as transparent as possible by seeing how easily it follows from Theorem 2.1.1, in which the relationships between $\mathcal{E}^u$ and $\mathcal{E}_\beta$ are expressed in terms of support properties of

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

In order to do this, we introduce for subsets B of Ω_n the following perturbations of the prior measures P_n:

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

We now think of the generalized canonical ensemble in a different light, not as a perturbation of the standard canonical ensemble defined in terms of P_n by adding the exponential factor $\exp[-a_n g(h_n)]$, but as a standard canonical ensemble corresponding to the new prior measures $P_{n,g}$. In other words, we write

$$P_{n,\beta,g}\{B\} = \frac{1}{\hat{Z}_n(\beta,g)} \cdot \int_B \exp[-a_n\langle\beta, h_n\rangle]\, dP_{n,g}.$$

We now reexpress the microcanonical ensemble P_n^u in a similar way. This ensemble is defined by conditioning the prior measures P_n on the set $\{h_n \in \{u\}^{(r)}\}$, where $\{u\}^{(r)}$ denotes the hypercube in $I\!R^\sigma$ with center u and side length $2r$. We introduce new conditioned measures

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

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 $P_{n,g}^{u,r}$, 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 $P_n^{u,r}$. As a result, the set of equilibrium macrostates for $P_{n,g}^{u,r}$ coincides with the set $\mathcal{E}^u$ of microcanonical equilibrium macrostates.

The asymptotic relationships (1.5) and (1.6) make it clear that 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 from the discussion in the preceding three paragraphs that the relationships between $\mathcal{E}^u$ and $\mathcal{E}(g)_\beta$ are expressed in terms of support and concavity properties of the function s_g obtained from s by replacing the rate function I in the definition of s by the new rate function I_g. Thus,

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

which differs from $s - g$ by a constant. This completes the derivation of Theorem 2.1.2 from Theorem 2.1.1.

In Section 2.9, we offer a second proof of Theorem 2.1.2. There it is proved directly from first principles without the use of Theorem 2.1.1.

For the purpose of applications the most important consequence of Theorem 2.1.2 is given in part (a), which we now discuss under the simplifying assumption that dom s is an open subset of $\mathbb{R}^\sigma$. We focus on $u \in$ 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 dom s is convex and open and if $s - g$ is strictly concave at all u, then $s - g$ has a strictly supporting hyperplane at all u [Prop. 2.2.9(b)] 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 this function 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 2.6.8, 2.6.9, and 2.6.10 several examples of universal equivalence are derived under natural smoothness conditions on s, while Theorem 2.6.11 derives a weaker form of universal equivalence for another class of microcanonical entropies s. 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 2.6.8, 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 dom s, then for any

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

$s(u) - \gamma u^2$ is strictly concave on dom s. By part (b) of Proposition 2.2.9 and part (a) of Theorem 2.1.2, it follows that the microcanonical ensemble and the Gaussian ensemble defined in terms of γ are universally equivalent; i.e., fully equivalent at all u except possibly relative boundary points of dom s. The strict concavity of $s(u) - \gamma u^2$ also implies that the generalized canonical free energy is differentiable on $I\!\!R$ [Thm. 2.6.4], a condition guaranteeing the absence of a discontinuous, first-order phase transition with respect to the Gaussian ensemble. Theorem 2.6.9 is the analogue of Theorem 2.6.8 that treats arbitrary dimension $\sigma \geq 2$. 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 $\gamma \to \infty$ [see (1.11)], full equivalence of ensembles should hold for each u and all sufficiently large γ. The bonus is that under the hypotheses of Theorems 2.6.8 and 2.6.9 universal equivalence of ensembles holds for all sufficiently large γ.

The criterion in Theorem 2.6.8 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. Suppose, for example, that dom s is a closed, bounded interval. If, as in the case of the Curie-Weiss-Potts model [12, 13], $s''(u) \to \infty$ as u

approaches a boundary point, then for any quadratic function g, $s - g$ is not strictly concave on the interior of $\mathrm{dom}\, s$. The situation in which $s''(u) \to \infty$ as u approaches a boundary point can often be handled by Theorem 2.6.11, which is a local version of Theorems 2.6.8 and 2.6.9.

Theorem 2.6.11 shows that if s is C^2 but s'' is not bounded above on the interior of $\mathrm{dom}\, s$, then for each u there exists a sufficiently large γ such that the microcanonical ensemble defined for this value of u and the Gaussian ensemble defined in terms of γ are fully equivalent. We would like to think that the smoothness hypothesis on s in this theorem as well as in Theorems 2.6.8 and 2.6.9 is in some sense generic for typical models in statistical mechanics. This should hold because in most cases the functions I and $\tilde{H}$ appearing in the definition of s are smooth functions of their arguments. To see how this affects the smoothness of s, consider any v such that for any u lying in some neighborhood of v there exists a unique $x = x_u \in \mathcal{X}$ satisfying $\tilde{H}(x) = u$ and $I(x) = -s(u)$. In the neighborhood of such a v, one expects that the corresponding elements x_u are smooth functions of u and thus that $s(u) = -I(x_u)$ is also a smooth function of u.

In Section 5 of [23], the results on ensemble equivalence summarized in Theorem 2.1.1 are extended to mixed canonical-microcanonical ensembles. Such ensembles arise, for example, in the study of soliton turbulence based on a class of wave equations of nonlinear Schrödinger-type [25]. The main theorems in the present chapter, including Theorem 2.1.2, can also be generalized to the setting of mixed ensembles. However, we omit these generalizations.

So far in this introduction, we have focused on equivalence and nonequivalence of ensembles at the level of equilibrium macrostates. One can also analyze ensemble equivalence and nonequivalence at the thermodynamic level, which focuses on relationships between the basic thermodynamic functions in the two ensembles, the microcanonical entropy $s(u)$ and the canonical free energy $\varphi(\beta)$. The theory of large deviations gives a variational formula for φ in terms of the rate function I and the interaction representation function $\tilde{H}$. In turn, this variational formula can be expressed as the Legendre-Fenchel transform s^* of s [Thm. 2.5.4(a)], showing that in general $\varphi = s^*$. However, the converse is not necessarily true. In fact, s can be expressed as the Legendre-Fenchel transform φ^* of φ if and only if s is concave on $I\!R^\sigma$ [Thm. 2.5.4(b)].

This result suggests a natural definition. The ensembles are said to be thermodynamically equivalent at a fixed value u if $s(u) = \varphi^*(u)$. Using the relationship $\varphi(\beta) = s^*(\beta)$, valid for all β, we can recast the condition for thermodynamic equivalence as $s(u) = s^{**}(u)$. Since s^{**} is concave on $I\!R^\sigma$ and since support and concavity properties of s imply full or partial equivalence of ensembles at the level of equilibrium macrostates, it should come as no surprise that there is a close relationship between the thermodynamic level and the macrostate level of ensemble equivalence. This relationship is spelled out in detail in Theorems 2.5.6 and 2.5.7.

Another contribution of the present chapter is to extend the concept of ensemble equivalence at the thermodynamic level to the relationship between the microcanonical and generalized canonical ensembles. As we show in Theorem 2.6.7, this relationship is obtained from that between the microcanonical and standard canonical ensembles by replacing s in the latter by $s - g$, where g is the function defining the generalized canonical ensemble. This extended formulation is facilitated by introducing two generalized forms of the Legendre-Fenchel transform, the properties of which are derived in Sections 2.2 and 2.3.

One of the seeds out of which the present chapter germinated is the paper [24], in which the authors study the equivalence of the microcanonical and canonical ensembles for statistical equilibrium models of coherent structures in two-dimensional and barotropic 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 [24], the authors 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 functional similar in form to the function

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

the minimum points of which define the set of equilibrium macrostates for the Gaussian ensemble [see (1.13)]. Such Lyapunov functionals arise in the study of constrained optimization problems, where they are known as augmented Lagrangians [4, 55].

Another seed out of which the present chapter germinated is the work of Kiessling and Lebowitz [46], in which Gaussian ensembles are used to study a point-vortex model of fluid turbulence. By sending $\gamma \to \infty$ after the fluid limit $n \to \infty$, they 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 chapter, 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 ∞.

Gaussian ensembles are also the subject of [10, 11, 43]. The first two of these papers use the ensembles to account for ensemble-dependent effects in finite systems and to carry out Monte Carlo simulations of phase transitions in Potts models. These simulations exhibit significant reductions in computer time in comparison with simulations based on standard canonical ensembles. The third paper is a theoretical study of the Gaussian ensemble, which derives it both from the analysis of a system attached to a finite reservoir and from the maximum entropy principle. The parameters β and γ on which the ensemble depends allow one to independently fix the energy of the system and the variance of the energy.

In addition to the connections with [10, 11, 43, 46], the present chapter also builds on the wide literature concerning equivalence of ensembles in statistical mechanics. An overview of this literature is given in the introduction to [51]. A number of papers on this topic, including [18, 23, 30, 33, 50, 51, 63], investigate equivalence of ensembles using the theory of large deviations. In [50, §7] and [51, §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 [23] 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.

Nonequivalence of ensembles at the thermodynamic level has been observed in a number of long-range, mean-field spin models, including the mean-field X-Y model [15] and the mean-field Blume-Emery-Griffith model [2, 3]. In [27] ensemble nonequivalence for the mean field Blume-Emery-Griffiths model was demonstrated to hold also at the level of equilibrium macrostates via numerical computations. For a mean-field version of the Potts model called the Curie-Weiss-Potts model, equivalence and nonequivalence of ensembles at the level of equilibrium macrostates is analyzed in detail in [12, 13]. In both the mean-field Blume-Emery-Griffiths model and the Curie-Weiss-Potts model, nonequivalence of ensembles arises from the different phase transition behavior of the two ensembles. The canonical ensemble exhibits a discontinuous, first-order phase transition, the set $\mathcal{E}_\beta$ changing discontinuously as β increases through a critical value β_c. The equilibrium macrostates that are skipped because of this discontinuous change in $\mathcal{E}_\beta$ appear in the microcanonical ensemble, which undergoes a continuous, second-order phase transition, the sets $\mathcal{E}^u$ changing continuously as u decreases. Ensemble nonequivalence has also been observed in models of turbulence [9, 24, 46, 61], models of plasmas [65], and gravitational systems [52]. Many of these models can also be analyzed by the methods of [23] and the present chapter. A detailed discussion of ensemble nonequivalence for models of coherent structures in turbulence is given in [23, §1.4].

We end this introduction by outlining the contents of this chapter. In Sections 2.2 and 2.3 we generalize the standard Legendre-Fenchel transform for concave functions, introducing two forms of a generalized Legendre-Fenchel transform that are suited for applications in statistical mechanics. The theory of these generalized transforms is illustrated in Section 2.4 for the example of a double-parabolic function. In Section 2.5 we present the hypotheses on the statistical mechanical models to which the theory of the present chapter applies, give a number of examples of such models, and then restate the results on ensemble equivalence and nonequivalence derived in [23]. The material in Section 2.5 is needed for Section 2.6, in which we generalize the results on ensemble equivalence and nonequivalence to the class of generalized canonical ensembles. This is based in part on the generalized Legendre-Fenchel transforms introduced in Sections 2.2 and 2.3. In Section 2.7 we give full details of the proof of Theorem 2.1.2 from Theorem 2.1.1 that is outlined in this introduction. In Section 2.8 we derive, under weaker assumptions on the models, large deviation principles with respect to the various ensembles, allowing us to define, and to study the relationships among, the corresponding sets of equilibrium macrostates in much greater generality. In Section 2.9 we give a second proof of Theorem 2.1.2, proving it directly from first principles and not from Theorem 2.1.1.

2.2 Generalized Legendre-Fenchel Transform, Part I

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 chapter, 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.

We begin by reviewing the basic theory of Legendre-Fenchel transforms for concave functions. Let σ be a positive integer. A function f on $\mathbb{R}^\sigma$ is said to be concave on $\mathbb{R}^\sigma$ if $-f$ is a proper convex function in the sense of [62, p. 24]; that is, f maps $\mathbb{R}^\sigma$ into $\mathbb{R} \cup \{-\infty\}$, $f \not\equiv -\infty$, and for all x and y in $\mathbb{R}^\sigma$ and all $\lambda \in (0,1)$

$$f(\lambda x + (1-\lambda)y) \geq \lambda f(x) + (1-\lambda) f(y).$$

A function f mapping a convex set K into $\mathbb{R}$ is said to be strictly concave on K if the inequality in the last display is strict for all $x \neq y$ in K and all $\lambda \in (0,1)$.

Let $f \not\equiv -\infty$ be a function mapping $\mathbb{R}^\sigma$ into $\mathbb{R} \cup \{-\infty\}$. For $\alpha \in \mathbb{R}^\sigma$ the Legendre-Fenchel transform of f is defined by [62, p. 308]

$$f^*(\alpha) = \inf_{x \in \mathbb{R}^\sigma} \{\langle \alpha, x \rangle - f(x)\},$$

and for $x \in \mathbb{R}^\sigma$ the Legendre-Fenchel transform of f^* is defined by

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

The first theorem gives three basic properties of the Legendre-Fenchel transform.

Because of property (c), when f is not concave or upper semicontinuous, we call f^{**} the concave, upper semicontinuous hull of f.

Theorem 2.2.1. *Let $f \not\equiv -\infty$ be a function mapping $I\!\!R^\sigma$ into $I\!\!R \cup \{-\infty\}$. The following conclusions hold.*

(a) *f^* is concave and upper semicontinuous on $I\!\!R^\sigma$.*

(b) *For all $x \in I\!\!R^\sigma$ we have $f^{**}(x) = f(x)$ if and only if f is concave and upper semicontinuous on $I\!\!R^\sigma$.*

(c) *If f is not concave and upper semicontinuous on $I\!\!R^\sigma$, then f^{**} is the smallest concave, upper semicontinuous function on $I\!\!R^\sigma$ that satisfies $f^{**}(x) \geq f(x)$ for all $x \in I\!\!R^\sigma$. In particular, if $f(x) > -\infty$, then $f^{**}(x) > -\infty$.*

Comments on the Proof. (a)–(b) These are analogues, for concave, upper semicontinuous functions, of properties of convex, lower semicontinuous functions proved in parts (a) and (e) of Theorem VI.5.3 in [21]. The similar proofs are omitted.

(c) For any x and α in $I\!\!R^\sigma$ we have $f(x) \leq \langle \alpha, x \rangle - f^*(\alpha)$ and thus

$$f(x) \leq \inf_{\alpha \in I\!\!R^\sigma} \{\langle \alpha, x \rangle - f^*(\alpha)\} = f^{**}(x).$$

Now let φ be any concave, upper semicontinuous function that satisfies $\varphi(x) \geq f(x)$ for all x. Then $\varphi^*(\alpha) \leq f^*(\alpha)$ for all α, and so by part (b) of this theorem applied to φ, $\varphi^{**}(x) = \varphi(x) \geq f^{**}(x)$ for all x. ■

As part (b) of Theorem 2.2.1 makes clear, unless f is concave and upper semicontinuous, the equation $f^{**}(x) = f(x)$ does not hold for all $x \in I\!\!R^\sigma$. In this section we generalize the Legendre-Fenchel transform in a simple and direct way so that we have equality for all x. The idea is to modify f by choosing a function g such that $f - g$ is concave and upper semicontinuous. Broad conditions under which such a function g exists are given in Theorems 2.2.14–2.2.16.

Let $f \not\equiv -\infty$ be a function mapping $I\!R^\sigma \to I\!R \cup \{-\infty\}$ and $g \not\equiv \infty$ any function mapping $I\!R^\sigma$ into $I\!R \cup \{\infty\}$. For $\alpha \in I\!R^\sigma$ the generalized Legendre-Fenchel transform is defined by

$$f^\sharp(\alpha) = f^\sharp(g, \alpha) = \inf_{x \in I\!R^\sigma} \{\langle \alpha, x\rangle + g(x) - f(x)\}, \tag{2.1}$$

where we define $\infty - (-\infty) = \infty$. For $x \in I\!R^\sigma$ the generalized Legendre-Fenchel transform of $f^\sharp$ is defined by

$$f^{\sharp\sharp}(x) = f^{\sharp\sharp}(g, x) = \inf_{\alpha \in I\!R^\sigma} \{\langle \alpha, x\rangle + g(x) - f^\sharp(g, \alpha)\}. \tag{2.2}$$

In the next elementary lemma we relate the generalized Legendre-Fenchel transform to the standard Legendre-Fenchel transform.

Lemma 2.2.2. (a) *For* $\alpha \in I\!R^d$, $f^\sharp(g, \alpha) = (f - g)^*(\alpha)$.

(b) *For* $x \in I\!R^d$, $f^{\sharp\sharp}(g, x) = g(x) + (f - g)^{**}(x)$.

(c) *For* $x \in I\!R^d$, $f^{\sharp\sharp}(g, x) \geq f(x)$.

Proof. Parts (a) and (b) follow immediately from the definitions, which imply that

$$f^\sharp(g, \alpha) = \inf_{x \in I\!R^\sigma} \{\langle \alpha, x\rangle - (f - g)(x)\} = (f - g)^*(\alpha)$$

and that

$$\begin{aligned} f^{\sharp\sharp}(g, x) &= g(x) + \inf_{\alpha \in I\!R^\sigma} \{\langle \alpha, x\rangle - (f - g)^*(\alpha)\} \\ &= g(x) + (f - g)^{**}(x). \end{aligned}$$

Since by part (c) of Theorem 2.2.1 $(f - g)^{**}(x) \geq (f - g)(x)$, it follows that

$$f^{\sharp\sharp}(g, x) = g(x) + (f - g)^{**}(x) \geq f(x).$$

This completes the proof. ■

Part (b) of the next theorem gives conditions on $f - g$ that are equivalent to the equality $f^{\sharp\sharp}(g, x) = f(x)$ for all $x \in I\!R^\sigma$.

Theorem 2.2.3. *Let $f \not\equiv -\infty$ be a function mapping $I\!R^\sigma \to I\!R \cup \{-\infty\}$ and $g \not\equiv \infty$ a function mapping R^d into $I\!R \cup \{\infty\}$. The following conclusions hold.*

(a) *For $x \in I\!R^\sigma$, $(f-g)^{**}(x) = (f-g)(x)$ if and only if $f^{\sharp\sharp}(g,x) = f(x)$.*

(b) *The following three statements are equivalent.*

(i) *$f - g$ is concave and upper semicontinuous on $I\!R^\sigma$.*

(ii) *For all $x \in I\!R^\sigma$, $(f-g)^{**}(x) = (f-g)(x)$.*

(iii) *For all $x \in I\!R^\sigma$, $f^{\sharp\sharp}(g,x) = f(x)$.*

Proof. (a) This follows from part (b) of Lemma 2.2.2.

(b) The equivalence of (i) and (ii) is the content of part (b) of Theorem 2.2.1. The equivalence of (ii) and (iii) follows from part (a) of the present theorem. ■

As we will explore in Sections 2.5 and 2.6, concavity and support properties of the microcanonical entropy s and of $s - g$ for appropriate functions g are directly related to questions of ensemble equivalence. These questions will be studied in this chapter at two levels. The thermodynamic level involves concavity properties of s and of $s-g$ while the macrostate level, which is the more fundamental of the two, involves support properties of s and of $s-g$. A basic fact is that if s has a strictly supporting hyperplane at some value u, then, in a sense to be made precise in Theorem 2.5.2, the microcanonical ensemble defined for this u is fully equivalent with the canonical ensemble. The results of the present section and the next section will allow us to extend this theorem and show that if there exists an appropriate function g such that $s - g$ has a strictly supporting hyperplane at some u, then the microcanonical ensemble defined for this u is fully equivalent with the generalized canonical ensemble defined in terms of this g [Thm. 2.6.2].

We now set the stage for this analysis. First, we give several definitions concerning support properties of functions. Then, in Proposition 2.2.9 we relate concavity and support properties of functions on $\mathbb{R}^\sigma$, showing among other facts that that if f is strictly concave on a subset of $\mathbb{R}^\sigma$, then f has a strictly supporting hyperplane at all points of this subset except possibly boundary points. Later this proposition will be applied to give criteria on f guaranteeing that there exists a function g such that $f - g$ has a strictly supporting hyperplane at all points of a given subset of $\mathbb{R}^\sigma$ [Thms. 2.2.14–2.2.16]. For $\alpha \in \mathbb{R}^\sigma$ we define $[\alpha, -1]$ to be the vector in $\mathbb{R}^{\sigma+1}$ whose first σ components agree with those of α and whose last component equals -1.

Definition 2.2.4. *Let $f \not\equiv -\infty$ be a function mapping $\mathbb{R}^\sigma$ into $\mathbb{R} \cup \{-\infty\}$.*

(a) *The domain of f, denoted by* $\operatorname{dom} f$*, is the set of points $x \in \mathbb{R}^\sigma$ for which $f(x) > -\infty$.*

(b) *Let x and α be points in $\mathbb{R}^\sigma$. We say that f has a supporting hyperplane at x with normal vector $[\alpha, -1]$ if*

$$f(y) \leq f(x) + \langle \alpha, y - x \rangle \ \text{ for all } y \in \mathbb{R}^\sigma.$$

(c) *Let f be concave on $\mathbb{R}^\sigma$. The superdifferential of f at x, denoted by $\partial f(x)$, is the set of α for which the inequality in part* (a) *holds for all y. The domain of ∂f, denoted by* $\operatorname{dom} \partial f$*, is the set of x for which $\partial f(x) \neq \emptyset$.*

(d) *Let x and α be points in $\mathbb{R}^\sigma$. We say that f has a strictly supporting hyperplane at x with normal vector $[\alpha, -1]$ if*

$$f(y) < f(x) + \langle \alpha, y - x \rangle \ \text{ for all } y \in \mathbb{R}^\sigma, y \neq x.$$

(e) *Let x and α be points in $\mathbb{R}^\sigma$. We say that f has a nonstrictly supporting hyperplane at x with normal vector $[\alpha, -1]$ if*

$$f(y) \leq f(x) + \langle \alpha, y - x \rangle \ \text{ for all } y \in \mathbb{R}^\sigma$$

and if equality holds for some $y \neq x$.

