Equivalence and nonequivalence of ensembles: Thermodynamic, macrostate, and measure levels

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We present general and rigorous results showing that the microcanonical and canonical ensembles are equivalent at all three levels of description considered in statistical mechanics – namely, thermodynamics, equilibrium macrostates, and microstate measures – whenever the microcanonical entropy is concave as a function of the energy density in the thermodynamic limit. This is proved for any classical many-particle systems for which thermodynamic functions and equilibrium macrostates exist and are defined via large deviation principles, generalizing many previous results obtained for specific classes of systems and observables. Similar results hold for other dual ensembles, such as the canonical and grand-canonical ensembles, in addition to path ensembles used for describing nonequilibrium systems driven in steady states.
I. INTRODUCTION

The problem of determining whether the microcanonical and canonical ensembles give the same predictions has a long history in statistical mechanics, starting from Boltzmann’s introduction of these ensembles as the ergode and holode [1], respectively, and Gibbs’s formulation of these ensembles in their modern probabilistic form [2]. Depending on the level of description considered, this equivalence problem takes different forms:

- **Thermodynamic equivalence:** Is the microcanonical thermodynamics of a system determined from the entropy as a function of its energy the same as the canonical thermodynamics determined from the free energy as function of temperature? Mathematically, this amounts to asking: are the entropy and free energy functions one-to-one related by Legendre transform?

- **Macrostate equivalence:** Is the set of equilibrium values of a certain macrostate (e.g., magnetization, energy, velocity distribution, etc.) determined in the microcanonical ensemble as a function of energy the same as the set of equilibrium values determined in the canonical ensemble? Is there a relationship between these two sets?

- **Measure equivalence:** Does the Gibbs distribution defining the canonical ensemble at the microstate level converge (in some sense to be made precise) to the microcanonical distribution defined by Boltzmann’s equiprobability postulate?

Many results have been derived over the years, providing conditions for equivalence at each of these levels, as well as conditions for relating one level to another; see, e.g., [3] for a review. It is known in particular that equivalence holds at the thermodynamic level whenever the entropy is concave and that this also implies, under additional conditions, the equivalence of the microcanonical and canonical ensembles at the macrostate level. Although the first result is general – it is just a mathematical statement about concave functions and the duality of Legendre transforms – the second has been derived by Ellis, Haven and Turkington [4] for a class of systems comprising mostly ideal (non-interacting), long-range, and mean-field systems. As for the measure level, a number of general results have been obtained by Lewis, Pfister and Sullivan [5–7], but have not been completely related to the two other levels for general systems and observables.

The aim of this paper is to solve these problems by proving in a general and rigorous way that equivalence actually holds at each of the level above under the same condition, namely the concavity of the entropy. The main ideas behind these results were presented in [8]; here we focus on giving proofs of these results, as well as on studying the measure level not considered in [8]. For the macrostate level, our results significantly generalize those of Ellis, Haven and Turkington [4] to any macrostate of any classical many-particle system for which equilibrium statistical mechanics is defined. The same results also imply equivalence results for the measure level, generalizing those of Lewis, Pfister and Sullivan [5–7] in terms of systems and observables considered and the way equivalence at this level is defined. In the end, our results show that all three equivalence levels coincide, in agreement with the general idea of statistical mechanics that the macroscopic world is a direct reflection of the microscopic world.

The concavity condition underlying the equivalence of ensembles is important because there are physical systems known to have nonconcave entropies in the thermodynamic limit. The common property of these systems is that they involve long-range interactions that asymptotically decay at large distances $r$ according to $r^{-\alpha}$ with $0 \leq \alpha \leq d$, where $d$ is the dimensionality of the system. Thus, the dividing line between equivalence and nonequivalence of ensembles is essentially between short- and long-range systems: the former have concave entropies, and are thus described equivalently by the microcanonical or the canonical ensemble, as proved by Ruelle [9] (see also [10]), whereas
the latter can have nonconcave entropies and therefore nonequivalent ensembles.\textsuperscript{1} Gravitating
particles are historically and physically the most important example of long-range systems showing
this behavior, as discovered by Lynden-Bell \cite{Lynden-Bell:1965} and Thirring \cite{Thirring:1966} in the late 1960s, and as
extensively studied since then; see \cite{Lai:2017, Weinberg:2018, Sachdev:2020} for recent reviews. Other examples include non-screened
plasma, dipolar systems, statistical models of two-dimensional turbulence, and mean-field systems
in general; see \cite{Lai:2017} for a review. Recently, experiments based on ion, cold atom and optical traps
have been proposed to observe long-range interactions and nonconcave entropies \cite{LongRangeExp}.\textsuperscript{2}