If $\sigma = 1$, then obviously a (strictly) supporting hyperplane with normal vector $[\alpha, -1]$ is a (strictly) supporting line with slope α. Before stating the proposition relating concavity and support properties of functions on $I\!R^\sigma$, we need several additional definitions. For A a subset of $I\!R^\sigma$, cl A denotes its closure.

Definition 2.2.5. *Let $f \not\equiv -\infty$ be a function mapping $I\!R^\sigma$ into $I\!R \cup \{-\infty\}$.*

(a) *The relative interior of* dom f*, denoted by* ri(dom f)*, is defined as the interior of* dom f *when considered as a subset of the smallest affine set that contains* dom f*. If* dom f = ri(dom f)*, then dom f is said to be relatively open.*

(b) *The relative boundary of* dom f *is defined as*

$$\text{rb(dom } f) = \text{cl(dom } f) \setminus \text{ri(dom } f).$$

Clearly, if the smallest affine set that contains dom f is $I\!R^\sigma$, then the relative interior of dom f equals the interior of dom f, which we denote by int(dom f).

When f is concave, the basic fact relating the sets dom f, ri(dom f), and dom ∂f is stated in the next lemma, which is proved in [62, Thm. 23.4]. According to this lemma, dom ∂f always contains ri(dom f) and differs from dom f, if at all, only in a subset of the relative boundary of dom f. By definition of dom ∂f, it follows that f has a supporting hyperplane at all points of dom f except possibly relative boundary points.

Lemma 2.2.6. *Let f be a concave function on $I\!R^\sigma$. Then*

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

It is easy to give examples of the various possibilities allowed by this lemma. For simplicity, we restrict to dimension $\sigma = 1$. If dom f is a nonempty, open interval, then ri(dom f) = dom f, and so the three subsets in the lemma are equal. Suppose, on the other hand, that dom f is a closed, bounded interval $[a, b]$ and f is differentiable on (a, b).

Then the boundary point a lies in dom ∂f if and only if $f'_+(a) = \lim_{x \to a^+} f'(x)$ is finite, in which case $\partial f(a) = (-\infty, (f')^+(a)]$. For any $\alpha \in \text{int}\, \partial f(a) = (-\infty, (f')^+(a))$, f has a strict supporting line at a with normal vector $[\alpha, -1]$ or equivalently slope α. Similarly the boundary point b lies in dom ∂f if and only if $(f')^-(b) = \lim_{x \to b^-} f'(x)$ is finite, in which case $\partial f(b) = [(f')^-(b), \infty)$. For any $\alpha \in \text{int}\, \partial f(b) = ((f')^+(b), \infty)$, f has a strict supporting line at b with normal vector $[\alpha, -1]$ or equivalently slope α. This example, as well as higher dimensional analogues, shows that in general one cannot expect equality in Lemma 2.2.6. This state of affairs leads to inevitable complications involving relative boundary points in the statements of many results concerning the existence of supporting hyperplanes.

Proposition 2.2.9 address support and strict concavity properties of functions on $I\!R^\sigma$. In order to prove part (b), we need the following technical lemma relating a concave function f with f^{**}, the concave, upper semicontinuous hull of f [Theorem 2.2.1(c)].

Lemma 2.2.7. *Let f be a concave function on $I\!R^\sigma$. The following conclusions hold.*

(a) *f^{**} agrees with f except possibly at relative boundary points of dom f. In particular, $f^{**}(x) = f(x)$ for all $x \in$* ri(dom f).

(b) dom f^{**} *differs from* dom f *at most by including some additional relative boundary points of* dom f. *In particular,* ri(dom f) $=$ ri(dom f^{**}).

Proof. Since f is a (proper) concave function on $I\!R^\sigma$, f^{**} coincides with the closure of f [62, Thm. 12.2]. Parts (a) and (b) of the lemma are consequences of Theorem 7.4 and Corollary 7.4.1 in [62]. ■

We also need the following one-dimensional result on extending strict concavity to points in dom f that lie in the relative boundary of dom f. Given points x and y in $I\!R^\sigma$, we denote by $L[x, y]$ the closed line segment defined by

$$L[x,y] = \{z \in I\!R^\sigma : z = \lambda x + (1-\lambda)y \text{ for some } 0 \leq \lambda \leq 1\}$$

and by $L[x,y)$ the half-closed line segment defined by

$$L[x,y) = \{z \in I\!R^\sigma : z = \lambda x + (1-\lambda)y \text{ for some } 0 < \lambda \leq 1\}.$$

Lemma 2.2.8. *Assume that* dom f *is convex,* f *is strictly concave on* ri(dom f)*, and* f *is continuous on* dom f. *Then for any* $x \in$ ri(dom f) *and any* $y \in$ dom f*,* f *is strictly concave on* $L[x,y]$.

Proof. If $y \in$ ri(dom f), then $L[x,y] \subset$ ri(dom f), and so f is strictly concave on $L[x,y]$ by hypothesis. We now assume that $y \in$ dom $f \setminus$ ri(dom f). The continuity of f on dom f allows us to extend the strict concavity of f on ri(dom f) to concavity on dom f. It follows that if f is not strictly concave on $L[x,y]$, then f must be affine on $L[x,y]$ and thus affine on $L[x,y)$. Since $L[x,y) \subset$ ri(dom f) [62, Thm. 6.1], this violates the strict concavity of f on ri(dom f). ■

In part (a) of the next proposition we show that if f has a supporting hyperplane at x, then $x \in$ dom f and $f^{**}(x) = f(x)$. Parts (b) and (c) relate strict concavity with the existence of a strictly supporting hyperplane. The proposition, especially part (b), will be applied a number of times in the sequel, including applications to statistical mechanics in Sections 2.5 and 2.6.

Proposition 2.2.9. *Let* $f \not\equiv -\infty$ *be a function mapping* $I\!R^\sigma$ *into* $I\!R \cup \{-\infty\}$. *The following conclusions hold.*

(a) *Assume that* f *has a supporting hyperplane at* x. *Then* $x \in$ dom f *and* $f^{**}(x) = f(x)$.

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

(c) *Assume that* f *has a strictly supporting hyperplane at all* x *in a convex subset* K *of* dom f. *Then* $f(x) = f^{**}(x)$ *for all* $x \in K$, *and* f *is strictly concave on* K.

Proof. (a) By assumption, there exists α with the property that for all y

$$f(y) \leq f(x) + \langle \alpha, y - x \rangle. \tag{2.3}$$

Choosing $y \in$ dom f, we see that $-\infty < f(x)$ and thus that $x \in$ dom f. The inequality in the last display implies that

$$\inf_{y \in I\!R^\sigma} \{\langle \alpha, y \rangle - f(y)\} = f^*(\alpha) \geq \langle \alpha, x \rangle - f(x).$$

It follows that $f(x) \geq \langle \alpha, x \rangle - f^*(\alpha) \geq f^{**}(x)$. Since in general $f(x) \leq f^{**}(x)$ [Thm. 2.2.1(c)], we conclude that $f(x) = f^{**}(x)$.

(b) The assumptions on f guarantee that f is concave on $I\!R^\sigma$. Since ri(dom f) $\subset$ dom ∂f [Lem. 2.2.6], for any $x \in$ ri(dom f) and any $\beta \in \partial f(x)$, f has a supporting hyperplane at x with normal vector $[\beta, -1]$; i.e.,

$$f(y) \leq f(x) + \langle \beta, y - x \rangle \text{ for all } y \in I\!R^\sigma. \tag{2.4}$$

If this hyperplane is not a strictly supporting hyperplane, then there exists $y_0 \in I\!R^\sigma$, $y_0 \neq x$ such that

$$f(y_0) = f(x) + \langle \alpha, y_0 - x \rangle. \tag{2.5}$$

Thus $y_0 \in$ dom f. Since f is strictly concave on $L[x, y_0]$ [Lem. 2.2.8], we have

$$\lambda f(x) + (1 - \lambda) f(y_0) < f(\lambda x + (1 - \lambda) y_0) \text{ for all } \lambda \in (0, 1).$$

Substituting (2.5) gives

$$f(x) + (1 - \lambda)\langle \alpha, y_0 - x\rangle < f(\lambda x + (1 - \lambda)y_0). \tag{2.6}$$

On the other hand, applying (2.4) to $y = \lambda x + (1 - \lambda)y_0$, we obtain

$$\begin{aligned} f(\lambda x + (1 - \lambda)y_0) &\leq f(x) + \langle \alpha, \lambda x + (1 - \lambda)y_0 - x\rangle \\ &= f(x) + (1 - \lambda) \cdot \langle \alpha, y_0 - x\rangle. \end{aligned}$$

This contradicts (2.6), proving that the supporting hyperplane at x with normal vector $[\alpha, -1]$ is a strictly supporting hyperplane. We have proved that f has a strictly supporting hyperplane at all $x \in$ 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 $x \in$ dom f. This completes the proof of part (b).

(c) Since a strictly supporting hyperplane is a supporting hyperplane, part (a) implies that $f(x) = f^{**}(x)$ for all $x \in K$. In order to prove that f is strictly concave on K, let $x \neq y$ be arbitrary points in K and let λ be an arbitrary number in $(0, 1)$. Our goal is to prove that

$$\lambda f(x) + (1 - \lambda)f(y) < f(\lambda x + (1 - \lambda)y). \tag{2.7}$$

Since f has a strictly supporting hyperplane at $z = \lambda x + (1 - \lambda)y$ and since z differs from both x and y, there exists $\alpha \in I\!R^\sigma$ such that

$$f(x) < f(z) + \langle \alpha, x - z\rangle = f(z) + \langle \alpha, (1 - \lambda)(x - y)\rangle \tag{2.8}$$

and

$$f(y) < f(z) + \langle \alpha, y - z\rangle = f(z) + \langle \alpha, \lambda(y - x)\rangle. \tag{2.9}$$

Multiplying (2.8) by λ, multiplying (2.9) by $1 - \lambda$, and adding yields (2.7). The proof of the proposition is complete. ■

An important aspect of concave duality is that the strict concavity of f is closely related to the smoothness of its Legendre-Fenchel transform f^*. Here are the relevant definitions followed by the statement of the duality.

Definition 2.2.10. *Let f be a concave function on $I\!\!R^\sigma$.*

(a) *f is said to be essentially smooth if $C = \text{int}(\text{dom}\, f)$ is nonempty, f is differentiable on C, and $\lim_{n\to\infty} \|\nabla f(x_n)\| = \infty$ whenever $x_1, x_2, \ldots$ is a sequence in C converging to a boundary point of C.*

(b) *f is said to be essentially strictly concave if f is strictly concave on every convex subset of* $\text{dom}\, \partial f = \{x \in I\!\!R^\sigma : \partial f(x) \neq 0\}$.

By Lemma 2.2.6, if a concave, upper semicontinuous function f is strictly concave on $\text{dom}\, f$, then f is essentially strictly concave, while if f is essentially strictly concave, then f is strictly concave on $\text{ri}(\text{dom}\, f)$. According to the next theorem, essential smoothness and essential strict concavity are dual properties.

Theorem 2.2.11. *Let f be a concave, upper semicontinuous function on $I\!\!R^\sigma$. Then f is essentially strictly concave if and only if f^* is essentially smooth.*

In applications to statistical mechanics, this theorem is particularly useful. Indeed, when f equals the microcanonical entropy, then f^* equals canonical free energy [Thm. 2.5.4(a)]. The essential smoothness of this function corresponds to the absence of a discontinuous, first-order phase transition with respect to the canonical ensemble.

We now change our emphasis in this section, no longer assuming that f is concave on $I\!\!R^\sigma$. We seek functions g mapping $I\!\!R^\sigma$ into $I\!\!R$ such that $f - g$ is strictly concave on $\text{dom}\, f$ or on the relative interior of this set. Then under additional assumptions Theorem 2.2.3 and Proposition 2.2.9 yield the equality $f^{\sharp\sharp}(g, \cdot) = f$ and the existence of a strict supporting hyperplane for $f-g$ at each point in dom f except possibly relative boundary points.

In Section 2.6 we will apply these ideas to the microcanonical entropy s. The existence of a function g such that $s-g$ has a strictly supporting hyperplane at each point in dom s except possibly relative boundary points guarantees that the microcanical ensemble and the generalized canonical ensemble defined in terms of g satisfy a strong form of equivalence known as universal equivalence [Thms. 2.6.7(d)]. In addition, if $s-g$ is strictly concave on dom s, then Theorem 2.2.11 implies that $(s-g)^*$ is essentially smooth. As in the case when $g=0$, this observation has an important implication in statistical mechanics. The function $(s-g)^*$ equals the generalized canonical free energy [Thm. 2.6.4(a)], the essential smoothness of which corresponds to the absence of a discontinuous, first-order phase transition with respect to the generalized canonical ensemble. The use of quadratic functions g to effect strict concavity and support properties of $s-g$ is particularly attractive. The resulting generalized canonical ensembles, known as Gaussian ensembles, lend themselves nicely to computations.

The next two theorems treat dimension $\sigma = 1$ and dimension $\sigma \geq 2$ separately. In them an easily verifiable criterion is given on a C^2 function f assuring that there exists a quadratic function g such that $f-g$ is strictly concave on dom f when $\sigma = 1$ and on int(dom f) when $\sigma \geq 2$. By part (b) of Proposition 2.2.9, this property implies that $f-g$ has a strictly supporting hyperplane at each point in dom f except possibly boundary points. The criterion is that all second-order partial derivatives of f are bounded above on the interior of dom f. As we show in part (a) of Theorem 2.2.12 in the case $\sigma = 1$, if $g(x) = \gamma x^2$, then $f-g$ is strictly concave on dom f for all $\gamma > \frac{1}{2} \sup_{x \in \text{int(dom } f)} f''(x)$. An analogous, but more complicated criterion is given in part (a) of Theorem 2.2.14 in the case $\sigma \geq 2$.

The criterion that all second-order partial derivatives of f are bounded above is essentially optimal for the existence of a fixed quadratic function g such that $f-g$ is strictly concave on the interior of dom f. Suppose, for example, that the dimension σ equals 1 and dom f is closed, bounded interval. If $f''(x) \to \infty$ as x approaches a boundary point, then for any quadratic function g, $(f-g)''$ is strictly positive on some open interval in dom f and so is convex on that interval [62, Thm. 4.4]. In particular, $f-g$ is not strictly concave on the interior of dom f.

The situation in which $f''(x) \to \infty$ as x approaches a boundary point can often be handled by Theorem 2.3.2, which is a local version of Theorems 2.2.12 and 2.2.14. Theorem 2.3.2 shows that if f is C^2 on an open set K and other conditions hold, then for each x in the interior of K there exists a quadratic function g depending, in general, on x such that $f-g$ has a strictly supporting hyperplane at x. When applied to the microcanonical entropy, this implies another form of universal equivalence of ensembles explained in Theorem 2.6.11 and in the paragraph following that theorem.

In Theorem 2.2.12 we consider dimension $\sigma = 1$, the most useful case for applications. In contrast to dimension $\sigma \geq 2$, the results for $\sigma = 1$ are also more complete. Not only do we have in (2.10) a simple criterion on γ guaranteeing that $f(x) - \gamma x^2$ is strictly concave on dom f, but also we prove in part (e) that $(f-g)^*$ is always essentially smooth, a substantial improvement over what holds in general when $\sigma \geq 2$. The criterion $\gamma > \gamma_0$ given in (2.10) is optimal in the sense that for any $\gamma < \gamma_0$, $f(x) - \gamma x^2$ is not strictly concave on dom f.

Theorem 2.2.12. *Assume that the dimension $\sigma = 1$. Let $f \not\equiv -\infty$ a function mapping $I\!R$ into $I\!R \cup \{-\infty\}$ such that* dom f *is a nonempty interval and f is continuous on* dom f. *In addition, assume that either f is strictly concave on* dom f *or that f is twice continuously differentiable on* int(dom f) *and f'' is bounded above on* int(dom f). *Then for all sufficiently large $\gamma \geq 0$ and $g(x) = \gamma x^2$, conclusions* (a)–(e) *hold. Specifically, if*

f is strictly concave on dom f*, then we choose any $\gamma \geq 0$, and otherwise we choose*

$$\gamma > \gamma_0 = \tfrac{1}{2} \cdot \sup_{x \in \text{int(dom } f)} f''(x). \tag{2.10}$$

(a) *$f - g$ is strictly concave and continuous on* dom f*.*

(b) *$f - g$ has a strict supporting hyperplane at each point in* dom f *except possibly boundary points; $f - g$ has a strictly supporting line at a boundary point if and only if the one-sided derivative of $f - g$ is finite at that boundary point.*

(c) *$f^{\sharp\sharp}(g, x) = f(x)$ for all $x \in$* dom f *except possibly boundary points.*

(d) *Assume that f is upper semicontinuous on $\mathbb{R}$; the latter condition is satisfied if* dom f *is closed. Then $f^{\sharp\sharp}(g, x) = f(x)$ for all $x \in \mathbb{R}$.*

(e) *$(f - g)^*$ is essentially smooth; in particular, $(f - g)^*$ is differentiable on the interior of its domain.*

Remark 2.2.13. The number γ_0, defined in (2.10) when f is not strictly concave on dom f, is nonnegative. Indeed, if we had $\gamma_0 < 0$, then we would have $f''(x) < 0$ for all $x \in$ dom f, and the proof of part (a) of the theorem with $\gamma = 0$ would show that f is strictly concave on dom f.

Proof. (a) If f is strictly concave on dom f, then $f(x) - \gamma x^2$ is also strictly concave on this set for any $\gamma \geq 0$. We now consider the case in which f is not strictly concave on dom f. If $g(x) = \gamma x^2$, then $f - g$ is continuous on dom f. If, in addition, we choose $\gamma > \gamma_0$ in accordance with (2.10), then for all $x \in$ int(dom f)

$$(f - g)''(x) = f''(x) - 2\gamma < 0.$$

A straightforward extension of the proof of Theorem 4.4 in [62], in which the inequalities in the first two displays are replaced by strict inequalities, shows that $-(f - g)$ is strictly convex on int(dom f) and thus that $f - g$ is strictly concave on int(dom f). The strict concavity of f on dom f follows from Lemma 2.2.8.

(b) The first assertion follows from part (a) of the present theorem and part (b) of Proposition 2.2.9 applied to $f - g$. Concerning the second assertion about boundary points, the reader is referred to the discussion following Lemma 2.2.6.

(c) Part (b) implies that $f-g$ has a strictly supporting hyperplane, and thus a supporting hyperplane, at each point in dom f except possibly relative boundary points. Hence by part (a) of Proposition 2.2.9 applied to $f - g$, for all $x \in$ dom f except possibly relative boundary points we have $(f-g)^{**}(x) = (f-g)(x)$ or equivalently $f^{\sharp\sharp}(g, x) = f(x)$ [Thm. 2.2.3(a)].

(d) If f is upper semicontinuous on $I\!R$ and $g(x) = \gamma x^2$, then $f - g$ is upper semicontinuous on $I\!R$. If dom f is closed, then the upper semicontinuity of f on $I\!R^\sigma$ follows immediately from the continuity of f on dom f. Part (a) implies that for any $\gamma > \gamma_0$, $f - g$ is strictly concave on dom f and thus is concave on $I\!R$. Since $f - g$ is upper semicontinuous of $I\!R$, part (b) of Theorem 2.2.3 allows us to conclude that $f^{\sharp\sharp}(g, x) = f(x)$ for all $x \in I\!R^\sigma$.

(e) Part (a) implies that $f - g$ is strictly concave on dom f and thus is essentially strictly concave. The essential smoothness of $(f - g)^*$ is a consequence of Theorem 2.2.11. The proof of the theorem is complete. ■

We now consider the analogue of Theorem 2.2.12 for arbitrary dimension $\sigma \geq 2$. In contrast to the case $\sigma = 1$, in which $f - g$ could always be extended to a strictly concave function on all of dom f, in this case there exists a quadratic g such that $f - g$ is strictly concave on the interior of dom f, but in general $f - g$ cannot be extended to a strictly concave function on all of dom f. One can easily find examples in which the boundary of dom f has flat portions, and $f - g$ is strictly concave on the interior of dom f and constant on these flat portions. As a result, unless dom f is open, we cannot in general apply Theorem 2.2.11 to conclude that $(f - g)^*$ is essentially smooth. In (2.11) an explicit criterion is given on γ guaranteeing that $f - \gamma\|\cdot\|^2$ is strictly concave on int(dom f). The criterion — namely, that $\gamma > \gamma_0$ — is optimal in the sense that for any $\gamma < \gamma_0$, $f - \gamma\|\cdot\|^2$ is not strictly concave on int(dom f). We denote by $\|\cdot\|$ and $\langle\cdot,\cdot\rangle$ the Euclidean norm and the Euclidean inner product on $I\!R^\sigma$.