The recent study of these long-range systems explains the need to revisit the equivalence problem.
Most works on ensemble equivalence assume that entropy is always concave either implicitly or
explicitly, and so naturally conclude that ensembles are always equivalent; see, e.g., \cite{Ruelle:1978, Gallavotti:1983, Gallavotti:1985}.
In Ruelle’s work \cite{Ruelle:1978}, this is not assumed but follows directly from the class of interactions considered,
namely short-range and tempered, for which it can be proved using subadditivity arguments that
the entropy exists and is concave in the thermodynamic limit. For a proof of this result for the
simpler case of finite-range systems, see Lanford \cite{Lanford:1975}.

Long-range systems can have nonconcave entropies precisely because the subadditivity argument
is not applicable: in the presence of long-range interactions, one cannot divide a system into
subsystems in such a way that the total energy of the system is extensive in the energies of the
subsystems \cite{Lai:2017}. The thermodynamic limit of this system can still be defined using Kac’s rescaling
prescription \cite{Kac:1949} for all the usual thermodynamic quantities (entropy, free energy, etc.), so that
statistical mechanics applies to long-range systems in the same way as for short-range systems
\cite{Lai:2017}. However, the difference is that the entropy function is not necessarily concave with long-range
interactions.

Here we investigate the consequences of this property for the equivalence of the microcanonical
and canonical ensembles in the case of general classical \( N \)-particle systems. Unlike several works
on the subject, we do not consider specific systems defined by a class of Hamiltonians, but rather
assume that the Hamiltonian is given and that the thermodynamic potentials and equilibrium
states obtained from this Hamiltonian exist in each ensemble and are characterized, as explained in
the next section, by well-defined large deviation principles. This is a natural assumption given, on
the one hand, that the equivalence problem has no meaning when thermodynamic potentials and
equilibrium states do not exist and, on the other, that all cases of thermodynamic behavior and
equilibrium states known to date are described by large deviation theory.\textsuperscript{3} With this assumption,
we then prove that ensemble equivalence holds at the thermodynamic, macrostate and measure
levels when the entropy is concave in the thermodynamic limit.

For simplicity, we focus in this paper on the microcanonical and canonical ensembles, but as
mentioned in Sec. VI the results proved also hold with minor modifications for other dual ensembles.
This includes, for example, the canonical and grand-canonical ensembles, the volume and pressure
ensembles, and the magnetization and magnetic field ensembles. In each case, the entropy function
entering in the equivalence condition has to be replaced by the thermodynamic potential of the
constrained ensemble considered, for example, the entropy as a function of the particle density for
the canonical ensemble. As shown in that section, the same notion of equivalence also applies to
nonequilibrium generalizations of the canonical and microcanonical ensembles defined for paths
of Markov processes. What underlies the problem of ensemble equivalence is in fact a general
relationship between the conditioning and the so-called tilting of probability measures \cite{Gallavotti:1983, Gallavotti:1985},
arising in many problems in probability theory, stochastic simulations, and the study of stochastic processes.

The organization of the paper is as follows. In Sec. II we define the microcanonical and canonical
ensembles, as well as the basic large deviation principles used to define the set of equilibrium

\textsuperscript{1} The presence of long-range interaction is a necessary but not sufficient condition for having nonconcave entropies,
so that not all long-range systems have nonconcave entropies.

\textsuperscript{2} There are strong reasons to believe that this cannot be otherwise: that is, many-body systems should have
equilibrium states in the thermodynamic limit only when they are described by large deviation theory or, more
precisely, when their distribution follows what is called the large deviation principle; see Sec. II.