Theorem 2.2.14. *Assume that the dimension $\sigma \geq 2$. Let $f \not\equiv -\infty$ be a function mapping $I\!R^\sigma$ into $I\!R \cup \{-\infty\}$ such that* dom f *is convex and has a nonempty interior and f is continuous on* dom f*. In addition, assume that either f is strictly concave on* int(dom f) *or that f is twice continuously differentiable on* int(dom f) *and all second-order partial derivatives of f are bounded above on* int(dom f)*. Then for all sufficiently large $\gamma \geq 0$ and $g(x) = \gamma\|x\|^2$, conclusions* (a)–(e) *hold. Specifically, if f is strictly concave on* int(dom f)*, then we choose any $\gamma \geq 0$, and otherwise we choose*

$$\gamma > \gamma_0 = \tfrac{1}{2} \cdot \sup_{x \in \text{int(dom } f)} \kappa(x), \tag{2.11}$$

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

(a) *$f - g$ is strictly concave on* int(dom f) *and on all closed line segments $L[x, y]$ for $x \in$* int(dom f) *and $y \in$* dom $f \cap$ rb(dom f)*. In addition, $f - g$ is concave and continuous on* dom f*.*

(b) *$f - g$ has a strictly supporting hyperplane at each point in* dom f *except possibly relative boundary points.*

(c) *$f^{\sharp\sharp}(g, x) = f(x)$ for all $x \in$* int(dom f)*.*

(d) *Assume that f is upper semicontinuous on $I\!R^\sigma$; the latter condition is satisfied if* dom f *is closed. Then $f^{\sharp\sharp}(g, x) = f(x)$ for all $x \in I\!R^\sigma$.*

(e) *Assume that* dom f *is open. Then $(f - g)^*$ is essentially smooth; in particular, $(f - g)^*$ is differentiable on the interior of its domain.*

Remark 2.2.15. The number γ_0, defined in (2.11) when f is not strictly concave on int(dom f), is nonnegative. Indeed, if we had $\gamma_0 < 0$, then the proof of part (a) of the theorem with $\gamma = 0$ would show that f is strictly concave on int(dom f).

Proof. (a) If f is strictly concave on int(dom f), then $f - \gamma\|\cdot\|^2$ is also strictly concave on this set for any $\gamma \geq 0$. We now consider the case in which f is not strictly concavity on int(dom f). If $g(x) = \gamma\|x\|^2$, then $f - g$ is continuous on dom f. For $x \in$ int(dom f), let $Q_x = \{\partial^2 f(x)/\partial x_i \partial x_j\}$ denote the Hessian matrix of f at x. We choose $\gamma > \gamma_0$ in accordance with (2.11), noting that

$$\begin{aligned} \gamma_0 &= \tfrac{1}{2} \cdot \sup_{x \in \text{int(dom } f)} \kappa(x) \\ &= \tfrac{1}{2} \cdot \sup_{x \in \text{int(dom } f)} \sup\{\langle Q_x \zeta, \zeta\rangle : \zeta \in I\!R^\sigma, \|\zeta\| = 1\}\,. \end{aligned} \tag{2.12}$$

Let I be the identity matrix. It follows that for any $x \in$ int(dom f) and all nonzero $z \in I\!R^\sigma$

$$\|z\|^2 \cdot [\langle Q_x z/\|z\|, z/\|z\|\rangle - 2\gamma] = \langle (Q_x - 2\gamma I)z, z\rangle < 0.$$

By analogy with the proof of Theorem 4.5 in [62], the strict concavity of $f - g$ on int(dom f) is equivalent to the strict concavity of the restriction of $f - g$ to each line segment in int(dom f). This, in turn, is equivalent to the strict concavity, for each $y \in$ int(dom f) and nonzero $z \in I\!R^\sigma$, of $\psi(\lambda) = (f - g)(y + \lambda z)$ on the open interval $G(y, z) = \{\lambda \in I\!R : y + \lambda z \in \text{int(dom } f)\}$. Since

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

ψ' is strictly decreasing on $G(y, z)$. A straightforward extension of the proof of Theorem 4.4 in [62], in which the inequalities in the first two displays are replaced by strict inequalities, shows that $-\psi$ is strictly convex on $G(y, z)$ and thus that ψ is strictly concave on $G(y, z)$. It follows that $f - g$ is strictly concave on int(dom f). Since f is continuous on dom f, Lemma 2.2.8 allows us to conclude that f is also strictly concave on all closed line segments $L[x, y]$ for $x \in$ int(dom f) and $y \in$ dom $f \cap$ rb(dom f). Since any point in dom $f \setminus$ int(dom f) is the limit of a sequence of points in int(dom f) [62, Thm. 6.1], the continuity of $f - g$ on dom f allows us to extend the strict concavity of $f - g$ on int(dom f) to the concavity of $f - g$ on dom f. This completes the proof of part (a).

(b)–(c) These are proved like parts (b)–(c) of Theorem 2.2.12.

(d) If f is upper semicontinuous on $I\!R^\sigma$ and $g(x) = \gamma\|x\|^2$, then $f - g$ is upper semicontinuous on $I\!R^\sigma$. If dom f is closed, then the upper semicontinuity of f on $I\!R^\sigma$ follows immediately from the continuity of f on dom f. Part (a) implies that for any $\gamma > \gamma_0$, $f - g$ is concave on dom f and thus is concave on $I\!R^\sigma$. Since $f - g$ is upper semicontinuous of $I\!R^\sigma$, by part (b) of Theorem 2.2.3 we conclude that $f^{\sharp\sharp}(x) = f(x)$ for all $x \in I\!R^\sigma$.

(e) If dom f is open, then part (a) implies that $f - g$ is strictly concave on dom f and thus is essentially strictly concave. The essential smoothness of $(f-g)^*$ is a consequence of Theorem 2.2.11. The proof of the theorem is complete. ■

In the next theorem we point out another class of functions f for which there exists a function g such that $f - g$ is strictly concave on dom f.

Theorem 2.2.16. *Let $f \not\equiv -\infty$ be a function mapping $I\!R^\sigma$ into $I\!R \cup \{-\infty\}$ such that* dom f *is convex, closed, and bounded and such that f is bounded and continuous on* dom f. *Then there exists a continuous function g mapping $I\!R^\sigma$ into $I\!R$ such that the following conclusions hold.*

(a) *$f - g$ is strictly concave and continuous on* dom f, *and $(f - g)^*$ is essentially smooth; in particular, $(f - g)^*$ is differentiable on the interior of its domain.*

(b) *$f - g$ has a strictly supporting hyperplane at each point in* dom f *except possibly relative boundary points.*

(c) $f^{\sharp\sharp}(g,x) = f(x)$ *for all* $x \in I\!\!R^\sigma$.

Proof. (a) Let h be any strictly concave function on $I\!\!R^\sigma$. Since h is continuous on $I\!\!R^\sigma$ [62, Cor. 10.1.1], h is bounded and continuous on $\mathrm{dom}\, f$. For $x \in \mathrm{dom}\, f$ define $g(x) = f(x) - h(x)$. Since g is bounded and continuous on the closed set $\mathrm{dom}\, f$, the Tietze Extension Theorem guarantees that g can be extended to a bounded, continuous function on $I\!\!R^\sigma$ [32, Thm. 4.16]. Then $f - g$ has the properties in part (a). The strict concavity of $f - g$ on $\mathrm{dom}\, f$ implies the essential smoothness of $(f - g)^*$ and thus its differentiability [Thm. 2.2.11].

(b) This follows from part (a) of the present theorem and part (b) of Proposition 2.2.9 applied to $f - g$.

(c) The function g constructed in the proof of part (a) is bounded and continuous on $I\!\!R^\sigma$. In addition, $f-g$ is strictly concave on $\mathrm{dom}\, f$ and thus concave on $I\!\!R^\sigma$. Since $f-g$ is continuous on the closed set $\mathrm{dom}\, f$, $f - g$ is also upper semicontinuous on $I\!\!R^\sigma$. The equality $f^{\sharp\sharp}(x) = f(x)$ for all x follows from Theorem 2.2.3. ■

Theorems 2.2.12 and 2.2.14, as well as a local version of these results to be presented in Theorem 2.3.2, highlight the ease with which one can find a quadratic function g such that $f - g$ has a strictly supporting hyperplane at a point at which f alone does not have this property. It is interesting that one can formulate such a support property in a geometrically obvious way in terms of paraboloids. Here are the relevant definitions.

Definition 2.2.17. *Let f be a function mapping $I\!\!R^\sigma$ into $I\!\!R \cup \{-\infty\}$, x and α points in $I\!\!R^\sigma$, and $\gamma \geq 0$.*

(a) *We say that f has a supporting paraboloid at $x \in I\!\!R^\sigma$ with parameters (α, γ) if*

$$f(y) \leq f(x) + \langle \alpha, y - x \rangle + \gamma \|y - x\|^2 \ \text{ for all } y \in I\!\!R^\sigma.$$

(b) *We say that f has a strictly supporting paraboloid at $x \in I\!R^\sigma$ with parameters (α, γ) if*

$$f(y) < f(x) + \langle \alpha, y - x \rangle + \gamma \|y - x\|^2 \text{ for all } y \in I\!R^\sigma, y \neq x.$$

If $\sigma = 1$, then we will refer to a (strictly) supporting paraboloid as a (strictly) supporting parabola. The next proposition relates support properties of $f - \gamma \|\cdot\|^2$ with the existence of a supporting paraboloid or a strictly supporting paraboloid for f.

Proposition 2.2.18. *Let $f \not\equiv -\infty$ be a function mapping $I\!R^\sigma$ into $I\!R \cup \{-\infty\}$, x and α points in $I\!R^\sigma$, and $\gamma \geq 0$. Then f has a* (*strictly*) *supporting paraboloid at x with parameters (α, γ) if and only if $f - \gamma \|\cdot\|^2$ has a* (*strictly*) *supporting hyperplane at x with normal vector $[\tilde{\alpha}, -1]$. The quantities α and $\tilde{\alpha}$ are related by $\tilde{\alpha} = \alpha - 2\gamma x$.*

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

$$f(y) - \gamma \|y\|^2 < f(x) - \gamma \|x\|^2 + \langle \tilde{\alpha}, y - x \rangle,$$

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

An immediate application of Proposition 2.2.18 is to the two scenarios treated in Theorems 2.2.12 and 2.2.14, in which we prove that for suitable quadratic functions g, $f - g$ has a strictly supporting hyperplane at each point in dom f except possibly relative boundary points.

Corollary 2.2.19. *We assume the hypotheses on f in Theorems* 2.2.12 *and* 2.2.14 *and choose $\gamma \geq 0$ in accordance with the statements of the theorems. Then f has a strictly supporting paraboloid at each point in* dom f *except possibly relative boundary points.*

This completes our discussion of properties of the generalized Legendre-Fenchel transforms $f^\sharp$ and $f^{\sharp\sharp}$. In the next section we present a generalization of the generalized Legendre-Fenchel transform that is particularly suited in applications to statistical mechanics.

2.3 Generalized Legendre-Fenchel Transform, Part II

The theory presented so far addresses the question of finding a single function g such that $f^{\sharp\sharp}(g,x) = f(x)$ for all $x \in \text{dom}\, f$. In a number of applications one is satisfied with a less stringent requirement; namely, for each x in a given set K find a function g depending on x and having the property that $f^{\sharp\sharp}(g,x) = f(x)$. In such applications one may also want to work with a fixed set $\mathcal{S}$ of functions g; e.g., the set of quadratic functions $\gamma\|x\|^2$ with $\gamma \geq 0$. This choice of $\mathcal{S}$ arises in the main result to be presented in this section, Theorem 2.3.2.

In order to extend the theory of the generalized Legendre-Fenchel transform to these cases, let $f \not\equiv -\infty$ be a function mapping $I\!R^\sigma$ into $I\!R \cup \{-\infty\}$ and $\mathcal{S}$ a set of functions $g \not\equiv \infty$ mapping $I\!R^\sigma$ into $I\!R \cup \{\infty\}$. For $\alpha \in I\!R^\sigma$ and $g \in \mathcal{S}$ we define $f^\sharp(g,\alpha)$ by (2.1); i.e.,

$$f^\sharp(g,\alpha) = \inf_{x \in I\!R^\sigma} \{\langle \alpha, x\rangle + g(x) - f(x)\}.$$

For $x \in I\!R^\sigma$ we then define

$$f^{\sharp\flat}(\mathcal{S},x) = \inf_{g \in \mathcal{S}} \inf_{\alpha \in I\!R^\sigma} \{\langle \alpha, x\rangle + g(x) - f^\sharp(g,\alpha)\}. \tag{3.1}$$

By (2.2) and part (b) of Lemma 2.2.2

$$f^{\sharp\flat}(\mathcal{S},x) = \inf_{g \in \mathcal{S}} f^{\sharp\sharp}(g,x) = \inf_{g \in \mathcal{S}} \{g(x) + (f-g)^{**}(x)\}. \tag{3.2}$$

Thus, if $\mathcal{S}$ consists of a single function g, then $f^{\sharp\flat}(\mathcal{S},x) = f^{\sharp\sharp}(g,x)$. Since $f^{\sharp\sharp}(g,x) \geq f(x)$ [Lem. 2.2.2(c)], it follows that

$$f^{\sharp\flat}(\mathcal{S},x) = \inf_{g\in\mathcal{S}} f^{\sharp\sharp}(g,x) \geq f(x). \tag{3.3}$$

Among other information, the next lemma indicates when the infimum in (3.3) is attained and equals $f(x)$. As we will see in the example to be discussed in the next section, one can have $f^{\sharp\flat}(\mathcal{S},x) = f(x)$ without the infimum in (3.3) being attained.

Lemma 2.3.1. (a) *For $x \in I\!\!R^\sigma$ and any $g \in \mathcal{S}$, $f^{\sharp\sharp}(g,x) \geq f^{\sharp\flat}(\mathcal{S},x) \geq f(x)$.*

(b) *Assume that for $x \in I\!\!R^\sigma$ there exists $g \in \mathcal{S}$ such that $(f-g)^{**}(x) = (f-g)(x)$ or equivalently $f^{\sharp\sharp}(g,x) = f(x)$. Then the infimum in* (3.3) *is attained at g and*

$$f^{\sharp\flat}(\mathcal{S},x) = f^{\sharp\sharp}(g,x) = f(x).$$

Proof. (a) This is obvious from (3.3).

(b) By part (a) of Theorem 2.2.3 $(f-g)^{**}(x) = (f-g)(x)$ if and only if $f^{\sharp\sharp}(g,x) = f(x)$. Hence part (b) follows from part (a). ■

Let f be a C^2 function on the interior of dom f. In Theorem 2.2.14 we prove that if all the second-order partial derivatives of f are bounded above, then there exists a quadratic function g such that $f-g$ is strictly concave on the interior of dom f and thus has a strictly supporting hyperplane at each point of that set. If the boundedness condition on the second-order partial derivatives is not satisfied, then in general one cannot expect to find a quadratic function g with these properties. Theorem 2.3.2 handles this case. It shows that f is C^2 on an open set K and other conditions hold, then for each $x \in K$ there exists a quadratic g depending on x such that $f-g$ has a strictly supporting hyperplane at x. When applied to the microcanonical entropy, this result implies a form of universal equivalence of ensembles explained in Theorem 2.6.11 and in the paragraph following that theorem. In that discussion we will also see that it encompasses a generic class of applications. A comprehensive example illustrating Theorem 2.3.2 is given in Section 2.4.

Before stating the theorem, we need several preliminaries. Let $f \not\equiv -\infty$ be a function mapping $I\!R^\sigma$ into $I\!R \cup \{-\infty\}$ and K an open subset of dom f on which f is C^2. For $x \in K$, $\alpha \in I\!R^\sigma$, and $\lambda \geq 0$, we define

$$D(x, \alpha, \lambda) = \left\{ y \in \text{dom}\, f : f(y) \geq f(x) + \langle \alpha, y - x \rangle + \lambda \|y - x\|^2 \right\}. \qquad (3.4)$$

Geometrically, this set contains all points for which the paraboloid with parameters (α, λ) passing through $(x, f(x))$ lies below the graph of f. Clearly, since $\lambda \geq 0$, we have $D(x, \alpha, \lambda) \subset D(x, \alpha, 0)$; the set $D(x, \alpha, 0)$ contains all points for which the graph of the hyperplane with normal vector $[\alpha, -1]$ passing through $(x, f(x))$ lies below the graph of f. Thus, in the next theorem the hypothesis that for each $x \in K$ the set $D(x, \nabla f(x), \lambda)$ is bounded for some $\lambda \geq 0$ is satisfied if dom f is bounded or, more generally, if $D(x, \nabla f(x), 0)$ is bounded. The latter set is bounded if, for example, $-f$ is superlinear; i.e., $\lim_{\|y\| \to \infty} f(y)/\|y\| = -\infty$. In the next section we treat an example in which f tends to $-\infty$ quadratically and thus $D(x, \nabla f(x), 0)$ is bounded for each x.

We next state Theorem 2.3.2, the main result in this section.

Theorem 2.3.2. *Let $f \not\equiv -\infty$ be a function mapping $I\!R^\sigma$ into $I\!R \cup \{-\infty\}$ and K an open subset of* dom f. *Assume that f is bounded above on $I\!R^\sigma$ and is twice continuously differentiable on K. Assume also that* dom f *is bounded or, more generally, that for every $x \in K$ there exists $\lambda \geq 0$ such that the set $D(x, \nabla f(x), \lambda)$ defined in* (3.4) *is bounded. The following conclusions hold.*

(a) *For each $x \in K$, define $\gamma_0(x) \geq 0$ by* (3.8). *Then for any $\gamma > \gamma_0(x)$, f has a strictly supporting paraboloid at x with parameters $(\nabla f(x), \gamma)$.*

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

(c) *Let* $\mathcal{S}$ *be the set of quadratic functions* $g_\gamma = \gamma\|\cdot\|^2$ *for* $\gamma \geq 0$*. Then for each* $x \in K$ *and any* $\gamma > \gamma_0(x)$

$$f^{\sharp\flat}(\mathcal{S}, x) = f^{\sharp\sharp}(g_\gamma, x) = f(x).$$

Proof. (a) Fix $x \in K$ and let $B(x, r) \subset K$ be an open ball with center x and positive radius r whose closure is contained in K. If $\sigma = 1$, then f'' is bounded above on $B(x, r)$, while if $\sigma \geq 2$, then all second-order partial derivatives of f are bounded above on $B(x, r)$. We now apply, to the restriction of f to $B(x, r)$, part (a) of Theorem 2.2.12 when $\sigma = 1$ and part (a) of Theorem 2.2.14 when $\sigma \geq 2$. We conclude that there exists a sufficiently large $A \geq 0$ such that $f - A\|\cdot\|^2$ is strictly concave on $B(x, r)$. Part (b) of Proposition 2.2.9 implies that when restricted to $B(x, r)$, $f - A\|\cdot\|^2$ has a strictly supporting hyperplane at x; that is, there exists $\theta \in I\!R^\sigma$ such that

$$f(y) - A\|y\|^2 < f(x) - A\|x\|^2 + \langle \theta, y - x \rangle \text{ for all } y \in B(x, r), y \neq x. \tag{3.5}$$

In fact, $\theta = \nabla(f - A\|\cdot\|^2)(x) = \nabla f(x) - 2Ax$ because $f - A\|\cdot\|^2$ is concave and differentiable on $B(x, r)$ [62, Thm. 25.1]. We rewrite the inequality in the last display as

$$f(y) < f(x) + \langle \nabla f(x), y - x \rangle + A\|y - x\|^2 \text{ for all } y \in B(x, r), y \neq x. \tag{3.6}$$

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 $f(y) = -\infty$ for $y \notin \text{dom} f$, the set where the inequality in the last display does not hold is $D(x, \nabla f(x), A)$. Since $A > \lambda$, we have $D(x, \nabla f(x), A) \subset D(x, \nabla f(x), \lambda)$, and since the latter set is assumed to be bounded, there exists $b \in (0, \infty)$ such that

$$D(x, \nabla f(x), A) \subset \{y \in I\!R^\sigma : \|y - x\| < b\}. \tag{3.7}$$

In addition, there exists $C \in (0, \infty)$ such that $f(y) \leq C$ for all $y \in I\!\!R^\sigma$.

Let γ be any number satisfying

$$\gamma > \gamma_0(x) = \max\left\{A, \frac{C - f(x) + \|\nabla f(x)\|b}{r^2}\right\}. \tag{3.8}$$

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

$$f(y) < f(x) + \langle \nabla f(x), y - x \rangle + \gamma \|y - x\|^2 \text{ for all } y \in I\!\!R^\sigma, y \neq x. \tag{3.9}$$

It suffices to prove (3.9) for all $y \in \text{dom} f$. Since $\gamma > A$ and since (3.6) is valid for all $y \in B(x, r)$, $y \neq x$, (3.9) is also valid for all $y \in B(x, r)$, $y \neq x$. In addition, for all $y \in \text{dom} f \setminus D(x, \nabla f(x), A)$

$$\begin{aligned} f(y) &< f(x) + \langle \nabla f(x), y - x \rangle + A\|y - x\|^2 \\ &\leq f(x) + \langle \nabla f(x), y - x \rangle + \gamma\|y - x\|^2, \end{aligned}$$

and so (3.9) is also valid for all such y. We finally show that (3.9) is valid for all $y \in D(x, \nabla f(x), A) \setminus B(x, r)$. This follows from the string of inequalities

$$\begin{aligned} & f(x) + \langle \nabla f(x), y - x \rangle + \gamma\|y - x\|^2 \\ & \quad > f(x) + \langle \nabla f(x), y - x \rangle + \gamma r^2 \\ & \quad > f(x) - \|\nabla f(x)\|b + C - f(x) + \|\nabla f(x)\|b \\ & \quad = C \\ & \quad \geq f(y). \end{aligned}$$

By proving that (3.9) is valid for all $y \in I\!\!R^\sigma$, we have completed the proof of part (a).

(b) This follows from part (a) of the present theorem and Proposition 2.2.18.

(c) By part (a), for each $x \in K$ and all sufficiently large $\gamma \geq 0$, $f - g_\gamma$ has a strictly supporting hyperplane, and thus a supporting hyperplane, at x. Hence by part (a) of

Proposition 2.2.9 applied to $f - g_\gamma$, we have $(f - g_\gamma)^{**}(x) = (f - g_\gamma)(x)$. Part (b) of Lemma 2.3.1 gives the desired conclusion; namely, that

$$f^{\sharp\flat}(\mathcal{S}, x) = f^{\sharp\sharp}(g_\gamma, x) = f(x).$$

This completes the proof of the theorem. ■

In the next section we analyze the fascinating example of the double-parabolic function, applying several results proved in the present and preceding sections.