\textsuperscript{3} With this assumption, we then prove that ensemble equivalence holds at the thermodynamic, macrostate and measure
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macrostates in each ensemble. This section follows the standard construction of these ensembles in terms of large deviations, which can be found for example in [26–29]. In Secs. III, we state some known definitions and results about thermodynamic equivalence, and then prove in Secs. IV and V equivalence results that relate this level to the macrostate and measure levels, respectively. The main insight used for proving equivalence at the macrostate level is an exact variational principle, stated in Sec. IV, relating the typical states and fluctuations of the microcanonical ensemble to those of the canonical ensemble. Rigorous proofs of all the results follow relatively directly using a combination of convex analysis results, summarized in Appendix A, and a fundamental result of large deviation theory known as Varadhan’s Theorem, stated in Appendix B. Finally, in Sec. VI, we show how to generalize our results to other dual equilibrium and nonequilibrium ensembles, as mentioned above.

II. NOTATIONS AND DEFINITIONS

We introduce in this section the notations used in the paper and recall the definitions of the microcanonical and canonical ensembles following the large deviation theory approach to statistical mechanics [26–29]. The notations closely follow those of [4].

A. Systems and macrostates

We consider a system of \( N \) classical particles with microscopic configuration or microstate \( \omega = (\omega_1, \omega_2, \ldots, \omega_N) \in \Lambda_N = \Lambda^N \), where \( \omega_i \) is the state of the \( i \)th particle taking values in some space \( \Lambda \). The physical properties of the system are described by its Hamiltonian or energy function \( H_N(\omega) : \Lambda_N \rightarrow \mathbb{R} \), from which we define the mean energy or energy per particle as \( h_N(\omega) = H(\omega)/N \). For simplicity, we do not consider the volume of the system, so that the thermodynamic limit is obtained by taking the limit \( N \rightarrow \infty \) with \( h_N \) kept constant. Systems with a volume are considered in Sec. VI, which treats the equivalence of the canonical and grand-canonical ensembles.

At the macroscopic level, the \( N \)-particle system is characterized in terms of a macrostate, defined mathematically as a function \( M_N : \Lambda_N \rightarrow \mathcal{M} \) taking values in some measurable space \( \mathcal{M} \). This macrostate can represent, for example, the mean magnetization of a spin system, in which case \( \mathcal{M} = [-1, 1] \), or the empirical distribution of velocities or positions of a gas of \( N \) particles, in which case \( \mathcal{M} \) is the space of normalized probability distributions. Note that the same symbol \( M_N \) is used to denote a single (scalar) macrostate, a vector macrostate representing a collection of different macrostates, or a function.

In the full setting of large deviation theory, \( \mathcal{M} \) is usually considered to be a general topological space known as a Polish space [30]. In this paper, we follow a more practical approach and consider \( \mathcal{M} \) to be a subset of \( \mathbb{R}^d \) with the usual Euclidean metric, so as not to deal with abstract topological issues. Empirical distributions and other similar macrostates defined over function spaces can be treated within this restriction using conventional discretizations and continuum limits.

To construct a statistical description of the \( N \)-particle system, we finally need a prior measure \( P_N \) on \( \Lambda_N \), whose basic element is denoted either by \( P_N(d\omega) \) or \( dP_N(\omega) \). In the physics literature, this prior is most often implicitly taken to be the (non-normalized) Lebesgue measure \( d\omega \). Here we follow [4] and make \( P_N \) explicit in the definition of statistical ensembles. This has the advantage of allowing one to consider models which do not necessarily comply with Boltzmann’s equiprobability postulate, and so for which the prior is not necessarily proportional to \( d\omega \). For a comparison of the two approaches, see Secs. 5.1 and 5.2 of [29].
B. Equilibrium ensembles

We consider throughout most of the paper the equilibrium properties of macrostates as calculated in the canonical and microcanonical ensembles. Generalizations of the results obtained for other ensembles are presented in Sec. VI.

The canonical ensemble is defined in the usual way by the microstate measure

\[ P_{N,\beta}(d\omega) = \frac{e^{-\beta H_N(\omega)}}{Z_N(\beta)} P_N(d\omega) \]  

where

\[ Z_N(\beta) = E_{P_N}[e^{-\beta H_N(\omega)}] = \int_{\Lambda_N} e^{-\beta H_N(\omega)} dP_N(\omega) \]

is the partition function normalizing \( P_{N,\beta} \) and \( \beta = (k_B T)^{-1} \) is the inverse temperature. From this measure, the probability of any event \( M_N \in A \) involving a macrostate \( M_N \) and some measurable subset \( A \) of \( \mathcal{M} \) is calculated as

\[ P_{N,\beta}\{M_N \in A\} = \int_{\Lambda_N} 1_A(M_N(\omega)) P_{N,\beta}(d\omega) = \int_{M_N^{-1}(A)} dP_{N,\beta}(\omega) \]

where

\[ M_N^{-1}(A) = \{ \omega \in \Lambda_N : M_N(\omega) \in A \} \]

is the pre-image of \( M_N \in A \).