2.4 Example of the Double-Parabolic Function

The example to be treated in this section illustrates several features of the generalized Legendre-Fenchel transforms $f^{\sharp\sharp}(g, x)$ and $f^{\sharp\flat}(\mathcal{S}, x)$ defined in (2.2) and (3.1). For the set of functions $\mathcal{S}$ we use the set of quadratic functions $g(x) = \gamma\|x\|^2$ for $\gamma \geq 0$.

The double-parabolic function that we analyze is defined for $x \in I\!R$ by

$$f(x) = \max\Big\{-\tfrac{1}{2}(x+1)^2, -\tfrac{1}{2}(x-1)^2\Big\} = \begin{cases} -\frac{1}{2}(x+1)^2 & \text{if } x < 0 \\ -\frac{1}{2}(x-1)^2 & \text{if } x \geq 0. \end{cases} \tag{4.1}$$

This function arises naturally in the theory of large deviations as negative the rate function of appropriately scaled normal random variables with random means ± 1 [41]. Specifically, let W_n be a sequence of normal random variables with mean 0 and variance n and let Y be an independent random variable for which $P\{Y = 1\} = P\{Y = -1\} = 1/2$. W_n satisfies the LDP with rate function $x^2/2$. By conditioning on the two values of Y, one easily shows that $Y + W_n$ satisfies the large deviation principle with rate function given by negative the function f in (4.1).

Clearly, f is concave on the set $|x| \geq 1$. A short calculation shows that

$$f^*(\alpha) = \inf_{x \in I\!R} \{\alpha x - f(x)\} = \begin{cases} -\frac{1}{2}(\alpha^2 - 2\alpha) & \text{if } \alpha < 0 \\ -\frac{1}{2}(\alpha^2 + 2\alpha) & \text{if } \alpha \geq 0 \end{cases}$$

and that

$$f^{**}(x) = \inf_{\alpha \in I\!R} \{\alpha x - f^*(\alpha)\} = \begin{cases} -\frac{1}{2}(x+1)^2 & \text{if } x \leq -1 \\ 0 & \text{if } x \in (-1, 1) \\ -\frac{1}{2}(x-1)^2 & \text{if } x \geq 1. \end{cases}$$

It follows that $f^{**}(x) = f(x)$ on the set $|x| \geq 1$, which is the set where f is concave. In accordance with part (c) of Theorem 2.2.1, f^{**} equals the concave, upper semicontinuous hull of f.

Our goal is to find a set of functions $\mathcal{S}$ having the property that $f^{\sharp\flat}(\mathcal{S}, x) = f(x)$ for all $x \in I\!R$. As we will see, this equality can be achieved by choosing $\mathcal{S}$ to be the set of quadratic functions γx^2 for $\gamma \geq 0$. According to part (a) of Lemma 2.3.1,

$$f^{\sharp\flat}(\mathcal{S}, x) = \inf_{g \in \mathcal{S}} f^{\sharp\sharp}(g, x). \tag{4.2}$$

For each $x \neq 0$ the infimum in (4.2) is attained at all $g_\gamma(y) = \gamma y^2$, where γ is is greater than or equal to a critical value γ_x depending on x [see (4.7)]; for all $\gamma \geq \gamma_x$, $f^{\sharp\sharp}(g_\gamma, x) = f(x)$. However, since $\gamma_x \to \infty$ as $x \to 0$, we cannot find a single $g \in \mathcal{S}$ such that $f^{\sharp\sharp}(g, x) = f(x)$ holds for all $x \neq 0$.

For $x = 0$ the situation is different. In this case the infimum in (4.2) is not attained at any $g \in \mathcal{S}$; instead, $f^{\sharp\flat}(\mathcal{S}, 0) = \lim_{\gamma \to \infty} f^{\sharp\sharp}(g_\gamma, 0)$. Alternatively, if one augments $\mathcal{S}$ with the function $\varphi(x)$ that equals 0 at $x = 0$ and equals ∞ at all $x \neq 0$, then the infimum in the formula

$$f^{\sharp\flat}(\mathcal{S} \cup \{\varphi\}, 0) = \inf_{g \in \mathcal{S} \cup \{\varphi\}} f^{\sharp\sharp}(g, 0)$$

is attained at $g = \varphi$ and $f^{\sharp\sharp}(\varphi, 0) = f(0)$. We express this by writing

$$f^{\sharp\flat}(\mathcal{S}, 0) = \lim_{\gamma\to\infty} f^{\sharp\sharp}(g_\gamma, 0) = f^{\sharp\sharp}(\varphi, 0).$$

The second equality is consistent with the fact that $\varphi = \lim_{\gamma\to\infty} g_\gamma$.

We now verify these statements both by explicit calculation and by applying the theory developed so far in this chapter. For $\gamma \geq 0$, define

$$f_\gamma(x) = f(x) - \gamma x^2.$$

This function has two symmetric maximum points at $\pm x_\gamma$, where

$$x_\gamma = \frac{1}{2\gamma + 1}. \tag{4.3}$$

The value of f_γ at these maxima is

$$f_\gamma(x_\gamma) = f_\gamma(-x_\gamma) = M_\gamma = -\frac{2\gamma^2}{(2\gamma+1)^2}. \tag{4.4}$$

First we calculate $f^{\sharp\flat}(\mathcal{S}, x)$ using (3.2):

$$f^{\sharp\flat}(\mathcal{S}, x) = \inf_{\gamma>0}\{\gamma x^2 + (f_\gamma)^{**}(x)\}. \tag{4.5}$$

Since

$$(f_\gamma)^*(\alpha) = \inf_{x\in I\!R}\{\alpha x - f_\gamma(x)\} = \begin{cases} -\dfrac{\alpha^2 - 2\alpha - 2\gamma}{4\gamma+2} & \text{if } \alpha < 0 \\ -\dfrac{\alpha^2 + 2\alpha - 2\gamma}{4\gamma+2} & \text{if } \alpha \geq 0 \end{cases}$$

and

$$(f_\gamma)^{**}(x) = \inf_{\alpha\in I\!R}\{\alpha x - (f_\gamma)^*(\alpha)\} = \begin{cases} f_\gamma(x) & \text{if } x \notin (-x_\gamma, x_\gamma) \\ M_\gamma & \text{if } x \in (-x_\gamma, x_\gamma), \end{cases}$$

it follows that

$$\gamma x^2 + (f_\gamma)^{**}(x) = \begin{cases} f(x) & \text{if } x \notin (-x_\gamma, x_\gamma) \\ \gamma x^2 + M_\gamma & \text{if } x \in (-x_\gamma, x_\gamma). \end{cases}$$

Thus by (4.5)

$$f^{\sharp\flat}(\mathcal{S},x) = \inf_{\gamma\geq 0}\Big\{f(x)\cdot 1_{(-x_\gamma,x_\gamma)^c}(x) + (\gamma x^2\ +\ M_\gamma)\cdot 1_{(-x_\gamma,x_\gamma)}\Big\}. \tag{4.6}$$

According to (3.3), for each $x \in I\!R$

$$f^{\sharp\flat}(\mathcal{S},x) = \inf_{g\in\mathcal{S}} f^{\sharp\sharp}(g,x) \geq f(x).$$

A consequence of (4.6) is that the formula

$$f^{\sharp\flat}(\mathcal{S},x) = f^{\sharp\sharp}(g_\gamma,x) = f(x)$$

is valid for any γ having the property that $x \notin (-x_\gamma, x_\gamma)$. Since $x_\gamma = 1/(2\gamma+1)$, this holds for any

$$\gamma \geq \gamma_x = \begin{cases} 0 & \text{if } |x| \geq 1 \\ \dfrac{1}{2}\left(\dfrac{1}{|x|} - 1\right) & \text{if } |x| < 1. \end{cases} \tag{4.7}$$

The critical value γ_x has the property that $x_{\gamma_x} = |x|$. Since $0 \in (-x_\gamma, x_\gamma)$ for all $\gamma \geq 0$, (4.6) also implies that

$$f^{\sharp\flat}(\mathcal{S},0) = \inf_{\gamma\geq 0} M_\gamma = \lim_{\gamma\to\infty} M_\gamma = -\frac{1}{2} = f(0).$$

This concludes the calculations showing that for all $x \in I\!R$

$$f^{\sharp\flat}(\mathcal{S},x) = \inf_{g\in\mathcal{S}} f^{\sharp\sharp}(g,x) = f(x),$$

that for $x \neq 0$ the infimum in this formula is attained at all g_γ for $\gamma \geq \gamma_x$, and that for $x = 0$ the infimum in this formula is not attained at any $g \in \mathcal{S}$.

Many features of these calculations can be determined directly from the theory that has been developed. For example, Theorem 2.3.2 can be applied to either of the open, convex sets $K^- = (-\infty, 0)$ or $K^+ = (0,\infty)$. Indeed f is bounded above by 0, and f is twice continuously differentiable on $K^- \cup K^+$. Furthermore, for any $x \in K^- \cup K^+$ the set

$$D(x, f'(x), 0) = \{y \in I\!R : f(y) \geq f(x) + f'(x)\cdot(y-x)\}$$

is bounded since as $|y| \to \infty$, $f(y)$ goes to $-\infty$ like $-y^2/2$. For $\gamma \geq 0$ we define $g_\gamma(x) = \gamma x^2$. Part (a) of Theorem 2.3.2 guarantees that for each $x \in K^- \cup K^+$ and all sufficiently large $\gamma \geq 0$, $f - g_\gamma$ has a strictly supporting line at each x. Part (b) of that theorem implies that for each $x \in K^- \cup K^+$, $f^{\sharp\flat}(\mathcal{S}, x) = f(x)$, where $\mathcal{S} = \{g_\gamma : \gamma \geq 0\}$. This conclusion of part (a) of Theorem 2.3.2 can also be determined from the graph of f, which makes it obvious that for each x satisfying $|x| \geq 1$, f has a strictly supporting line at x and that for each x satisfying $0 < |x| < 1$, f has a strictly supporting parabola at x of the form $\alpha(y - x) + \gamma(y - x)^2$ for sufficiently large $\gamma \geq 0$. By part (b) of Proposition 2.2.18 we conclude that for each x satisfying $0 < |x| < 1$, $f - g_\gamma$ has a strict supporting line at x for sufficiently large $\gamma \geq 0$.

We have now completed our analysis of two forms of generalized Legendre-Fenchel transforms. In the next section we review the results on ensemble equivalence and nonequivalence proved in [23], which rely in part on properties of the standard Legendre-Fenchel transform. In Section 2.6 these results are extended to the context of generalized canonical ensembles, using properties of the generalized Legendre-Fenchel transforms derived in Sections 2.2 and 2.3.

2.5 Two Levels of Ensemble Equivalence and Nonequivalence

In [23] a general theory was developed for studying equivalence and nonequivalence of the microcanonical and canonical ensembles for a class of statistical mechanical models of coherent structures in turbulence. The notational changes between that paper and the present chapter are discussed in two paragraphs appearing just before Example 2.5.1. As we point out, all the results in [23] can be applied to a much wider class of models, including those considered in the present chapter, by making superficial changes in notation.

The general theory of ensemble equivalence and nonequivalence in [23] is based on the theory of large deviations and the theory of concave functions. In the present section we review the basic results in that paper, augmenting them by showing how to relate ensemble equivalence and nonequivalence at two separate, but related levels: the thermodynamic level and the level of equilibrium macrostates. In the next section we will show 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. The thermodynamic level of ensemble equivalence is formulated in terms of the generalized Legendre-Fenchel transforms introduced in Sections 2.2 and 2.3.

The statistical mechanical models that we consider are defined in terms of the following quantities.

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

- A sequence of positive scaling constants $a_n \to \infty$ 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 $n \in I\!N$ a sequence of Hamiltonians $\{H_{n,i}, i = 1, \ldots, \sigma\}$, which are measurable functions mapping Ω_n into $I\!R$. For $\omega \in \Omega_n$ we define

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

  h_n maps Ω_n into $I\!R^\sigma$.

A large deviation analysis of the general model is possible provided that we can find, as specified in the next four items, a hidden space, a hidden process, and a sequence of interaction representation functions and provided that the hidden process satisfies the large deviation principle (LDP) on the hidden space.

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

2. **Hidden process.** This is 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.** This is a sequence $\{\tilde{H}_i, i = 1, \ldots, \sigma\}$ of bounded, continuous functions mapping $\mathcal{X}$ into $\mathbb{R}$ such that as $n \to \infty$

$$h_{n,i}(\omega) = \tilde{H}_i(Y_n(\omega)) + \mathrm{o}(1) \quad \text{uniformly for } \omega \in \Omega_n; \tag{5.1}$$

i.e. $\lim_{n\to\infty} \sup_{\omega\in\Omega_n} |h_{n,i}(\omega) - \tilde{H}_i(Y_n(\omega))| = 0$. We define $\tilde{H} = (\tilde{H}_1, \ldots, \tilde{H}_\sigma)$, which maps $\mathcal{X}$ into $\mathbb{R}^\sigma$.

4. **LDP for the hidden process.** 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 $\mathcal{X}$ the large deviation upper bound

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

is valid, and for any open subset G of $\mathcal{X}$ the large deviation lower bound

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

is valid.

According to item 3, the interaction representation functions $\tilde{H}_i$ are bounded. Because of (5.1) the functions $h_{n,i}$ are also bounded. In Section 2.8 we show that all the results in this chapter are valid under much weaker hypotheses on $\tilde{H}_i$.

After explaining the differences in notation between [23] and the present chapter, we give a number of examples of models that can be studied by the methods of these two papers.

Notational changes between [23] and the present chapter. In [23] the general theory of ensemble equivalence and nonequivalence is formulated for a class of statistical mechanical models of coherent structures in turbulence. These models are typically defined on a fixed domain, and the associated equilibrium macrostates are studied in the continuum limit. In the present chapter we use the notation suitable for lattice spin models, which are typically defined on a sequence of expanding domains and for which the equilibrium macrostates are studied in the thermodynamic limit or infinite-volume limit. *With only superficial changes in notation, all the results in* [23] *are applicable here. In turn, all the results derived here are applicable to the models considered in* [23].

In [23] the quantities $H_{n,i}$ and $H_n = (H_{n,1}, \ldots, H_{n,\sigma})$ play the role that the quantities $h_{n,i} = \frac{1}{a_n} H_{n,i}$ and h_n play in the present chapter. Thus in [23] the asymptotic relationship (5.1) is replaced by

$$H_{n,i}(\omega) = \tilde{H}_i(Y_n(\omega)) + \text{o}(1) \text{ uniformly for } \omega \in \Omega.$$

There are also differences in the definitions of the ensembles. In the present chapter the canonical ensemble $P_{n,\beta}$ is defined in (5.2) with the exponential factor $\exp[-a_n\langle\beta, h_n\rangle]$, and the equilibrium macrostates are studied in terms of the $n \to \infty$ limit of the $P_{n,\beta}$-distributions of Y_n. By contrast, in [23] the canonical ensemble $P_{n,\beta}$ is defined with the exponential factor $\exp[-\langle\beta, H_n\rangle]$. The equilibrium macrostates are studied in terms of the $n \to \infty$ limit of the $P_{n,a_n\beta}$-distributions of Y_n, in which β is scaled by a_n. In the present chapter the microcanonical ensemble $P_n^{u,r}$ is defined in (5.7) by conditioning h_n to lie in a hypercube with center u and side-length $2r$. By contrast, in [23] the microcanonical ensemble $P_n^{u,r}$ is defined by conditioning H_n to lie in a hypercube with center u and side-length $2r$. In both papers the equilibrium macrostates with respect to the microcanonical ensemble are studied in terms of the $n \to \infty$ limit of the $P_n^{u,r}$-distributions of Y_n. This completes our discussion of the notational differences between [23] and the present chapter. $\blacksquare$

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 [23] and the present chapter. 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 fluid turbulence, the fifth a model of two-dimensional and barotropic, quasi-geostrophic turbulence, and the sixth a model of soliton turbulence.

Example 2.5.1.

1. Mean-field Blume-Emery-Griffiths model. The Blume-Emery Griffiths model [6] 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. This mean-field model is defined on the set $\{1, 2, \ldots, n\}$. 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 Hamiltonians are 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 hidden space for this model is the set of probability measures on Λ, the hidden process is the empirical measure associated with the spin configuration 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 [26], which also analyzes the phase transition in the model. Equivalence and nonequivalence of ensembles for this model is studied at the thermodynamic level in [2, 3, 27] and at the level of equilibrium macrostates in [27].

2. Curie-Weiss-Potts model. The Curie-Weiss-Potts model is a long-range, mean-field approximation to the well known Potts model [69]. It is defined on the set $\{1, 2, \ldots, n\}$. The spin at site $j \in \{1, 2, \ldots, n\}$ is denoted by ω_j, a quantity taking values in the set Λ consisting of the q coordinate vectors $\theta^i \in I\!R^q$, where $q \geq 3$ 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 $\frac{1}{q}\sum_{i=1}^{q} \delta_{\theta^i}$, and for $\omega = (\omega_1, \ldots, \omega_n) \in \Omega_n$ the Hamiltonians are 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 hidden space for the Curie-Weiss-Potts model is the set of probability measures on Λ, the hidden process is the empirical measure 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 [12], which together with [13] gives a complete analysis of ensemble equivalence and nonequivalence at the level of equilibrium macrostates.

3. Short-range spin systems. Short-range spin systems such as the Ising model on $Z\!\!Z^d$

and numerous generalizations can also be handled by the methods of this chapter. 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 [21]. The even more sophisticated analysis of multi-dimensional models is carried out in [31, 56]. For these spin systems the hidden space is the space of translation-invariant probability measures on $\mathbb{Z}^d$, the hidden process the empirical process, and the rate function in the associated LDP the mean relative entropy.

4. A model of fluid turbulence. The Miller-Robert model is a model of coherent structures for an ideal, two-dimensional fluid governed by the vorticity transport equation [54, 60]. The large deviation analysis of this model carried out in [8] gives a rigorous derivation of maximum entropy principles governing the equilibrium behavior of the ideal fluid. The hidden space equals the space of probability measures on the unit torus.

5. A model of two-dimensional and barotropic, quasi-geostrophic turbulence. A generalization of the Miller-Robert model describing coherent structures in two-dimensional and barotropic, quasi-geostrophic turbulence is presented in [24]. This paper also studies ensemble nonequivalence via numerical computations and presents new results on the nonlinear stability of the steady mean flows corresponding to microcanonical equilibrium macrostates. The large deviation analysis of this model is carried out in [22]. The hidden space equals $L^2(\Lambda)$, where Λ is a rectangle in $\mathbb{R}^2$.

6. A model of soliton turbulence. A model of coherent structures in soliton turbulence based on a class of dispersive wave equations of nonlinear Schrödinger-type is studied in [25]. The large deviation analysis of this model given in [25] derives rigorously a concentration phenomenon involving the long-time behavior of solutions of these equations. The hidden space is $L^2(\Lambda)$, where Λ is a bounded domain in $\mathbb{R}^d$. $\blacksquare$

We now return to the general theory, first introducing the canonical ensemble, the canonical free energy, the microcanonical entropy, and the microcanonical ensemble and then analyzing the relationships among these objects. 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

$$P_{n,\beta}\{B\} = \frac{1}{Z_n(\beta)} \cdot \int_B \exp[-a_n \langle \beta, h_n \rangle] \, dP_n. \tag{5.2}$$

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

The basic thermodynamic function for the canonical ensemble is the canonical free energy, defined for $\beta \in \mathbb{R}^\sigma$ by

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

It is proved in [23, Thm. 2.4] that this limit exists and is given by

$$\varphi(\beta) = \inf_{y \in \mathcal{X}} \{ I(y) + \langle \beta, \tilde{H}(y) \rangle \} \tag{5.3}$$

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

$$I_\beta(x) = I(x) + \langle \beta, \tilde{H}(x) \rangle - \varphi(\beta). \tag{5.4}$$

As the 0-set of this rate function, the set

$$\mathcal{E}_\beta = \{ x \in \mathcal{X} : I_\beta(x) = 0 \} \tag{5.5}$$

is nonempty and compact. Let A be any Borel subset of $\mathcal{X}$ whose closure $\bar{A}$ satisfies $\bar{A} \cap \mathcal{E}_\beta = \emptyset$ and define $I_\beta(\bar{A}) = \inf_{x \in \bar{A}} I_\beta(x)$. Then $I_\beta(\bar{A}) > 0$, and so by the large deviation upper bound

$$P_{n,\beta}\{Y_n \in A\} \leq \text{const} \cdot e^{-a_n I_\beta(\bar{A})/2} \to 0 \text{ as } n \to \infty.$$

This limit justifies calling $\mathcal{E}_\beta$ the set of canonical equilibrium macrostates.

The basic thermodynamic function for the microcanonical ensemble is the microcanonical entropy, defined for $u \in I\!\!R^\sigma$ by

$$s(u) = -\inf\{I(x) : x \in \mathcal{X}, \tilde{H}(x) = u\}. \tag{5.6}$$

Since I maps $\mathcal{X}$ into $[0, \infty]$, s maps $I\!\!R^\sigma$ into $[-\infty, 0]$. We define $\text{dom}\, s$ to be the set of $u \in I\!\!R^\sigma$ for which $s(u) > -\infty$. In general, $\text{dom}\, s$ is nonempty since $-s$ is a rate function [23, Prop. 3.1(a)]. For each $u \in \text{dom}\, s$, $r > 0$, $n \in I\!\!N$, and set $B \in \mathcal{F}_n$ the microcanonical ensemble is defined to be the conditioned measure

$$P_n^{u,r}\{B\} = P_n\{B \mid h_n \in \{u\}^{(r)}\}, \tag{5.7}$$

where $\{u\}^{(r)} = [u_1 - r, u_1 + r] \times \cdots \times [u_\sigma - r, u_\sigma + r]$. As shown in [23, p. 1027], if $u \in \text{dom}\, s$, 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.