The microcanonical ensemble is defined, on the other hand, from Boltzmann’s equiprobability postulate by assigning a constant weight to all microstates \( \omega \) having an energy \( H_N(\omega) = U \). Probabilistically, this is made precise by conditioning the prior \( P_N \) on the set of microstates having a mean energy \( h_N(\omega) \) lying in the “thickened” energy shell \([u-r,u+r]\):

\[ P_N^u(d\omega) = P_N\{d\omega|h_N \in [u-r,u+r]\}, \quad r > 0. \]

By Bayes’ Theorem, this becomes

\[ P_N^u(d\omega) = \frac{1_{[u-r,u+r]}(h_N(\omega))}{P_N\{h_N \in [u-r,u+r]\}} P_N(d\omega), \]

where \( 1_A(x) \) is the indicator function of the set \( A \) and

\[ P_N\{h_N \in [u-r,u+r]\} = \int_{\Lambda_N} 1_{[u-r,u+r]}(h_N(\omega)) dP_N(\omega) \]

is a normalizing factor representing the mean energy distribution with respect to the prior \( P_N \). The need to consider the mean energy rather than the energy in the definition of \( P_N^u \) arises because of the thermodynamic limit, whereas the thickened energy shell is there to make \( P_N^u \) a well defined measure; see [8] for the more physical but less rigorous approach based on densities and Dirac delta functions instead of indicator functions.

In the remaining, it will be implicit that \( r \to 0 \), so we omit this symbol when writing the microcanonical measure. Moreover, we will simplify the notation by denoting the infinitesimal interval \([u-r,u+r]\) by \( du \) so as to write the microcanonical ensemble at mean energy \( u \) as

\[ P_N^u(d\omega) = P_N\{d\omega|h_N \in du\} = \frac{1_{du}(h_N(\omega))}{P_N\{h_N \in du\}} P_N(d\omega). \]
From this microstate measure, the macrostates probabilities at fixed energy are then calculated, as in the canonical case, using

\[ P_N^u \{ M_N \in A \} = \int_{A_N} 1_A(M_N(\omega)) \, P_N^u(d\omega) = \int_{M_N^{-1}(A)} dP_N^u(\omega). \] (9)

For a more general definition of the microcanonical ensemble based on conditionings involving events of the form \( h_N \in A_N \) with \( \{ A_N \} \) a sequence of sets, see [7].

C. Large deviation principles

The stability of equilibrium systems observed physically at the macroscopic scale is due mathematically to the fact that large fluctuations of macrostates are extremely unlikely – in fact, exponentially unlikely with the system size – which implies that \( P_{N,\beta} \) and \( P_N^u \) must concentrate exponentially at the macrostate level around certain values corresponding to equilibrium states.

This exponential concentration of measures is known in probability theory as the large deviation principle (LDP) and is defined as follows. Consider first the canonical ensemble. We say that \( M_N \) satisfies the LDP with respect to \( P_{N,\beta} \) if there exists a lower semicontinuous function \( I_\beta \) such that

\[ \limsup_{N \to \infty} \frac{1}{N} \ln P_{N,\beta} \{ M_N \in C \} \leq - \inf_{m \in C} I_\beta(m) \] (10)

for any closed sets \( C \) and

\[ \liminf_{N \to \infty} \frac{1}{N} \ln P_{N,\beta} \{ M_N \in O \} \geq - \inf_{m \in O} I_\beta(m) \] (11)

for any open sets \( O \).3 The function \( I_\beta \) is called the rate function; in [5–7], it is also called the Ruelle-Lanford (R-L) function. In the microcanonical ensemble, we say similarly that \( M_N \) satisfies the LDP with respect to \( P_N^u \) if the same limits exist for a (lower semicontinuous) rate function \( I^u \).