It is proved in [23, Thm. 3.2] that with respect to $P_n^{u,r}$, Y_n satisfies the LDP on $\mathcal{X}$, in the double limit $n \to \infty$ and $r \to 0$, with rate function

$$I^u(x) = \begin{cases} I(x) + s(u) & \text{if } \tilde{H}(x) = u \\ \infty & \text{otherwise.} \end{cases} \tag{5.8}$$

As the 0-set of this rate function, for $u \in \text{dom}\, s$ the set

$$\mathcal{E}^u = \{x \in \mathcal{X} : I^u(x) = 0\}. \tag{5.9}$$

is nonempty and compact. It is called the set of microcanonical equilibrium macrostates. This nomenclature is justified by the large deviation principle as we outlined in the case of the canonical ensemble.

In the remainder of this section we state the results proved in [23] concerning ensemble equivalence and nonequivalence at the level of equilibrium macrostates. We also relate this level with the thermodynamic level of ensemble equivalence and nonequivalence.

The problem of ensemble equivalence and nonequivalence at the macrostate level involves relationships between the sets $\mathcal{E}_\beta$ and $\mathcal{E}^u$ of equilibrium macrostates for the two ensembles. These sets are defined in (5.5) and (5.9), respectively. The next theorem, proved in Theorems 4.4, 4.6, and 4.8 in [23], gives necessary and sufficient conditions, in terms of support properties of s, for ensemble equivalence and nonequivalence. Part (a) states that for any $\beta \in I\!R^\sigma$ canonical equilibrium macrostates can always be realized microcanonically. However, the converse is not necessarily true. According to part (d), for a given $u \in \operatorname{dom} s$ microcanonical equilibrium macrostates cannot be realized canonically unless s has a supporting hyperplane at u. We conclude that at the level of equilibrium macrostates the microcanonical ensemble is the richer of the two ensembles.

For the definitions of supporting hyperplane and strictly supporting hyperplane in the next theorem, the reader is referred to Definition 2.2.4.

Theorem 2.5.2. *In parts* (b), (c)*, and* (d)*,* u *denotes any point in* $\operatorname{dom} s$*.*

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

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

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

(c) **Partial equivalence.** *There exists $\beta \in I\!\!R^\sigma$ 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 $[\beta, -1]$.*

(d) **Nonequivalence.** *For all $\beta \in I\!\!R^\sigma$, $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ if and only if s has no supporting hyperplane at u. Except possibly for relative boundary points of* dom s*, the latter condition is equivalent to the nonconcavity of s at u* [Thm. 2.5.7(b)].

Theorem 4.10 in [23] states an alternative version of part (a) of Theorem 2.5.2, in which the set $\tilde{H}(\mathcal{E}_\beta)$ is replaced by $\partial\varphi(\beta) \cap \{u \in I\!\!R^\sigma : s(u) = s^{**}(u)\}$. We next present a third version of part (a) that is useful in applications [12].

Corollary 2.5.3. *For $\beta \in I\!\!R^\sigma$ we define A_β to be the set of $u \in$* 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 (a) of Theorem 2.5.2 implies that if $u \in \tilde{H}(\mathcal{E}_\beta)$, then $\mathcal{E}^u \subset \mathcal{E}_\beta$. From parts (b) and (c) 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 thus

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

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

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

This completes the proof. ■

One of our goals is find concavity and support conditions on the microcanonical entropy guaranteeing that the two ensembles are fully equivalent at all points $u \in$ dom s

except possibly relative boundary points. If this is the case, then we say that the ensembles are **universally equivalent**. As stated in part (d) of Theorem 2.5.7, a condition implying that the ensembles are universally equivalent is that s is strictly concave on $\operatorname{dom} s$.

Having completed our analysis of ensemble equivalence at the level of equilibrium macrostates, we end the section by relating this to 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 the context of statistical mechanical models in a natural way. Formula (5.3) makes it clear that the canonical free energy φ is a finite, concave function on $\mathbb{R}^\sigma$; by [62, Thm. 10.1] it is also continuous on $\mathbb{R}^\sigma$ and therefore upper semicontinuous. Replacing the infimum over $y \in \mathcal{X}$ in (5.3) 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 (5.6) of the microcanonical entropy s, we see that for all $\beta \in \mathbb{R}^\sigma$

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

This calculation shows that φ, the basic thermodynamic function in the canonical ensemble, can always be expressed as the Legendre-Fenchel transform of s, the basic thermodynamic function in the microcanonical ensemble. However, the converse need not be true. In fact, by part (b) of Theorem 2.2.1 $s(u) = \varphi^*(u)$ 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 mirrors what we have already seen at the level of equilibrium macrostates; namely, of the two ensembles the microcanonical ensemble is the more fundamental.

The next theorem records these facts in parts (a) and (b). Part (c) uses Theorem 2.2.11 to assert that if s is strictly concave on dom s, then φ is differentiable on $I\!\!R^\sigma$, a property implying that the canonical ensemble does not exhibit a discontinuous, first-order phase transition. The concept of essential smoothness appearing in part (c) of the theorem is defined in part (a) of Definition 2.2.10. Part (d) gives additional properties of s that will be used later in this chapter. The first assertion in part (d) is a consequence of the contraction principle and the general assumptions on the model [23, p. 1026]. It is reproved under weaker assumptions in Proposition 2.8.1 in the present chapter. The second assertion in part (d) follows from the definition of s and the facts that I is nonnegative and lower semicontinuous and $\tilde{H}$ is continuous.

Theorem 2.5.4. (a) *The canonical free energy φ is a finite, concave, continuous function on $I\!\!R^\sigma$, and $\varphi(\beta) = s^*(\beta)$ for all $\beta \in I\!\!R^\sigma$.*

(b) *For all $u \in I\!\!R^\sigma$, $s(u) = \varphi^*(u)$, or equivalently $s(u) = s^{**}(u)$, if and only if s is concave on $I\!\!R^\sigma$.*

(c) *If* dom s *is convex and s is strictly concave on dom s, then φ is essentially smooth; in particular, φ is differentiable on $I\!\!R^\sigma$.*

(d) *With respect to P_n, the sequences $\tilde{H}(Y_n)$ and h_n satisfy the* LDP *on $I\!\!R^\sigma$ with rate function $-s$. The function s is nonpositive and upper semicontinuous on $I\!\!R^\sigma$.*

Given $u \in$ dom s, we say that s is concave at u if $s(u) = s^{**}(u)$ and that s is nonconcave at u if $s(u) \neq s^{**}(u)$. Since $s(u) \leq s^{**}(u)$ is always valid [Thm. 2.2.1(c)], s is nonconcave at u if and only if $s(u) < s^{**}(u)$. In the physical literature thermodynamic equivalence of ensembles at $u \in$ dom s is traditionally formulated in terms of the equality $s(u) = \varphi^*(u) = s^{**}(u)$. Here are the relevant definitions.

Definition 2.5.5. *Let u be a point in* dom s*.*

(a) *The microcanonical and canonical ensembles are said to be thermodynamically equivalent at* u *if* $s(u) = s^{**}(u)$.

(b) *The ensembles are said to be thermodynamically nonequivalent at* u *if* $s(u) \neq s^{**}(u)$.

In summary, the ensembles are thermodynamically equivalent at u *if and only if* s *is concave at* u.

In order to avoid the technicalities associated with relative boundary points of dom s, we will first assume that dom s is an open subset of $I\!R^\sigma$. Although this assumption is not valid in many applications, introducing it allows us to considerably simplify the exposition. As we will soon see in Theorem 2.5.6, under this assumption the relationships between ensemble equivalence and nonequivalence at the thermodynamic level and at the level of equilibrium macrostates are especially clean. In Theorem 2.5.7 we will drop the assumption that dom s is open and give the more complicated relationships between these two levels that are necessitated by the presence of relative boundary points.

Part (a) of Theorem 2.5.6 characterizes, in terms of the set of points at which s is concave, the set of points at which s has a supporting hyperplane. Part (b) gives a useful criterion for selecting points at which s has a supporting hyperplane. Parts (c) and (d) fill in a small gap in [23]. Part (c) relates thermodynamic equivalence with full or partial equivalence of ensembles at the level of equilibrium macrostates. According to part (d), if s is strictly concave on its domain, then s has a strictly supporting hyperplane at all points in its domain. In combination with Theorem 2.5.2, part (d) gives a criterion for deciding when the two ensembles are universally equivalent; i.e., equivalent at all points $u \in$ dom s.

In order to state Theorem 2.5.6, we introduce the set C consisting of all $u \in I\!R^\sigma$ such that s has a supporting hyperplane at u; that is,

$$C = \{u \in I\!\!R^\sigma : \exists \beta \in I\!\!R^\sigma \ni s(v) \leq s(u) + \langle \beta, v - u \rangle \, \forall v \in I\!\!R^\sigma\}. \tag{5.10}$$

We also define

$$\Gamma = \{u \in I\!\!R^\sigma : s(u) = s^{**}(u)\}. \tag{5.11}$$

Thus $u \in \Gamma \cap \text{dom}\, s$ if and only if s is concave at u or equivalently the ensembles are thermodynamically equivalent at u.

In part (a) of the next proposition, $\text{dom}\, \partial s^{**}$ denotes the set of points u for which the superdifferential of s^{**} at u is nonempty [Defn. 2.2.4(c)]. In the proof of Theorem 2.5.6 as well as in the proof of its generalization given in Theorem 2.5.7, we will refer to Lemma 2.2.6, which states that if f is concave on $I\!\!R^\sigma$, then

$$\text{ri}(\text{dom}\, f) \subset \text{dom}\, \partial f \subset \text{dom}\, f. \tag{5.12}$$

This will be applied in the proof of part (a) to $f = s$ when s is concave on $I\!\!R^\sigma$ and in the proof of part (b) to $f = s^{**}$.

Theorem 2.5.6. *We assume that* $\text{dom}\, s$ *is an open subset of* $I\!\!R^\sigma$. *The following conclusions hold.*

(a) $C = \Gamma \cap \text{dom}\, \partial s^{**}$. *In particular, if s is concave on $I\!\!R^\sigma$, then* $C = \text{dom}\, \partial s = \text{dom}\, s$, *and so s has a supporting hyperplane at all points of* $\text{dom}\, s$.

(b) $C = \Gamma \cap \text{dom}\, s$.

(c) *The microcanonical and 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.*

(d) *Assume that* $\text{dom}\, s$ *is convex and open and that s is strictly concave on* $\text{dom}\, s$. *Then s has a strictly supporting hyperplane at all* $u \in \text{dom}\, s$, *and the ensembles are universally equivalent; i.e., fully equivalent at all $u \in$ dom s.*

Proof. (a) The assertion that $C = \Gamma \cap \text{dom}\, \partial s^{**}$ is proved in part (a) of Lemma 4.1 in [23]. A special case of this — namely, $C \subset \Gamma$ — is proved in part (a) of Proposition 2.2.9. If in addition s is concave on $I\!R^\sigma$, then by the definitions of the sets, $C = \text{dom}\, \partial s$. Since dom s is open, ri(dom $s) = \text{dom}\, s$, and so (5.12) implies that $C = \text{dom}\, s$. By the definition of C, this implies that s has a supporting hyperplane at all points in dom s.

(b) By part (a), $C \subset \Gamma$. In addition, if $u \in C$, then there exists $\beta \in I\!R^\sigma$ such that

$$s(v) \leq s(u) + \langle \beta, v - u \rangle \text{ for all } v \in I\!R^\sigma,$$

and so $u \in \text{dom}\, s$. It follows that $C \subset \Gamma \cap \text{dom}\, s$. Conversely, if $u \in \Gamma \cap \text{dom}\, s$, then $s(u) = s^{**}(u)$ and, since dom $s \subset \text{dom}\, s^{**}$ and dom s is open, we also have $u \in$ ri(dom $s) \subset$ ri(dom $s^{**})$. Since ri(dom $s^{**})$ is a subset of dom ∂s^{**} [see (5.12)], it follows that $\Gamma \cap \text{dom}\, s \subset \Gamma \cap \text{dom}\, \partial s^{**}$. Since by part (a) $\Gamma \cap \text{dom}\, \partial s^{**}$ equals C, we have completed the proof that $C = \Gamma \cap \text{dom}\, s$.

(c) If the ensembles are thermodynamically equivalent at $u \in \text{dom}\, s$, then $s(u) = s^{**}(u)$, and so $u \in \Gamma \cap \text{dom}\, s$. Hence by part (b) $u \in C$. Parts (b) and (c) of Theorem 2.5.2 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, then by parts (b) and (c) of Theorem 2.5.2 we have $u \in C$ and thus, by part (a) of the present theorem, $u \in \Gamma$. We conclude that the ensembles are thermodynamically equivalent at u.

(d) Since s is strictly concave on the open set dom s, s is continuous on dom s [62, Thm. 10.1]. Part (b) of Proposition 2.2.9 then implies that s has a strictly supporting hyperplane at all $u \in \text{dom}\, s$. The fact that the ensembles are universally equivalent is a consequence of part (b) of Theorem 2.5.2. The proof of the theorem is complete. ■

We end this section by dropping the assumption in Theorem 2.5.6 that dom s is an open subset of $I\!R^\sigma$ and giving in Theorem 2.5.7 the general relationships between ensemble equivalence and nonequivalence at the thermodynamic level and at the level of equilibrium macrostates. Because of the presence of relative boundary points, the relationships between these two levels are more complicated than in Theorem 2.5.6, in which we assumed that dom s is open. The sets C and Γ in the next proposition are defined in (5.10) and (5.11).

Theorem 2.5.7. *In contrast to Theorem* 2.5.6*, we no longer assume that* dom s *is an open subset of* $I\!\!R^\sigma$*. The following conclusions hold.*

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

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

(c) *If the microcanonical and 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*.*

(d) *Assume that* dom s *is convex and* s *is strictly concave on* ri(dom s) *and continuous on* dom s*. Then* s *has a strictly supporting hyperplane at all* $u \in \text{dom}\, s$ *except possibly relative boundary points, and the ensembles are universally equivalent; i.e., fully equivalent at all* $u \in \text{dom}\, s$ *except possibly relative boundary points.*

Proof. (a) The assertion that $C = \Gamma \cap \text{dom}\, \partial s^{**}$ is proved in part (a) of Lemma 4.1 in [23]. If in addition s is concave on $I\!\!R^\sigma$, then by the definitions of the sets, $C = \text{dom}\, \partial s$. By (5.12) s has a supporting hyperplane at all points in dom s except possibly relative boundary points.

(b) If $u \in \Gamma \cap \text{ri}(\text{dom}\, s)$, then $s(u) = s^{**}(u)$ and $u \in \text{ri}(\text{dom}\, s^{**})$, which in turn is a subset of dom ∂s^{**} [see (5.12)]. Hence $\Gamma \cap \text{ri}(\text{dom}\, s) \subset \Gamma \cap \text{dom}\, \partial s^{**}$, which by part (a) equals C. This proves the first inclusion in part (b). The second inclusion in part (b) is proved as in the proof of part (b) of Theorem 2.5.6.

(c) If the ensembles are thermodynamically equivalent at $u \in \text{ri}(\text{dom}\, s)$, then $s(u) = s^{**}(u)$, and so $u \in \Gamma \cap \text{ri}(\text{dom}\, s)$. Hence by part (b) of the present proposition, $u \in C$. Parts (b) and (c) of Theorem 2.5.2 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, then by parts (b) and (c) of Theorem 2.5.2 we have $u \in C$ and thus, by part (a) of the present theorem, $u \in \Gamma$. We conclude that the ensembles are thermodynamically equivalent at u.

(d) Part (b) of Proposition 2.2.9 implies that s has a strictly supporting hyperplane at all $u \in \text{dom}\, s$ except possibly relative boundary points. The fact that the ensembles are universally equivalent is a consequence of part (b) of Theorem 2.5.2. The proof of the theorem is complete. ■

In the next section we generalize the results just presented to the setting of generalized canonical ensembles.

2.6 Generalized Canonical Ensembles

In this section we introduce a new class of canonical ensembles called generalized canonical ensembles. One of the main results is to show that when the standard canonical ensemble is nonequivalent to the microcanonical ensemble on some 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. As in the theory developed in [23], the new results concerning the generalized canonical ensemble address both the thermodynamic level and the macrostate level of ensemble equivalence. The thermodynamic level is expressed in terms of the generalized Legendre-Fenchel transforms that were introduced in Section 2.2 and 2.3. A special case of the generalized canonical ensembles are Gaussian ensembles, defined by adding an appropriate quadratic term to the exponent in the standard canonical ensemble [10, 11, 43].

The new ensembles are defined in terms of a continuous function g mapping $I\!R^\sigma$ into $I\!R$. For each $n \in I\!N$ and $\beta \in I\!R^\sigma$ we define the generalized partition function

$$Z_{n,g}(\beta) = \int_{\Omega_n} \exp[-a_n\langle\beta, h_n\rangle - a_n g(h_n)]\, dP_n. \tag{6.1}$$

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

$$P_{n,\beta,g}\{B\} = \frac{1}{Z_{n,g}(\beta)} \cdot \int_B \exp[-a_n\langle\beta, h_n\rangle - a_n g(h_n)]\, dP_n. \tag{6.2}$$

We call $P_{n,\beta,g}$ the generalized canonical ensemble.

The basic thermodynamic function for the generalized canonical ensemble is the generalized canonical free energy. For $\beta \in I\!R^\sigma$ it is defined by

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

The next theorem expresses this limit in terms of a variational formula and shows that with respect to the generalized canonical ensemble the hidden process Y_n satisfies an LDP.

Theorem 2.6.1. *Let g be a continuous function mapping $I\!R^\sigma$ into $I\!R$, in terms of which the generalized canonical ensemble* (6.2) *is defined. The following conclusions hold.*

(a) *$\varphi_g(\beta)$ exists and is given by*

$$\varphi_g(\beta) = \inf_{y\in\mathcal{X}}\{I(y) + \langle\beta, \tilde{H}(y)\rangle + g(\tilde{H}(y))\}. \tag{6.3}$$

(b) *With respect to* $P_{n,\beta,g}$, Y_n *satisfies the LDP on* $\mathcal{X}$ *with the rate function*

$$I_{\beta,g}(x) = I(x) + \langle \beta, \tilde{H}(x) \rangle + g(\tilde{H}(x)) - \varphi_g(\beta). \tag{6.4}$$

Proof. We will prove that for any bounded, continuous function f mapping $\mathcal{X}$ into $I\!R$

$$\begin{aligned} \lim_{n\to\infty} \frac{1}{a_n} \log \int_{\Omega_n} \exp[a_n f(Y_n) - a_n \langle \beta, h_n \rangle - a_n g(h_n)]\, dP_n \\ = \sup_{y\in\mathcal{X}} \{ f(y) - \langle \beta, \tilde{H}(y) \rangle - g(\tilde{H}(y)) - I(y) \}. \end{aligned} \tag{6.5}$$

Not only does this limit with $f = 0$ give part (a) of the theorem, but also it implies that

$$\lim_{n\to\infty} \frac{1}{a_n} \log \int_{\Omega_n} \exp[a_n f(Y_n)]\, dP_{n,\beta,g} = \sup_{y\in\mathcal{X}} \{ f(y) - I_{\beta,g}(y) \}.$$

This limit, known as the Laplace principle for Y_n with respect to $P_{n,\beta,g}$, is equivalent to the LDP stated in part (b) of the theorem [19, Thms. 1.2.1, 1.2.3].

We now prove the limit (6.5). Pick $M < \infty$ sufficiently large so that

$$\sup_{x\in\mathcal{X}} \{ \|h_n(x)\|, \|\tilde{H}(x)\| \} \leq M.$$

This is possible by (5.1) and the boundedness of $\tilde{H}$. It follows from [21, Lem. II.7.4] that

$$\begin{aligned} &\left| \frac{1}{a_n} \log \int_{\Omega_n} \exp[a_n f(Y_n) - a_n \langle \beta, h_n \rangle - a_n g(h_n)]\, dP_n \right. \\ &\quad \left. - \ \frac{1}{a_n} \log \int_{\Omega_n} \exp[a_n f(Y_n) - a_n \langle \beta, \tilde{H}(Y_n) \rangle - a_n g(\tilde{H}(Y_n))] dP_n \right| \\ &\quad \leq \| \langle \beta, h_n \rangle - \langle \beta, \tilde{H}(Y_n) \rangle \|_\infty + \| g(h_n) - g(\tilde{H}(Y_n)) \|_\infty . \end{aligned}$$

By (5.1) and the uniform continuity of g on $\{y \in R^\sigma : \|y\| \leq M\}$, the terms in the last line of this display converge to 0 as $n \to \infty$. Thus (6.5) is proved once we show that

$$\begin{aligned} \lim_{n\to\infty} \frac{1}{a_n} \log \int_{\Omega_n} \exp[a_n f(Y_n) - a_n \langle \beta, \tilde{H}(Y_n) \rangle - a_n g(\tilde{H}(Y_n))]\, dP_n \\ = \sup_{y\in\mathcal{X}} \{ f(y) - \langle \beta, \tilde{H}(y) \rangle - g(\tilde{H}(y)) - I(y) \}. \end{aligned}$$

Since Y_n satisfies the LDP with respect to P_n, it also satisfies the Laplace principle with respect to P_n [19, Thms. 1.2.1]. This gives the limit in the last display since f, $\tilde{H}$, and $g \circ \tilde{H}$ are all bounded, continuous functions mapping $\mathcal{X}$ into $I\!\!R$. The proof of the theorem is complete. ■

As we have just seen, the generalized canonical ensemble $P_{n,\beta,g}$ is defined in terms of a continuous function g mapping $\mathcal{X}$ into $I\!\!R$. With respect to these measures Y_n satisfies the LDP with rate function $I_{\beta,g}$ defined in (6.4). As in the case of the standard canonical ensemble considered in Section 2, the set

$$\mathcal{E}(g)_\beta = \{x \in \mathcal{X} : I_{\beta,g}(x) = 0\} \tag{6.6}$$

is called the set of generalized canonical equilibrium macrostates.