For most applications in physics, this definition can be simplified by considering nice rate functions and sets for which the upper and lower bounds are the same (typically, continuous rate functions and finite intervals or balls). With this in mind, we can express the LDP for a real observable \( M_N \) simply as

\[ \lim_{N \to \infty} -\frac{1}{N} \ln P_{N,\beta} \{ M_N \in [m-r, m+r] \} = I_\beta(m) \] (12)

with the limit \( r \to 0 \) implicit as before. If \( M_N \) is a vector taking values in \( \mathbb{R}^n \), then the interval \([m-r, m+r]\) is replaced by an infinitesimal ball \( B_r(m) = \{ m' \in M : \| m - m' \| \leq r \} \) centered at \( m \) to obtain the same limit. In both cases, it is convenient to summarize the limit defining the LDP using the logarithmic equivalence notation

\[ P_{N,\beta} \{ M_N \in dm \} \asymp e^{-N I_\beta(m)} \, dm \] (13)

where \( dm \) denotes an infinitesimal interval or ball centered at \( m \) [26–28]. This way, we emphasize the two fundamental properties of the LDP, namely the exponential decay of probabilities with \( N \), except at points where the rate function vanishes, and the fact that this decay is in general only

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3 We should define the LDP, more precisely, for the sequence \( \{ P_{N,\beta} \} \) of probability measures associated with the sequence \( \{ M_N \} \) of random variables. Here we simplify the presentation by referring directly to macrostates and their probabilities.
approximately exponential in $N$, that is, exponential in $N$ up to first order in the exponent. A similar notation holds obviously for the microcanonical LDP.

The simplification of the two bounds in the definition of the LDP is convenient but not crucial for the results discussed in the remainder of the paper. In particular, all the large deviation results stated hold under the full definition given above, which is due to Varadhan [32]. For more details about LDPs defined in the context of statistical mechanics, the lower semicontinuity of rate functions, and the $\asymp$ notation, see [26–29].

D. Equilibrium macrostates

The LDP of $M_N$ with respect to $P_{N}^{u}$ and $P_{N,\beta}$ imply, as mentioned before, that these measures concentrate exponentially with $N$ on certain points of $\mathcal{M}$ corresponding physically to the typical or equilibrium values of $M_N$ obtained in the thermodynamic limit. Mathematically, these points must correspond to minima and zeros of $I^{u}$ and $I_{\beta}$, since rate functions are always non-negative. This justifies defining the set $\mathcal{E}^{u}$ of equilibrium values of the macrostate $M_N$ in the microcanonical ensemble at mean energy $u$ as

$$\mathcal{E}^{u} = \{ m \in \mathcal{M} : I^{u}(m) = 0 \}$$

(14)

and the set of equilibrium values of $M_N$ in the canonical ensemble at inverse temperature $\beta$ as

$$\mathcal{E}_{\beta} = \{ m \in \mathcal{M} : I_{\beta}(m) = 0 \}.$$  

(15)

The former definition formalizes Einstein’s observation that microcanonical equilibrium states maximize the macrostate entropy, which is identified as $-I^{u}(m)$, whereas the latter formalizes Landau’s later observation that canonical equilibrium states minimize the canonical macrostate free energy, identified as the rate function $I_{\beta}(m)$. More information about these definitions and identifications can be found in [26–28], [5–7], and Secs. 5.3 and 5.4 of [29]. In [5–7], the equilibrium macrostate sets are called the concentration sets.

As observed by Lanford [24] (see also [4–7]), the interpretation of the elements of $\mathcal{E}^{u}$ or $\mathcal{E}_{\beta}$ as equilibrium states is rigorously justified when these sets contain one element. In this common case, it is relatively easy to show that the microcanonical or canonical measure of $M_N$ is exponentially concentrated on a single value, so that $M_N$ converges in probability to this typical value in the limit $N \to \infty$. A proof of this result, which establishes a Law of Large Numbers for $M_N$, can be found for example in Theorems 2.5 and 3.6 of [4].

There is a problem, however, when $\mathcal{E}^{u}$ or $\mathcal{E}_{\beta}$ contains more than one elements for a given value of their parameters, which arises typically when there is phase coexistence at a first-order phase transition. In this case, there are two possibilities: i) all the elements of $\mathcal{E}^{u}$ or $\mathcal{E}_{\beta}$ are concentration points of $M_N$ and so correspond to ‘real’ equilibrium states; or ii) some of these elements correspond to points where the probability of $M_N$ decays sub-exponentially with $N$. Here we consider mostly the first case; the second involves corrections to the LDP of $P_{N}^{u}$ or $P_{N,\beta}$ far beyond the scope of this paper. For a discussion of these corrections in the context of the 2D Ising model, see, e.g., Examples 5.4 and 5.6 of [29].