The main goal of this section is to analyze the equivalence and nonequivalence of the microcanonical and generalized canonical ensembles both at the level of equilibrium macrostates and at the thermodynamic level. The analysis at the former level is presented in Theorem 2.6.2. The function g used in the definition of the generalized canonical ensemble affects the formulation in a simple yet fundamental way. Essentially all the results in Section 2.5 concerning equivalence and nonequivalence of the microcanonical and standard canonical ensembles generalize to the present setting by replacing the microcanonical entropy s by $s - g$. This phenomenon will be elucidated in Section 2.7.

The most important repercussion of this fact is the ease with which one can prove that the microcanonical and generalized canonical ensembles are universally equivalent in those cases in which full or even partial equivalence does not hold in the setting of the preceding section. In order to achieve universal equivalence, one merely chooses g so that $s - g$ is strictly concave on $\operatorname{dom} s$. One has considerable freedom doing this since the only requirement is that g be continuous. Several useful examples, three of which involve quadratics, are given in Theorems 2.6.9–2.6.11.

We now present the main result of this section, Theorem 2.6.2, which gives necessary and sufficient conditions, in terms of support properties of $s - g$, for ensemble equivalence and nonequivalence at the level of equilibrium macrostates. This equivalence and nonequivalence is expressed in terms of relationships between the set $\mathcal{E}^u$ of microcanonical equilibrium macrostates, defined in (5.9), and the set $\mathcal{E}(g)_\beta$ of generalized canonical equilibrium macrostates, defined in (6.6).

Two proofs of the next theorem will be presented. In Section 2.7 we give an elementary proof of Theorem 2.6.2, deriving it from Theorem 2.5.2, its analogue for the canonical ensemble. In Section 2.9, Theorem 2.6.2 is proved directly from first principles without the use of Theorem 2.5.2. Of these two proofs, the one given in Section 2.9 was worked out first. Although it has the virtue of being self-contained, the proof given in Section 2.7 illuminates much more clearly how Theorem 2.6.2 follows immediately from Theorem 2.5.2 by replacing s in the latter theorem by $s - g$.

As in the preceding section, where we considered the standard canonical ensemble, Theorems 2.6.4 and 2.6.2 show that for a general function g the microcanonical ensemble is the more basic of the two ensembles, both at the thermodynamic level and at the level of equilibrium macrostates. However, as we will see in Theorems 2.6.9–2.6.11, the considerable freedom that one has in choosing g often makes it possible to pick a suitable g such that the microcanonical and generalized canonical ensembles are universally equivalent.

Theorem 2.6.2. *Let g be a continuous function mapping $I\!R^\sigma$ into $I\!R$, in terms of which the generalized canonical ensemble* (6.2) *is defined. The following conclusions hold. In parts* (b), (c), *and* (d), u *denotes any point in* dom s.

(a) **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*

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

(b) **Full equivalence.** *There exists* $\beta \in I\!\!R^\sigma$ *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* $[\beta, -1]$.

(c) **Partial equivalence.** *There exists* $\beta \in I\!\!R^\sigma$ *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* $[\beta, -1]$.

(d) **Nonequivalence.** *For all* $\beta \in I\!\!R^\sigma$, $\mathcal{E}^u \cap \mathcal{E}(g)_\beta = \emptyset$ *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 [Thm. 2.6.7(b)].

The next corollary gives an alternative version of part (a) of Theorem 2.6.2. It follows from the theorem in the same way that Corollary 2.5.3 follows from Theorem 2.5.2, which is the analogue of Theorem 2.6.2 for the canonical ensemble.

Corollary 2.6.3. *Let* g *be a continuous function mapping* $I\!\!R^\sigma$ *into* $I\!\!R$*, in terms of which the generalized canonical ensemble* (6.2) *is defined. For* $\beta \in I\!\!R^\sigma$ *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 function g, in terms of which the generalized canonical ensemble is defined, is assumed to be a continuous function mapping $I\!\!R^\sigma$ into $I\!\!R$. In addition, the interaction representation functions $\tilde{H}_i$ appearing in item 3 at the beginning of Section 2.5 are assumed to be bounded, continuous functions mapping the hidden space $\mathcal{X}$ into $I\!\!R$ and satisfying (5.1). The continuity of g and the boundedness and continuity of $\tilde{H}_i$ are required to derive the LDPs for Y_n with respect to $P_n^{u,r}$ [23, Thm. 3.2] and $P_{n,\beta,g}$ [Thm. 2.6.1]. In Section 2.9 we derive these two LDPs under weaker assumptions on $\tilde{H}_i$.

The relationships between the sets $\mathcal{E}^u$ and $\mathcal{E}(g)_\beta$ in the Theorem 2.6.2 are valid under much weaker assumptions on both g and $\tilde{H}_i$ that guarantee that these sets are nonempty. The set $\mathcal{E}^u$ is nonempty if $\tilde{H}_i$ is only continuous, while $\mathcal{E}(g)_\beta$ is nonempty if g and $\tilde{H}_i$ are bounded below and lower semicontinuous. In general, 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 2.5.2.

Having completed our analysis of ensemble equivalence at the level of equilibrium macrostates, we now relate this with ensemble equivalence at the thermodynamic level. The thermodynamic level of ensemble equivalence is formulated in terms of the generalized Legendre-Fenchel transform defined in (2.1) with the same function g used to define the generalized canonical ensemble. To see this, we start with the variational formula for $\varphi_g(\beta)$ given in part (a) of Theorem 2.6.1. 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 $u \in I\!R^\sigma$ and using the definition (5.6) of the microcanonical entropy s, we see that for all $\beta \in I\!R^\sigma$

$$\begin{aligned}
\varphi_g(\beta) &= \inf_{u \in I\!R^\sigma} \{\langle \beta, u\rangle + g(u) + \inf\{I(y) : y \in I\!R^\sigma, \tilde{H}(y) = u\}\} \\
&= \inf_{u \in I\!R^\sigma} \{\langle \beta, u\rangle + g(u) - s(u)\} \\
&= (s-g)^*(\beta) \;=\; s^\sharp(g, \beta).
\end{aligned}$$

This expresses $\varphi_g(\beta)$ as the generalized Legendre-Fenchel transform $s^\sharp(g,\beta)$ of s. Whether this transform can be inverted to express $s(u)$ as $\varphi_g^\sharp(g,u)$ is answered by Theorem 2.2.3. We record the facts in parts (a) and (b) of Theorem 2.6.4, which is the generalized canonical analogue of Theorem 2.5.4. In part (c) we apply Theorem 2.2.11 to conclude that if $s-g$ is strictly concave, then $\varphi_g = (s-g)^*$ is differentiable on $I\!R^\sigma$. The nondifferentiability of $\varphi_g(\beta)$ signals the presence of a discontinuous, first-order phase transition with respect to the generalized canonical ensemble. In Theorems 2.6.9–2.6.10 we point out several cases in which the conclusion of part (c) of Theorem 2.6.4 is valid.

Theorem 2.6.4. *Let g be a continuous function mapping $I\!R^\sigma$ into $I\!R$. In terms of g we define the generalized canonical ensemble* (6.2) *and the generalized Legendre-Fenchel transforms* (2.1) *and* (2.2)*. The following conclusions hold.*

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

(b) *For all $u \in I\!R^\sigma$, $s(u) = \varphi_g{}^\sharp(g, u)$ or equivalently $s(u) = s^{\sharp\sharp}(g, u)$ if and only if $s - g$ is concave on $I\!R^\sigma$.*

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

The properties of s expressed in part (b) of Theorem 2.6.4 motivate the following definition of the thermodynamic equivalence of the microcanonical and generalized canonical ensembles. This definition is the generalized canonical analogue of Definition 2.5.5. In Theorem 2.6.7 the thermodynamic equivalence of these ensembles will be related to the equivalence of the ensembles at the level of equilibrium macrostates.

Definition 2.6.5. *Let u be a point in* dom s *and g a continuous function mapping $I\!R^\sigma$ into $I\!R$, in terms of which the generalized canonical ensemble* (6.2) *is defined.*

(a) *The microcanonical and generalized canonical ensembles are said to be thermodynamically equivalent at u if $s(u) = s^{\sharp\sharp}(g, u)$.*

(b) *The ensembles are said to be thermodynamically nonequivalent at u if $s(u) \neq s^{\sharp\sharp}(g, u)$.*

In summary, the ensembles are thermodynamically equivalent at u if and only if $s - g$ is concave at u.

Part (b) of Theorem 2.6.4 gives a necessary and sufficient condition under which one can express $s(u)$, for all $u \in I\!R^\sigma$, in terms of $\varphi_g^\sharp(g, u)$ for a fixed function g. In the next theorem we explore a possibility that arises in a number of applications; namely, writing $s(u) = \varphi_g^\sharp(g, u)$ for all u in a given subset K of dom s, where the function g depends on u. This representation involves the generalized Legendre-Fenchel transform $s^{\sharp\flat}$ defined in (3.1). In Theorem 2.6.11 we point out a case for which the conclusion of Theorem 2.6.6 is valid; in this case $\mathcal{S}$ equals the set of nonnegative quadratic functions.

Theorem 2.6.6. *Let $\mathcal{S}$ be a set of continuous functions mapping $I\!\!R^\sigma$ into $I\!\!R$ and K a subset of* dom s*. For each $g \in \mathcal{S}$ we define the generalized canonical ensemble* (6.2)*. Then for each $u \in K$ we can write $s(u) = s^{\sharp\flat}(\mathcal{S}, u)$ provided that there exists $g \in \mathcal{S}$ such that $(s - g)^{**}(u) = s(u)$ or equivalently $s^{\sharp\sharp}(g, u) = s(u)$.*

Proof. This is an immediate consequence of part (b) of Lemma 2.3.1. ■

Theorem 2.6.6 suggests a generalized formulation of ensemble equivalence at the thermodynamic level. The microcanonical and generalized canonical ensembles are said to be thermodynamically equivalent at $u \in K$ relative to the set $\mathcal{S}$ if there exists $g \in \mathcal{S}$ such that $s(u) = s^{\sharp\sharp}(g, u)$. Otherwise, the ensembles are said to be thermodynamically nonequivalent at u relative to the set $\mathcal{S}$.

Theorem 2.6.2 expresses, in terms of support properties of $s - g$, the equivalence and nonequivalence of the microcanonical and generalized canonical ensembles at the macrostate level. In Theorem 2.6.7 we relate these results to ensemble equivalence and nonequivalence at the thermodynamic level [Defn. 2.6.5]. Because this theorem is proved exactly like Theorem 2.5.7, which is its analogue in Section 5, the proof is omitted. Part (d) of Theorem 2.6.7 shows that if $s - g$ is strictly concave on dom s, then $s - g$ has a strictly supporting hyperplane at all points in dom s except possibly at relative boundary points. In combination with part (b) of Theorem 2.6.2, this gives a criterion for the two ensembles to be universally equivalent. This criterion is applied in Theorems

2.6.8–2.6.10.

Let g be a continuous function mapping $I\!\!R^\sigma$ into $I\!\!R$, in terms of which we define the generalized canonical ensemble in (6.2). In the next proposition $C(g)$ denotes the set consisting of all $u \in I\!\!R^\sigma$ such that $s - g$ has a supporting hyperplane at u. That is,

$$C(g) = \{u \in I\!\!R^\sigma : \exists \beta \in I\!\!R^\sigma \ni (s-g)(v) \leq (s-g)(u) + \langle \beta, v - u \rangle \ \forall v \in I\!\!R^\sigma\}. \quad (6.7)$$

We also define

$$\Gamma(g) = \{u \in I\!\!R^\sigma : s(u) = s^{\sharp\sharp}(g, u)\}. \quad (6.8)$$

Thus $u \in \Gamma(g) \cap \operatorname{dom} s$ if and only if the ensembles are thermodynamically equivalent at u.

Since g is finite on $I\!\!R^\sigma$, in general $\operatorname{dom}(s - g) = \operatorname{dom} s$. If, as in Theorem 2.5.6, $\operatorname{dom} s$ is an open subset of $I\!\!R^\sigma$, then the statement of the following theorem would be somewhat simplified.

Theorem 2.6.7. *Let g be a continuous function mapping $I\!\!R^\sigma$ into $I\!\!R$, in terms of which the generalized canonical ensemble in* (6.2) *is defined. The following conclusions hold.*

(a) $C(g) = \Gamma(g) \cap \operatorname{dom} \partial(s - g)^{**}$. *In particular, if $s - g$ is concave on $I\!\!R^\sigma$, then $C(g) = \operatorname{dom} \partial(s - g)$, and so $s - g$ has a supporting hyperplane at all points of* $\operatorname{dom}(s - g) = \operatorname{dom} s$ *except possibly relative boundary points.*

(b) $\Gamma(g) \cap \operatorname{ri}(\operatorname{dom} s) \subset C(g) \subset \Gamma(g) \cap \operatorname{dom} s$.

(c) *If the microcanonical and generalized canonical ensembles are thermodynamically equivalent at $u \in \operatorname{ri}(\operatorname{dom} s)$, then the ensembles are either fully or partially equivalent at u. Conversely, if the ensembles are either fully or partially equivalent at $u \in \operatorname{dom} s$, then the ensembles are thermodynamically equivalent at u.*

(d) *Assume that* $\operatorname{dom} s$ *is convex and $s - g$ is strictly concave on* $\operatorname{ri}(\operatorname{dom} s)$ *and continuous on* $\operatorname{dom} s$. *Then $s - g$ has a strictly supporting hyperplane at all $u \in \operatorname{dom} s$*

except possibly relative boundary points, and the ensembles are universally equivalent; i.e., fully equivalent at all $u \in$ dom s except possibly relative boundary points.

When the dimension $\sigma = 1$, Theorem 2.6.8 gives a useful and applicable criterion guaranteeing the existence of a quadratic function g such that $s - g$ is strictly concave on dom s. The criterion — 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 $s - g$. Suppose, for example, that dom s is a closed, bounded interval. If, as in the case of the Curie-Weiss-Potts model [12], $s''(u) \to \infty$ as u approaches a boundary point, then for any quadratic function g, $s - g$ is not strictly concave on the interior of dom s. The situation in which $s''(u) \to \infty$ as u approaches a boundary point can often be handled by Theorem 2.6.11, which is a local version of Theorems 2.6.8 and 2.6.9.

The strict concavity of $s - g$ on 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., $s^{\sharp\sharp}(g, u) = s(u)$. As we note in part (e) of Theorem 2.6.8, the strict concavity of $s - g$ also implies that the generalized canonical free energy $\varphi_g = (s - g)^*$ is differentiable on $I\!R$, a condition guaranteeing the absence of a discontinuous, first-order phase transition with respect to the Gaussian ensemble.

Theorem 2.6.8. *Assume that the dimension $\sigma = 1$ and that dom s is a nonempty interval. Assume also that s is continuous on* dom s*, s is twice continuously differentiable on* int(dom s)*, and s'' is bounded above on* int(dom s)*. Then for all sufficiently large $\gamma \geq 0$ and $g(u) = \gamma u^2$, conclusions* (a)–(e) *hold. Specifically, if s is strictly concave on* dom s*, then we choose any $\gamma \geq 0$, and otherwise we choose*

$$\gamma > \gamma_0 = \tfrac{1}{2} \cdot \sup_{u \in \text{int(dom } s)} s''(u). \tag{6.9}$$

(a) $s - g$ *is strictly concave and continuous on* dom s.

(b) $s - g$ *has a strictly supporting line, and* s *has a strictly supporting paraboloid, at each point in* 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 ensemble and the Gaussian ensemble defined in terms of this* g *are universally equivalent; i.e., fully equivalent at all* $u \in$ dom s *except possibly boundary points.*

(d) $s^{\sharp\sharp}(g, u) = s(u)$ *for all* $u \in I\!R$.

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

Proof. The properties listed in parts (a)–(b) and (d)–(e) are immediate consequences of Theorem 2.2.12, Proposition 2.2.18, and the fact that s is upper semicontinuous on $I\!R^\sigma$ [Thm. 2.5.4(d)]. The property listed in part (c) follows from part (a) of the present theorem and part (d) of Theorem 2.6.7. ∎

We now consider the analogue of Theorem 2.6.8 for arbitrary dimension $\sigma \geq 2$. In contrast to the case $\sigma = 1$, in which $s - g$ could always be extended to a strictly concave function on all of dom s, in this case there exists a quadratic g such that $s - g$ is strictly concave on the interior of dom s, but in general $s - g$ cannot be extended to a strictly concave function on all of dom s. As a result, unless dom s is open, we cannot apply Theorem 2.2.11 to conclude that the generalized canonical free energy $\varphi_g = (s - g)^*$ is differentiable on $I\!R^\sigma$.

Theorem 2.6.9. *Assume that the dimension* $\sigma \geq 2$ *and that* dom s *is convex and has nonempty interior. Assume also that* s *is continuous on* dom s, s *is twice continuously* *differentiable on* int(dom s), *and all second-order partial derivatives of* s *are bounded above on* int(dom s). *Then for all sufficiently large* $\gamma \geq 0$ *and* $g(u) = \gamma\|u\|^2$, *conclusions* (a)–(e) *hold. Specifically, if* s *is strictly concave on* int(dom s), *then we choose any* $\gamma \geq 0$, *and otherwise we choose*

$$\gamma > \gamma_0 = \tfrac{1}{2} \cdot \sup_{u \in \mathrm{int(dom}\, s)} \kappa(u), \tag{6.10}$$

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

(a) $s - g$ *is strictly concave on* int(dom s) *and concave and continuous on dom* s.

(b) $s-g$ *has a strictly supporting hyperplane, and* s *has a strictly supporting paraboloid, at each point in* dom s *except possibly boundary points.*

(c) *The microcanonical ensemble and the Gaussian ensemble defined in terms of this* g *are universally equivalent; i.e., fully equivalent at all* $u \in$ dom s *except possibly boundary points.*

(d) $s^{\sharp\sharp}(g, u) = s(u)$ *for all* $u \in I\!\!R^\sigma$.

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

Proof. The properties listed in parts (a)–(b) and (d)–(e) are immediate consequences of Theorem 2.2.14, Proposition 2.2.18, and the fact that s is upper semicontinuous on $I\!\!R^\sigma$ [Thm. 2.5.4(d)]. The property listed in part (c) follows from part (a) of the present theorem and part (d) of Theorem 2.6.7. ■

In the next theorem we give other conditions on s guaranteeing conclusions similar to those in Theorems 2.6.8 and 2.6.9.

Theorem 2.6.10. *Assume that* dom s *is convex and closed and* s *is bounded and continuous on* dom s. *Then there exists a continuous function* g *mapping* $I\!\!R^\sigma$ *into* $I\!\!R$ *such that the following conclusions hold.*

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

(b) $s - g$ *has a strictly supporting hyperplane at each point in* dom s *except possibly relative boundary points.*

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

(d) $s^{\sharp\sharp}(g, u) = s(u)$ *for all* $u \in I\!R^\sigma$.

Proof. The properties listed in parts (a), (b), and (d) are immediate consequences of Theorem 2.2.16. The property listed in part (c) follows from part (a) of the present theorem and part (d) of Theorem 2.6.7. ■

Suppose that s is C^2 on the interior of 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 dom s is a closed, bounded interval of $I\!R$ and $s''(u) \to \infty$ as u approaches the right hand endpoint of dom s [12]. It also arises in the example of the double parabola treated Section 2.4. In such cases one cannot expect that the conclusions of Theorem 2.6.9 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 dom s and thus that the ensembles are universally equivalent.

Theorem 2.6.11, a local version of Theorems 2.6.9 and 2.6.8, 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 $K =$ int(dom s) and the second-order partial derivatives of s are all not bounded above on K. In Theorem 2.6.11 additional conditions are given guaranteeing that for each $u \in K$ there exists a quadratic g depending on u such that $s - g$ has a strictly supporting hyperplane at u. This, in turn, implies a form of universal equivalence of ensembles that is weaker than that in Theorems 2.6.9 and 2.6.8 but is still useful. In contrast to Theorem 2.6.9, which states that $s^{\sharp\sharp}(g, u) = s(u)$ for all u, in Theorem 2.6.11 we prove the alternative representation $s^{\sharp\flat}(\mathcal{S}, u) = s(u)$ for all u in K, where $\mathcal{S}$ is the set of quadratic functions $\gamma\|\cdot\|^2$ for $\gamma \geq 0$. This alternative representation is necessitated by the fact that the quadratic g depends on u.

In this theorem we restrict ourselves to finding a quadratic $g = \gamma\|\cdot\|^2$ depending on u such that $s - g$ has a strictly supporting hyperplane at u. 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 $s - g$ has a strictly supporting hyperplane cannot decrease. Because of part (a) of Theorem 2.6.2, this can be restated in terms of ensemble equivalence. Let $\mathcal{E}(\gamma)_\beta$ be the set defined in (1.13). Defining

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

we have $U_{\gamma_1} \subset U_{\gamma_2}$ whenever $\gamma_2 > \gamma_1$ and $\cup_{\gamma > 0} U_\gamma = K$. This phenomenon is investigated in detail in [13] for the Curie-Weiss-Potts model.

For $u \in K$ and $\lambda \geq 0$, the set $D(u, \nabla s(u), \lambda)$ appearing in the statement of Theorem 2.6.11 is defined by

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

Parts (a), (b), and (c) of Theorem 2.6.11 are direct consequences of Theorem 2.3.2. Part (d) of Theorem 2.6.11 follows from part (b) of Theorem 2.6.2. The hypothesis in Theorem 2.3.2 that s is bounded above on $I\!R^\sigma$ is automatic since s is nonpositive on $I\!R^\sigma$.

Theorem 2.6.11. *Let* K *an open subset of* dom s *and assume that* s *is twice continuously differentiable on* K. *Assume also that* dom s *is bounded or, more generally, that for* *every* $u \in \operatorname{int} K$ *there exists* $\lambda \geq 0$ *such that* $D(u, \nabla s(u), \lambda)$ *is bounded. The following conclusions hold.*

(a) *For each* $u \in K$*, define* $\gamma_0(u) \geq 0$ *like* $\gamma_0(x)$ *in* (3.8)*, replacing* $f(x)$ *and* $\nabla f(x)$ *by* $s(u)$ *and* $\nabla s(u)$*. 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* $g = \gamma \| \cdot \|^2$*. Then* $s - g$ *has a strictly supporting hyperplane at* u *with normal vector* $[\nabla s(u) - 2\gamma u, -1]$*.*

(c) *Let* $\mathcal{S}$ *be the set of quadratic functions* $g_\gamma = \gamma \| \cdot \|^2$ *for* $\gamma \geq 0$*. Then for each* $u \in K$ *and any* $\gamma > \gamma_0(u)$

$$s^{\sharp\flat}(\mathcal{S}, u) = s^{\sharp\sharp}(g_\gamma, u) = s(u).$$

(d) *For each* $u \in K$ *choose* $g = \gamma \| \cdot \|^2$ *such that, in accordance with part* (a)*,* $s - g$ *has a strictly supporting hyperplane at* u*. Then the microcanonical ensemble and the Gaussian ensemble defined in terms of this* g *are fully equivalent at* u*.*

This theorem suggests an extended form of the notion of universal equivalence of ensembles. In Theorems 2.6.8–2.6.10 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 ensemble and the generalized canonical ensemble defined in terms of this g are universally equivalent. In Theorem 2.6.11 we can also achieve full equivalence of ensembles for all $u \in K$. However, in contrast to Theorem 2.6.9, 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 2.6.11 by saying that the microcanonical ensemble and the Gaussian ensembles are **universally equivalent on *K* relative to the set of nonnegative quadratic functions**.

Away from phase transitions, the smoothness hypothesis on s in Theorem 2.6.11 is generic for typical models in statistical mechanics. By definition, a point u_c at which s is not differentiable represents a first-order microcanonical phase transition [27, Fig. 3]. A point u_c at which s is differentiable but not twice differentiable represents a second-order microcanonical phase transition [27, Fig. 4]. If follow that s is smooth on any open set K not containing such phase transitions in its closure. Hence, if the other conditions in Theorem 2.6.11 are valid, then the microcanonical and Gaussian ensembles are universally equivalent on K relative to the set of quadratic functions. If, in fact, there are no phase transitions in the microcanonical ensemble, then s is smooth on all of int(dom s). This implies the universal equivalence of the two ensembles provided that the other conditions in Theorems 2.6.8 and 2.6.9 are valid.

This completes our discussion of the generalized canonical ensemble and its equivalence with the microcanonical ensemble. In the next section we give an elementary proof of Theorem 2.6.2, the main result stated in the present section.

2.7 Proof of Theorem 2.6.2 from Theorem 2.5.2

Theorem 2.6.2 states equivalence and nonequivalence results at the level of equilibrium macrostates for the microcanonical and generalized canonical ensembles. In this section we give an elementary proof of Theorem 2.6.2, deriving it from Theorem 2.5.2, its analogue for the standard canonical ensemble. In Section 2.9, Theorem 2.6.2 is proved directly from first principles without the use of Theorem 2.5.2.

The goal of the elementary proof of Theorem 2.6.2 is to elucidate why the relationships between the sets of microcanonical and generalized canonical equilibrium macrostates as expressed in this theorem are given so simply in terms of support properties of $s - g$. We carry this out via the following observations.

- In (6.2) the generalized canonical ensemble is introduced as a perturbation of the canonical ensemble defined in terms of the prior measures P_n by adding the extra exponential factor $\exp[-a_n g(h_n)]$.

- Think of the generalized canonical ensemble in a different light: not as a perturbation of the standard canonical ensemble, but as a standard canonical ensemble corresponding to a perturbation of the prior measures P_n. This perturbation, defined in (7.1) in terms of the function g, is denoted by $P_{n,g}$.

- The perturbations $P_{n,g}$ of P_n have the property that the microcanonical ensemble defined in terms of P_n and the microcanonical ensemble defined in terms of $P_{n,g}$ are asymptotically equal, in the large deviation sense, as $n \to \infty$ and $r \to 0$. This is shown in (7.2) and (7.3).

- A straightforward calculation shows that the microcanonical entropy s_g associated with the perturbed prior measures $P_{n,g}$ equals $s - g -$ const [Thm. 2.7.1]. As Theorem 2.5.2 then indicates, the relationships between the sets of microcanonical and generalized canonical equilibrium macrostates is simply expressed in terms of support properties of $s_g = s - g -$ const, or equivalently in terms of support properties of $s - g$. Theorem 2.6.2 is thus proved.

We now present the details. Let g be a continuous function mapping $I\!R^\sigma$ into $I\!R$. Let $(\Omega_n, \mathcal{F}_n, P_n)$ be a sequence of probability spaces in terms of which the statistical mechanical models are defined. For any set $B \in \mathcal{F}_n$ we define measures on $\mathcal{F}_n$ by

$$P_{n,g}\{B\} = \int_B \exp[-a_n g(h_n)]\, dP_n \cdot \frac{1}{\int_{\Omega_n} \exp[-a_n g(h_n)]\, P_n}. \tag{7.1}$$

For $\beta \in I\!R^\sigma$ it is clear that the generalized canonical ensemble $P_{n,\beta,g}$ introduced in (6.2) equals the standard canonical ensemble defined in terms of the new prior measures $P_{n,g}$; i.e., for any $B \in \mathcal{F}_n$

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

It follows that the set of equilibrium macrostates with respect to the canonical ensemble defined in terms of the new prior measures $P_{n,g}$ coincides with the set $\mathcal{E}(g)_\beta$ introduced in (6.6).

The microcanonical ensemble is defined by conditioning the prior measures on the set $\{h_n \in \{u\}^{(r)}\}$, where $\{u\}^{(r)} = [u_1 - r, u_1 + r] \times \cdots \times [u_\sigma - r, u_\sigma + r]$. We label these conditioned measures $P_n^{u,r}$ and $P_{n,g}^{u,r}$ depending on whether the prior measures are P_n or $P_{n,g}$, respectively. For any set $B \in \mathcal{F}_n$, $P_n^{u,r}$ is defined in by

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

while

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

Since $P_{n,g}$ differs from P_n only through the exponential factor $\exp[-a_n g(h_n)]$, conditioning $P_{n,g}$ on $\{h_n \in \{u\}^{(r)}\}$ reduces essentially to conditioning P_n on $\{h_n \in \{u\}^{(r)}\}$. In fact, because g is continuous, the two conditioned measures become asymptotically equal, in the large deviation sense, as $n \to \infty$ and $r \to 0$.

In order to prove this, we fix $u \in \text{dom}\, s$ and define

$$\begin{aligned} b(r) = \sup\{g(x) : x \in I\!R^\sigma, \|x - u\| \leq r\} \\ - \inf\{g(x) : x \in I\!R^\sigma, \|x - u\| \leq r\}. \end{aligned}$$

Since g is continuous, $b(r) \to 0$ as $r \to 0$. We consider any sequence of sets B_n in $\mathcal{F}_n$; in particular, $B_n = \{Y_n \in A\}$ for A an open or closed subset of $\mathcal{X}$. The easy estimate

$$\exp[-a_n b(r)]\, P_n^{u,r}\{B_n\} \leq P_{n,g}^{u,r}\{B_n\} \leq \exp[a_n b(r)]\, P_n^{u,r}\{B_n\}$$

implies that

$$\lim_{r\to 0}\liminf_{n\to\infty}\frac{1}{a_n}\log P^{u,r}_{n,g}\{B_n\} = \lim_{r\to 0}\liminf_{n\to\infty}\frac{1}{a_n}\log P^{u,r}_{n}\{B_n\} \tag{7.2}$$

and

$$\lim_{r\to 0}\limsup_{n\to\infty}\frac{1}{a_n}\log P^{u,r}_{n,g}\{B_n\} = \lim_{r\to 0}\limsup_{n\to\infty}\frac{1}{a_n}\log P^{u,r}_{n}\{B_n\}. \tag{7.3}$$

It follows that with respect to $P^{u,r}_{n,g}$, Y_n satisfies the LDP with the same rate function as in the LDP for Y_n with respect to $P^{u,r}_n$. As a result, the set of equilibrium macrostates with respect to $P^{u,r}_{n,g}$ coincides with the set $\mathcal{E}^u$ of microcanonical equilibrium macrostates introduced in (5.9).

In order to complete the proof of Theorem 2.6.2, we must identify the microcanonical entropy associated with the new prior measures $P_{n,g}$. The formula for this quantity is given in the next theorem.

Theorem 2.7.1. *Let g be a continuous function mapping $I\!R^\sigma$ into $I\!R$. Then for $u \in \text{dom}\, s$ the microcanonical entropy s_g corresponding to the measures $P_{n,g}$ defined in* (7.1) *is given by*

$$s_g(u) = s(u) - g(u) - \sup_{v\in\text{dom}\, s}\{s(v) - g(v)\}. \tag{7.4}$$

Proof. By Theorem 2.6.1, with respect to $P_{n,g}$, Y_n satisfies the LDP with rate function

$$I_g(x) = I(x) + g(\tilde{H}(x)) - \inf_{y\in\mathcal{X}}\{I(y) + g(\tilde{H}(y))\}.$$

The formula for s_g is obtained by adapting (5.6) to the current situation, replacing the original rate function I by I_g. It follows that

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

Clearly $s_g(u) > \infty$ if and only if $s(u) > \infty$, and so the domains of the two functions coincide. In order to obtain (7.4), we write

$$
\begin{aligned}
&\inf_{y \in \mathcal{X}} \{I(y) + g(\tilde{H}(y))\} \\
&\quad = - \sup_{v \in \text{dom}\, s} \Big(-\{I(y) + g(\tilde{H}(y)) : y \in \mathcal{X}, \tilde{H}(y) = v\} \Big) \\
&\quad = - \sup_{v \in \text{dom}\, s} \{s(v) - g(v)\}.
\end{aligned}
$$

This completes the proof. ■

We now see that Theorem 2.6.2 is an immediate consequence of Theorem 2.5.2. Indeed, the discussion leading up to Theorem 2.7.1 shows that the relationship between the sets $\mathcal{E}^u$ and $\mathcal{E}(g)_\beta$ of equilibrium macrostates is described by support properties of s_g, as detailed in Theorem 2.5.2. However, s_g and $s - g$ have the identical support properties; i.e., the first function has a supporting hyperplane at some u or a strictly supporting hyperplane at some u or no supporting hyperplane at some u if and only the second function has the same property. Replacing s in Theorem 2.5.2 by $s - g$ gives Theorem 2.6.2. This completes the proof of the latter theorem.

2.8 LDPs for the Three Ensembles Under Weaker Conditions

In this section we prove LDPs for Y_n with respect to the microcanonical ensemble, the standard canonical ensemble, and the generalized canonical ensemble under weaker conditions than those in [23] and in this chapter. These extensions are important because the LDPs are used to define the corresponding sets of equilibrium macrostates in terms of the 0-sets of the rate functions. These sets are $\mathcal{E}^u$, defined in (5.9); $\mathcal{E}_\beta$, defined in (5.5); and $\mathcal{E}(g)_\beta$, defined in (6.6). A consequence of proving the three LDPs under weaker conditions is to generalize Theorems 2.5.2 and 2.6.2 to this broader setting. Theorem

2.5.2 gives relationships between $\mathcal{E}^u$ and $\mathcal{E}_\beta$ while Theorem 2.6.2 does the same for $\mathcal{E}^u$ and $\mathcal{E}(g)_\beta$.

Except for changes in notation, the assumptions in [23] on the statistical mechanical models coincide with those given near the start of Section 2.5 of the present chapter. Among other matters, in this section we seek to weaken the assumptions on the interaction representation functions $\tilde{H}_i$ given in item 3 in paragraph 3 of that section. There we assume that $\{\tilde{H}_i, i = 1, \ldots, \sigma\}$ is a sequence of bounded, continuous function mapping $\mathcal{X}$ into $I\!R$ such that as $n \to \infty$

$$h_{n,i}(\omega) = \tilde{H}_i(\omega) + \mathrm{o}(1) \quad \text{uniformly for } \omega \in \Omega_n. \tag{8.1}$$

As we will see, the assumption that $\tilde{H}_i$ is bounded can be considerably weakened.

We start with the LDP with respect to the microcanonical ensemble $P_n^{u,r}$ defined in (5.7). In this case Y_n satisfies the LDP on $\mathcal{X}$, in the double limit $n \to \infty$ and $r \to 0$, with rate function I^u defined in (5.8) [23, Thm. 3.2]. An examination of the proof reveals that the boundedness of $\tilde{H}_i$ is not needed at all. All that is required is that each $\tilde{H}_i$ is continuous and that (8.1) holds. As we prove in the next proposition, under these hypotheses $\tilde{H}(Y_n) = (\tilde{H}_1(Y_n), \ldots, \tilde{H}_\sigma(Y_n))$ and h_n satisfy the LDP with respect to the prior measures P_n with rate function $-s$. With this LDP in hand, the proof of the LDP for Y_n with respect to $P_n^{u,r}$ given in Theorem 3.2 in [23] goes over without change.

Proposition 2.8.1. *We assume the conditions on the statistical mechanical models given near the start of Section* 2.5*, except that in item* 3 *we drop the assumption that each* $\tilde{H}_i$ *is bounded on* $\mathcal{X}$*. Then with respect to the prior measures* P_n*,* $\tilde{H}(Y_n)$ *and* h_n *satisfy the LDP on* $I\!R^\sigma$ *with rate function* $-s$*.*

Proof. By assumption, with respect to P_n, Y_n satisfies the LDP on $\mathcal{X}$ with rate function I. Since $\tilde{H}$ is a continuous function mapping $\mathcal{X}$ into $I\!R^\sigma$, the contraction principle [17, Thm. 4.2.1] implies that with respect to P_n, $\tilde{H}(Y_n)$ satisfies the LDP on $I\!\!R^\sigma$ with rate function

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

This function coincides with $-s(u)$. When expressed in terms of the equivalent Laplace principle, this means that for any bounded, continuous function f mapping $I\!\!R^\sigma$ into $I\!\!R$

$$\lim_{n\to\infty} \frac{1}{a_n} \log \int_{\Omega_n} \exp[a_n f(\tilde{H}(Y_n))]\, dP_n = \sup_{u \in I\!\!R^\sigma} \{f(\tilde{H}(u)) + s(u)\}.$$

Because of the uniform estimate (8.1) relating each $h_{n,i}$ and $\tilde{H}_i(Y_n)$, the Laplace principle for $\tilde{H}(Y_n)$ readily extends to the Laplace principle for h_n with rate function $-s$. Since the Laplace principle and the LDP are equivalent, the last display implies that with respect to P_n, h_n satisfies the LDP on $I\!\!R^\sigma$ with rate function $-s$. This completes the proof. ■

We next turn to the standard canonical ensemble $P_{n,\beta}$ defined in (5.2). In this case Y_n satisfies the LDP on $\mathcal{X}$ with rate function I_β defined in (5.4). As in the case of the microcanonical ensemble, the assumptions on $\tilde{H}_i$ can also be weakened. Besides the continuity of each $\tilde{H}_i$ and the approximation property (8.1), a minimal condition on $\tilde{H}_i$ is that these functions are bounded below on $\mathcal{X}$, or more generally, that they are bounded below on the union of the supports of Y_n. Because of (8.1), this boundedness condition implies that the interaction functions $h_{n,i}$ are also bounded below, thus guaranteeing that the canonical ensemble is well-defined.

We claim that if the $\tilde{H}_i$ are continuous and bounded below on the union of the supports of Y_n, then with respect to $P_{n,\beta}$, Y_n satisfies the LDP on $\mathcal{X}$ with the same rate function I_β. In order to see this, we follow the pattern of proof of Theorem 2.6.1, which shows that the LDP for Y_n with respect to $P_{n,\beta}$ holds if for any bounded, continuous function f mapping $\mathcal{X}$ into $I\!R$

$$\lim_{n\to\infty}\frac{1}{a_n}\log\int_{\Omega_n}\exp[a_n f(Y_n) - a_n\langle\beta, h_n\rangle]\,dP_n \tag{8.2}$$
$$= \sup_{y\in\mathcal{X}}\{f(y) - \langle\beta, \tilde{H}(y)\rangle - I(y)\}.$$

Since (8.1) implies that

$$\lim_{n\to\infty}\left|\frac{1}{a_n}\log\int_{\Omega_n}\exp[a_n f(Y_n) - a_n\langle\beta, h_n\rangle]\,dP_n - \frac{1}{a_n}\log\int_{\Omega_n}\exp[a_n f(Y_n) - a_n\langle\beta, \tilde{H}(Y_n)\rangle]dP_n\right| = 0,$$

it suffices to prove (8.2) with h_n replaced by $\tilde{H}(Y_n)$. The desired limit is a consequence of Theorem 1.3.4 in [19]. This completes the proof.

In the next theorem we record these LDPs with respect to the microcanonical and standard canonical ensembles.

Theorem 2.8.2.

(a) *We assume the conditions on the statistical mechanical models given near the start of Section* 2.5, *except that in item* 3 *we drop the assumption that each* $\tilde{H}_i$ *is bounded on* $\mathcal{X}$. *Then 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*

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

(b) *We assume the conditions on the statistical mechanical models given near the start of Section* 2.5, *except that in item* 3 *we replace the assumption that each* $\tilde{H}_i$ *is bounded on* $\mathcal{X}$ *with the assumption that each* $\tilde{H}_i$ *is bounded below on the union of the supports of* Y_n. *Then with respect to the canonical ensemble* $P_{n,\beta}$, Y_n *satisfies the LDP on* $\mathcal{X}$ *with rate function*

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

We finally turn to the generalized canonical ensemble $P_{n,\beta,g}$, defined in (6.2) in terms of a continuous function g mapping $I\!\!R^\sigma$ into $I\!\!R$. In this case the LDP for Y_n is shown to hold in Theorem 2.6.1; the rate function $I_{\beta,g}$ is defined in (6.4). The main result in this section is to prove this LDP under weaker conditions on $\tilde{H}_i$ and g. The first case is where $\tilde{H}_i$ is no longer bounded on $\mathcal{X}$ but is bounded below on the union of the supports of the Y_n. Then a minimal condition on g guaranteeing that the generalized canonical ensemble is well defined is that g is bounded below on the union of the ranges of $\tilde{H}(Y_n)$. The second case is where no boundedness condition on $\tilde{H}_i$ is assumed at all. Then a minimal condition on g guaranteeing that the generalized canonical ensemble is well defined is that g is superlinear; i.e.,

$$\lim_{\|x\|\to\infty} \frac{g(x)}{\|x\|} = \infty.$$

These two sets of assumptions are given in parts (a) and (b) of the next theorem. We prove the LDP under the assumptions in part (b). The proof can easily be adapted to handle the assumptions in part (a).