E. Thermodynamic potentials

Before we proceed to discuss the equivalence of the microcanonical and canonical ensembles, we need to define two additional functions, corresponding to the thermodynamic potentials of each
ensemble. The first is the **canonical free energy** or **specific free energy** defined as

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

with \(\beta \in \mathbb{R}\). This function is also sometimes called the **pressure** [9] following its interpretation in the grand-canonical ensemble. Its domain or essential domain is denoted by

\[
\text{dom } \varphi = \{ \beta \in \mathbb{R} : \varphi(\beta) > -\infty \}.
\]

In large deviation theory, \(\varphi(\beta)\) is up to a sign the scaled cumulant generating function of the mean energy \(h_N\) with respect to the prior \(P_N\); see (2). We define this function in the mathematical rather than physics way without a \(1/\beta\) pre-factor in order for \(\varphi(\beta)\) to be everywhere concave. To be more precise, \(\varphi(\beta)\) is by definition a finite, concave and upper semicontinuous function; by concavity, it is also continuous in the interior of its domain [4].

In the microcanonical ensemble, the thermodynamic potential to consider is the **microcanonical entropy** or **specific entropy**, defined as

\[
s(u) = \lim_{r \to 0} \lim_{N \to \infty} \frac{1}{N} \ln P_N\{h_N \in [u - r, u + r]\},
\]

\(P_N\) being again the prior measure. The domain of this function is

\[
\text{dom } s = \{ u \in \mathbb{R} : s(u) > -\infty \}
\]

and is assumed to coincide with the range of \(h_N\). It is clear from the large deviation point of view that the definition of \(s(u)\) is equivalent to an LDP for the mean energy \(h_N\) with respect to \(P_N\), which we write without a minus sign to comply with the physics notation. With the asymptotic notation, we thus express this LDP as

\[
P_N\{h_N \in du\} \asymp e^{Ns(u)} du,
\]

where \(du = [u - r, u + r]\) as before.

The entropy function \(s(u)\) is upper semicontinuous, but not necessarily concave, as often assumed. Following the introduction, it is the system studied and the form of its Hamiltonian \(H_N\) that determines whether or not the entropy is concave. For short-range systems, \(s(u)\) is concave, but for long-range systems, it can be nonconcave. This is the starting point of nonequivalent ensembles.

### III. THERMODYNAMIC EQUIVALENCE

We begin our study of the equivalence problem with the (lowest) thermodynamic level. As mentioned in the introduction, the problem at this level is to determine whether there is a correspondence between the two equilibrium thermodynamic behaviors of an \(N\)-particle system obtained in the microcanonical and canonical ensembles via the entropy \(s(u)\) and free energy \(\varphi(\beta)\), respectively. The large deviation nature of these two functions implies that they must be related by Legendre transform, so that the mathematical question that we face is: What are the conditions guaranteeing that the Legendre transform between \(s(u)\) and \(\varphi(\beta)\) is involutive, that is, self-inverse?

These conditions have been studied in many works; see [3] for a review. We repeat these conditions in this section to make the presentation self contained and introduce some definitions and concepts of convex analysis that will be used in the next sections.
A. Equivalence results

To discuss the thermodynamic equivalence of the canonical and microcanonical ensembles, we obviously need $\varphi$ and $s$ to exist:

**Assumptions (Existence of thermodynamic potentials).**

(A1) The limit defining $\varphi(\beta)$ exists and yields a function different than 0 or $\infty$ everywhere;

(A2) $h_N$ satisfies the LDP with respect to the prior measure $P_N$ with entropy function $s(u)$.