Theorem 2.8.3. *Let g be a continuous function mapping $I\!\!R^\sigma$ into $I\!\!R$, in terms of which the generalized canonical ensemble $P_{n,\beta,g}$ is defined. We assume the conditions on the statistical mechanical models given near the start of Section* 2.5, *except for either of the following changes.*

(a) *In item* 3 *we replace the assumption that each $\tilde{H}_i$ is bounded on $\mathcal{X}$ with the assumption that each $\tilde{H}_i$ is bounded below on the union of the supports of Y_n. We also add the assumption that g is bounded below on the union of the supports of $\tilde{H}(Y_n)$.*

(b) *In item* 3 *we drop the assumption that each $\tilde{H}_i$ is bounded on $\mathcal{X}$ and add the assumption that g is superlinear.*

Under the assumptions either in part (a) *or in part* (b), *with respect to $P_{n,\beta,g}$, Y_n*

satisfies the LDP *on* $\mathcal{X}$ *with rate function*

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

Proof under the assumptions in part (b). Let f be an arbitrary bounded, continuous function mapping $\mathcal{X}$ into $I\!R$. For any set $B \in \mathcal{F}_n$ we define

$$F_n(B) = \int_B \exp[a_n f(Y_n) - a_n \langle \beta, h_n \rangle - a_n g(h_n)]\, dP_n$$

and

$$D_n(B) = \int_B \exp[a_n f(Y_n) - a_n \langle \beta, \tilde{H}(Y_n) \rangle - a_n g(\tilde{H}(Y_n)]\, dP_n.$$

For simplicity, we will denote $F_n(\Omega_n)$ by F_n and $D_n(\Omega_n)$ by D_n. As in the case of Theorem 2.6.1, we can prove the present theorem by showing that

$$\lim_{n\to\infty} \frac{1}{a_n} \log F_n = \sup_{y \in \mathcal{X}} \{ f(y) - \langle \beta, \tilde{H}(y) \rangle - g(\tilde{H}(y)) - I(y) \}. \tag{8.3}$$

By hypothesis on $\tilde{H}$ and g, the function $\langle \beta, \tilde{H} \rangle + g \circ \tilde{H}$ is continuous and bounded below on $\mathcal{X}$. Since Y_n satisfies the LDP on $\mathcal{X}$, and hence the Laplace principle on $\mathcal{X}$, with rate function I, Theorem 1.3.4 in [19] implies that

$$\lim_{n\to\infty} \frac{1}{a_n} \log D_n = \sup_{y \in \mathcal{X}} \{ f(y) - \langle \beta, \tilde{H}(y) \rangle - g(\tilde{H}(y)) - I(y) \}.$$

Hence, in order to complete the proof, we must show that

$$\lim_{n\to\infty} \left| \frac{1}{a_n} \log F_n - \frac{1}{a_n} \log D_n \right| = 0. \tag{8.4}$$

According to Proposition 2.8.1, the sequences h_n and $\tilde{H}(Y_n)$ satisfy the LDP on $I\!R^\sigma$, and hence the Laplace principle on $I\!R^\sigma$, with rate function $-s$. Since the function on $I\!R^\sigma$ mapping $y \mapsto \langle \beta, y \rangle + g(y)$ is continuous and bounded below, Theorem 1.3.4 in [19] gives the limits

$$\begin{aligned} \lim_{n\to\infty} \frac{1}{a_n} \log \int_{\Omega_n} \exp[-a_n \langle \beta, h_n \rangle - a_n g(h_n)]\, dP_n \\ = \sup_{u \in I\!R^\sigma} \{ -\langle \beta, u \rangle - g(u) + s(u) \} \end{aligned} \tag{8.5}$$

and

$$\lim_{n\to\infty} \frac{1}{a_n} \log \int_{\Omega_n} \exp[-a_n\langle\beta, \tilde{H}(Y_n)\rangle - a_n g(\tilde{H}(Y_n)]\, dP_n \qquad (8.6)$$
$$= \sup_{u\in I\!R^\sigma} \{-\langle\beta, u\rangle - g(u) + s(u)\}.$$

We now choose $\alpha > 0$ sufficiently large to satisfy

$$\sup_{u\in I\!R^\sigma} \{-\langle\beta, u\rangle - g(u) + s(u)\} > -\alpha + \|f\|_\infty.$$

Combining this inequality with (8.5) and (8.6), we see that for all sufficiently large n

$$F_n \geq \exp[-a_n\|f\|_\infty]\ \exp[-a_n\alpha + a_n\|f\|_\infty] = \exp[-a_n\alpha] \qquad (8.7)$$

and

$$D_n \geq \exp[-a_n\|f\|_\infty]\ \exp[-a_n\alpha + a_n\|f\|_\infty] = \exp[-a_n\alpha]. \qquad (8.8)$$

We compare these bounds with bounds on the quantities $F_n(\{\|h_n\| > M\})$ and $D_n(\{\|\tilde{H}(Y_n)\| > M-1\})$ for a suitable choice of M. Since g is superlinear, there exists $M < \infty$ such that

$$\text{if } \|u\| > M-1, \text{ then } \langle\beta, u\rangle + g(u) \geq 2\alpha + \|f\|_\infty.$$

Thus if $\|u\| > M-1$, then for any $x \in \mathcal{X}$

$$-f(x) + \langle\beta, u\rangle + g(u) \geq -\|f\|_\infty + 2\alpha + \|f\|_\infty = 2\alpha.$$

It follows that for all $n \in I\!N$ that

$$0 \leq F_n(\{\|h_n\| > M\}) \leq F_n(\{\|h_n\| > M-1\}) \leq e^{-2a_n\alpha} \qquad (8.9)$$

and

$$0 \leq D_n(\{\|\tilde{H}(Y_n)\| > M-1\}) \leq e^{-2a_n\alpha}. \qquad (8.10)$$

We need the following simple lemma.

Lemma 2.8.4. *Let α be a positive number and b_n and c_n positive sequences such that for all sufficiently large n*

$$b_n + c_n \geq e^{-a_n \alpha} \textit{ and } 0 \leq b_n \leq e^{-2a_n \alpha}.$$

Then

$$\lim_{n\to\infty} \left| \frac{1}{a_n} \log(b_n + c_n) - \frac{1}{a_n} \log(c_n) \right| = 0.$$

Proof. For all sufficiently large n

$$c_n = b_n + c_n - b_n \geq e^{-a_n \alpha} - e^{-2a_n \alpha} \geq \frac{1}{2} e^{-a_n \alpha}.$$

Therefore, for all sufficiently large n we have $0 \leq b_n/c_n \leq 2e^{-a_n \alpha}$. Hence b_n/c_n converges to 0 as $n \to \infty$. It follows that

$$\lim_{n\to\infty} \left| \frac{1}{a_n} \log(b_n + c_n) - \frac{1}{a_n} \log(c_n) \right| = \lim_{n\to\infty} \left| \frac{1}{a_n} \log(1 + \frac{b_n}{c_n}) \right| = 0.$$

This completes the proof. ■

We apply the lemma to

$$F_n = F_n(\{\|h_n\| \leq M\}) + F_n(\{\|h_n\| > M\})$$

and to

$$D_n = D_n(\{\|\tilde{H}(Y_n)\| \leq M - 1\}) + D_n(\{\|\tilde{H}(Y_n)\| > M - 1\}).$$

Using (8.7)–(8.10), we obtain

$$\lim_{n\to\infty} \left| \frac{1}{a_n} \log(F_n) - \frac{1}{a_n} \log(F_n(\{\|h_n\| \leq M\}) \right| = 0 \tag{8.11}$$

and

$$\lim_{n\to\infty} \left| \frac{1}{a_n} \log(D_n) - \frac{1}{a_n} \log(D_n(\{\|\tilde{H}(Y_n)\| \leq M - 1\}) \right| = 0. \tag{8.12}$$

The approximation property expressed in (8.1) shows that for all sufficiently large n

$$\{\|\tilde{H}(Y_n)\| \leq M - 1\} \subset \{\|h_n\| \leq M\}$$

and hence that

$$D_n(\{\|\tilde{H}(Y_n)\| \leq M - 1\}) \leq D_n(\{\|h_n\| \leq M\}).$$

Thus for all sufficiently large n

$$\begin{aligned} 0 &\leq \frac{1}{a_n}\log(D_n) - \frac{1}{a_n}\log(D_n(\{\|h_n\| \leq M\}) \\ &\leq \frac{1}{a_n}\log(D_n) - \frac{1}{a_n}\log(D_n(\{\|\tilde{H}(Y_n)\| \leq M - 1\}). \end{aligned}$$

By (8.12) we have

$$\lim_{n\to\infty}\left|\frac{1}{a_n}\log(D_n) - \frac{1}{a_n}\log(D_n(\{\|h_n\| \leq M\}))\right| = 0. \tag{8.13}$$

We complete the proof of (8.4) by comparing $F_n(\{\|h_n\| \leq M\})$ and $D_n(\{\|h_n\| \leq M\})$. By (8.1), for all sufficiently large n

$$\{\|h_n\| \leq M\} \subset \{\|h_n\| \leq M + 1\} \cap \{\|\tilde{H}(Y_n)\| \leq M + 1\}.$$

Lemma II.7.4 in [21] then implies that

$$\begin{aligned} &\left|\frac{1}{a_n}\log(F_n(\{\|h_n\| \leq M\})) - \frac{1}{a_n}\log(D_n(\{\|h_n\| \leq M\}))\right| \\ &\quad\leq \|\langle\beta, h_n\rangle - \langle\beta, \tilde{H}(Y_n)\rangle\|_\infty + \sup_{\{\|h_n\| \leq M\}} |g(h_n) - g(\tilde{H}(Y_n))| \\ &\quad\leq \|\langle\beta, h_n\rangle - \langle\beta, \tilde{H}(Y_n)\rangle\|_\infty \\ &\qquad\qquad + \sup_{\{\|h_n\| \leq M+1\} \cap \{\|\tilde{H}(Y_n)\| \leq M+1\}} |g(h_n) - g(\tilde{H}(Y_n))|. \end{aligned}$$

Since g is uniformly continuous on $\{\|u\| \leq M + 1\}$, (8.1) gives the limit

$$\lim_{n\to\infty}\left|\frac{1}{a_n}\log(F_n(\{\|h_n\| \leq M\}) - \frac{1}{a_n}\log(D_n(\{\|h_n\| \leq M\})\right| = 0. \tag{8.14}$$

Combining (8.11), (8.13), and (8.14), we obtain the desired limit (8.4). This completes the proof of the theorem under the assumptions in part (b). ■

2.9 Direct Proof of Theorem 2.6.2

In this section we give a direct proof of Theorem 2.6.2 from first principles. The proof will be facilitated by using the following characterizations of the set $\mathcal{E}^u$ of microcanonical equilibrium macrostates, defined in (5.9), and the set $\mathcal{E}(g)_\beta$ of generalized canonical equilibrium macrostates, defined in (6.6). These characterizations are immediate from the definitions of the rate functions I^u and $I_{\beta,g}$, in terms of which the two sets of equilibrium macrostates are defined.

- For $u \in \text{dom}\, s$, $x \in \mathcal{E}^u$ if and only if $I(x) < \infty$ and x minimizes $I(y)$ over $y \in \mathcal{X}$ subject to the constraint $\tilde{H}(y) = u$.

- For $\beta \in I\!R^\sigma,\ x \in \mathcal{E}(g)_\beta$ if and only if x minimizes $\langle \beta, \tilde{H}(y)\rangle + g(\tilde{H}(y)) + I(y)$ over $y \in \mathcal{X}$.

Throughout this section g is a continuous function mapping $I\!R^\sigma$ into $I\!R$, in terms of which the generalized canonical ensemble (6.2) is defined. The function s denotes the microcanonical entropy defined in (5.6). The proof of Theorem 2.6.2 depends on the next lemma, which relates the sets $\mathcal{E}^u$ and $\mathcal{E}(g)_\beta$ and the existence of a supporting hyperplane for $h = s - g$ at u with normal vector $[\beta, -1]$ [Defn. 2.2.4(b)].

Lemma 2.9.1. *Define* $h = s - g$.

(a) *For some* u *and* β *in* $I\!R^\sigma$, $h(v) \leq h(u) + \langle \beta, v - u\rangle$ *for all* $v \in I\!R^\sigma$ *if and only if* $\mathcal{E}^u \neq \emptyset$ *and* $\mathcal{E}^u \subset \mathcal{E}(g)_\beta$.

(b) *We assume that for some* $u \in \text{dom}\, s$ *and* $\beta \in I\!R^\sigma$, $\mathcal{E}^u \cap \mathcal{E}(g)_\beta \neq \emptyset$. *The following conclusions hold.*

(i) $h(v) \leq h(u) + \langle \beta, v - u\rangle$ *for all* $v \in I\!R^\sigma$.

(ii) $\mathcal{E}^u \subset \mathcal{E}(g)_\beta$.

Proof. (a) We assume that for some u and β in $I\!\!R^\sigma$

$$h(v) \leq h(u) + \langle \beta, v - u \rangle \text{ for all } v \in I\!\!R^\sigma.$$

Then $u \in \text{dom}\, h = \text{dom}\, s$, and hence $\mathcal{E}^u \neq \emptyset$. Also, since $h = s - g$, the inequality in the last display is equivalent to

$$\begin{aligned}
\langle \beta, u \rangle + g(u) - s(u) &= \inf_{v \in I\!\!R^\sigma} \{\langle \beta, v \rangle + g(v) - s(v)\} \\
&= \varphi_g(\beta) \\
&= \inf_{y \in \mathcal{X}} \{\langle \beta, \tilde{H}(y) \rangle + g(\tilde{H}(y)) + I(y)\}.
\end{aligned}$$

If x is an arbitrary point in $\mathcal{E}^u$, then $\tilde{H}(x) = u$ and $I(x) = -s(u)$. It follows that

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

and thus that $x \in \mathcal{E}(g)_\beta$. We have proved that $\mathcal{E}^u \subset \mathcal{E}(g)_\beta$, as claimed.

Since $\mathcal{E}^u \neq \emptyset$ and $\mathcal{E}(g)_\beta \subset \mathcal{E}^u$ imply that $\mathcal{E}^u \cap \mathcal{E}_\beta \neq \emptyset$, the converse in part (a) is a consequence of part (b), which we now prove.

(b)(i) If x is a point in $\mathcal{E}^u \cap \mathcal{E}(g)_\beta$, then $\tilde{H}(x) = u$ and $I(x) = -s(u)$. Since $x \in \mathcal{E}(g)_\beta$, we have

$$\begin{aligned}
&\langle \beta, \tilde{H}(x) \rangle + g(\tilde{H}(x)) + I(x) \\
&\quad = \inf_{y \in \mathcal{X}} \{\langle \beta, \tilde{H}(y) \rangle + g(\tilde{H}(y)) + I(y)\} \\
&\quad = \varphi_g(\beta).
\end{aligned}$$

Thus for any $v \in I\!\!R^\sigma$

$$\begin{aligned}
\langle \beta, u \rangle + g(u) - s(u) &= \varphi_g(\beta) \\
&= \inf_{w \in I\!\!R^\sigma} \{\langle \beta, w \rangle + g(w) - s(w)\} \\
&\leq \langle \beta, v \rangle + g(v) - s(v).
\end{aligned}$$

This implies that $h(v) \le h(u) + \langle \beta, v - u \rangle$ for all $v \in I\!\!R^\sigma$.

(b)(ii) This follows from parts (b)(i) and (a) of this lemma. ■

We now prove Theorem 2.6.2.

Proof of part (a). We first prove that for any $\beta \in I\!\!R^\sigma$, $\tilde{H}(\mathcal{E}(g)_\beta) \subset \operatorname{dom} s$. Let u be any point in $\tilde{H}(\mathcal{E}(g)_\beta)$ and x any point in $\mathcal{E}(g)_\beta$. Since $I_{\beta,g}(x) = 0$, we have

$$\begin{aligned} & I(x) + \langle \beta, \tilde{H}(x) \rangle + g(\tilde{H}(x)) \\ & \quad = \inf_{y \in \mathcal{X}} \{ I(y) + \langle \beta, \tilde{H}(y) \rangle + g(\tilde{H}(y)) \} < \infty. \end{aligned}$$

Hence by the definition of s, $s(u) \ge -I(x) > -\infty$, and therefore $u \in \operatorname{dom} s$. Since $u \in \tilde{H}(\mathcal{E}(g)_\beta)$ is arbitrary, the desired set inclusion is proved.

We next prove that

$$\mathcal{E}(g)_\beta \subset \bigcup_{u \in \tilde{H}(\mathcal{E}(g)_\beta)} \mathcal{E}^u. \tag{9.1}$$

Let x be any point in $\mathcal{E}(g)_\beta$ and set $u = \tilde{H}(x) \in \tilde{H}(\mathcal{E}(g)_\beta)$. Then for any $y \in \mathcal{X}$ satisfying $\tilde{H}(y) = u$

$$\begin{aligned} I(x) + \langle \beta, \tilde{H}(x) \rangle + g(\tilde{H}(x)) & = I(x) + \langle \beta, u \rangle + g(u) \\ & \le I(y) + \langle \beta, u \rangle + g(u). \end{aligned}$$

It follows that x minimizes $I(y)$ over $y \in \mathcal{X}$ satisfying $\tilde{H}(y) = u$ and therefore that $x \in \mathcal{E}^u$. Since $x \in \mathcal{E}(g)_\beta$ is arbitrary, the proof of (9.1) is complete.

We complete the proof of part (a) by showing that for any $\beta \in I\!\!R^\sigma$ and any $u \in \tilde{H}(\mathcal{E}(g)_\beta)$ we have $\mathcal{E}^u \subset \mathcal{E}(g)_\beta$. Any $u \in \tilde{H}(\mathcal{E}(g)_\beta)$ has the form $u = \tilde{H}(x)$ for some $x \in \mathcal{E}(g)_\beta$. As shown in the preceding paragraph, $x \in \mathcal{E}^u$. Hence $\mathcal{E}^u \cap \mathcal{E}(g)_\beta \ne \emptyset$, and so by part (b)(ii) of Lemma 2.9.1 we conclude that $\mathcal{E}^u \subset \mathcal{E}(g)_\beta$, as claimed. ■

Proof of part (b). We start by assuming that $s-g$ has a strictly supporting hyperplane at $u \in \operatorname{dom} s$ with normal vector $[\beta, -1]$. Setting $h = s - g$, we have

$$h(v) < h(u) + \langle \beta, v-u \rangle \text{ for all } v \in I\!\!R^\sigma, v \neq u. \tag{9.2}$$

According to part (a) of Lemma 2.9.1, $\mathcal{E}^u \subset \mathcal{E}(g)_\beta$. Suppose that $\mathcal{E}^u \neq \mathcal{E}(g)_\beta$. Part (a) of the present theorem then implies that there exists $w \neq u$ such that $\mathcal{E}^w \neq \emptyset$ and $\mathcal{E}^w \subset \mathcal{E}(g)_\beta$. This in turn allows us again to apply part (a) of Lemma 2.9.1, obtaining

$$h(v) \leq h(w) + \langle \beta, v-w \rangle \text{ for all } v \in I\!\!R^\sigma.$$

Substituting $v = u$ gives

$$\begin{aligned} -\infty \;<\; h(u) \;&\leq\; h(w) + \langle \beta, u-w \rangle \\ &<\; h(u) + \langle \beta, w-u \rangle + \langle \beta, u-w \rangle \;=\; h(u); \end{aligned}$$

the second strict inequality follows from (9.2) for $v = w$. The contradiction that $h(u) < h(u)$ proves that $\mathcal{E}^u = \mathcal{E}(g)_\beta$.

We now prove the converse. If $\mathcal{E}^u = \mathcal{E}(g)_\beta$ for some $\beta \in I\!\!R^\sigma$, then by part (a) of Lemma 2.9.1 $h = s - g$ satisfies

$$h(v) \leq h(u) + \langle \beta, v-u \rangle \text{ for all } v \in I\!\!R^\sigma;$$

i.e., $s-g$ has a supporting hyperplane at u with normal vector $[\beta, -1]$. Now assume that $s-g$ does not have a strictly supporting hyperplane at u. Then there exists $w \neq u$ such that

$$h(w) = h(u) + \langle \beta, w-u \rangle.$$

Thus $w \in \operatorname{dom} s$, $\mathcal{E}^w \neq \emptyset$, and for all $v \in I\!\!R^\sigma$

$$\begin{aligned} h(v) \;&\leq\; h(u) + \langle \beta, v-u \rangle \\ &=\; h(w) - \langle \beta, w-u \rangle + \langle \beta, v-u \rangle \\ &=\; h(w) + \langle \beta, v-w \rangle. \end{aligned}$$

Hence by part (a) of Lemma 2.9.1 $\mathcal{E}^w \subset \mathcal{E}(g)_\beta$, and this in turn yields $\mathcal{E}^w \subset \mathcal{E}^u$. However, this is impossible because $w \neq u$ and so $\mathcal{E}^u \neq \mathcal{E}^w$. We conclude that $s - g$ has a strictly supporting hyperplane at u with normal vector $[\beta, -1]$. This completes the proof of part (b).

Proof of part (c). We assume that $s - g$ has a nonstrictly supporting hyperplane at u with normal vector $[\beta, -1]$. Then by part (a) of Lemma 2.9.1 $\mathcal{E}^u \subset \mathcal{E}(g)_\beta$. If in fact $\mathcal{E}^u = \mathcal{E}(g)_\beta$, then by part (b) of the present theorem $s - g$ has a strictly supporting hyperplane at u with normal vector $[\beta, -1]$. This contradiction proves that $\mathcal{E}^u \subset \mathcal{E}(g)_\beta$ and $\mathcal{E}^u \neq \mathcal{E}(g)_\beta$.

We prove the converse by assuming that $\mathcal{E}^u \subset \mathcal{E}(g)_\beta$ and $\mathcal{E}^u \neq \mathcal{E}(g)_\beta$. Since $\mathcal{E}^u \subset \mathcal{E}(g)_\beta$, part (a) of Lemma 2.9.1 implies that $h = s - g$ satisfies

$$h(v) \leq h(u) + \langle \beta, v - u \rangle \text{ for all } v \in I\!\!R^\sigma. \tag{9.3}$$

Since $\mathcal{E}^u \neq \mathcal{E}(g)_\beta$, part (a) of the present theorem implies that there exists $w \neq u$ such that $\mathcal{E}^w \neq \emptyset$ and $\mathcal{E}^w \subset \mathcal{E}(g)_\beta$. Again applying part (a) of Lemma 2.9.1, we have

$$h(v) \leq h(w) + \langle \beta, v - w \rangle \text{ for all } v \in I\!\!R^\sigma. \tag{9.4}$$

Substituting $v = u$ in (9.4) and using (9.3) give

$$\begin{aligned} -\infty \ < \ h(u) \ &\leq \ h(w) + \langle \beta, u - w \rangle \\ &\leq \ h(u) + \langle \beta, w - u \rangle + \langle \beta, u - w \rangle \ = \ h(u). \end{aligned}$$

Thus $h(u) = h(w) + \langle \beta, u - w \rangle$. Since $w \neq u$, we have shown that $s - g$ has a nonstrictly support hyperplane at u with normal vector $[\beta, -1]$. This completes the proof of part (c).

Proof of part (d). If $h = s - g$ does not have a supporting hyperplane at u, then for any $\beta \in I\!\!R^\sigma$ the inequality $h(v) \leq h(u) + \langle \beta, v - u \rangle$ does not hold for all $v \in I\!\!R^\sigma$. Part (b)(i) of Lemma 2.9.1 implies that for all $\beta \in I\!\!R^\sigma$, $\mathcal{E}^u \cap \mathcal{E}(g)_\beta = \emptyset$, as claimed.

We prove the converse by assuming that for all $\beta \in I\!\!R^\sigma$, $\mathcal{E}^u \cap \mathcal{E}(g)_\beta = \emptyset$ but that $s - g$ has a supporting hyperplane at u. Then by part (a) there exists $\beta' \in I\!\!R^\sigma$ such that $\mathcal{E}^u \subset \mathcal{E}(g)_{\beta'}$. This contradiction shows that $s - g$ does not have a supporting hyperplane at u. The proof of the theorem is complete. $\blacksquare$

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