The assumptions are not independent, for if $s$ exists, then $\varphi$ also exists and is given by the Legendre-Fenchel transform (or conjugate) of $s$:

$$\varphi(\beta) = \inf_{u \in \mathbb{R}} \{ \beta u - s(u) \}. \quad (21)$$

This result holds in the thermodynamic limit for any system and implies our first result about equivalence, namely: the canonical thermodynamic behavior of a system, as encoded in $\varphi(\beta)$ as a function of the inverse temperature of some external heat bath, can always be determined from the microcanonical ensemble knowing $s(u)$. The rigorous proof of this transform follows using Varadhan’s generalization of the Laplace principle; see Sec. II.7 of [26], Sec. 4 of [4] or Appendix B. Following the theory of convex functions [33], we denote this Legendre transform by $\varphi = s^\ast$.

What is interesting for the equivalence problem is that the inverse transform does not always hold. To see this, define the Legendre-Fenchel transform of $\varphi$, which corresponds to the double Legendre-Fenchel transform ($s^\ast)^\ast = s^{**}$ of $s$:

$$s^{**}(u) = \inf_{\beta \in \mathbb{R}} \{ \beta u - \varphi(\beta) \} = \inf_{\beta \in \mathbb{R}} \{ \beta u - s^\ast(\beta) \}. \quad (22)$$

This is a concave and upper semicontinuous function such that $s^{**}(u) \geq s(u)$ for all $u \in \text{dom } s$, corresponding geometrically to the concave envelope or concave hull of $s(u)$ [33]. As a result, if $s$ is concave, then $s = s^{**}$ and the Legendre-Fenchel transform is dual: $\varphi = s^\ast$ and $s = \varphi^\ast$. In this case, we say that we have thermodynamic equivalence, since $\varphi$ and $s$ can be transformed into one another. However, if $s$ is not concave, that is, if $s \neq s^{**}$, then there are some parts of $s$ that do not correspond to the Legendre-Fenchel transform of $\varphi$ and thus cannot be obtained from the canonical ensemble. In this case, we say that we have thermodynamic nonequivalence of ensembles [4]. Physically, this means that a system having a nonconcave entropy must have thermodynamic properties as a function of the mean energy that cannot be accounted for within the canonical ensemble as a function of temperature (for otherwise $s$ and $\varphi$ would be related by Legendre-Fenchel transform).

This definition of thermodynamic equivalence is global as it is based on the whole functions $s$ and $\varphi$. Clearly, a local definition can also be given by comparing $s(u)$ and $s^{**}(u)$ directly for specific values of the mean energy $u$. In this case, it is convenient to define $s(u)$ as being concave at $u \in \text{dom } s$ if $s(u) = s^{**}(u)$ and nonconcave otherwise.

**Definition 1 (Thermodynamic equivalence).**

(a) If $s(u)$ is concave at $u$, then the microcanonical ensemble at mean energy $u$ is said to be thermodynamically equivalent with the canonical ensemble;

(b) If $s(u)$ is nonconcave at $u$, then the microcanonical ensemble at mean energy $u$ is thermodynamically nonequivalent with the canonical ensemble.
This definition is illustrated in Fig. 1.

Note that, although the term or relation ‘equivalent’ is symmetric (as in ‘equal’), there is a directionality in the interpretation of equivalence in that, as noted before, the whole of \( \varphi \) can always be obtained by Legendre-Fenchel transform from \( s \), but \( s \) cannot always be obtained from \( \varphi \). We will see in the next section that this property leads to a similar ‘directionality’ in the equivalence of the microcanonical and canonical ensembles at the macrostate level.

The next result gives a more geometric characterization of thermodynamic equivalence based on subdifferentials and supporting lines. These concepts, which are important for the next sections, are defined in Appendix A and illustrated in Fig. 1. For the purpose of this paper, the main property of concave points to note is that they admit supporting lines except possibly at boundary points; see Appendix A for more details.

**Proposition 2.** Except possibly at boundary points of \( s \), we have the following:

(a) If \( s \) admits a supporting line at \( u \), then the microcanonical ensemble at \( u \) is thermodynamically equivalent with the canonical ensemble for all \( \beta \in \partial s(u) \);

(b) If \( s \) does not admit a supporting line at \( u \), then the microcanonical ensemble at \( u \) is thermodynamically nonequivalent with the canonical ensemble for all \( \beta \in \mathbb{R} \).

The characterization of \( \beta \) in terms of the subdifferential \( \partial s(u) \) of \( s(u) \) follows from the fact that the Legendre-Fenchel transform is equal to

\[
s(u) = \beta u - \varphi(\beta)
\]

for all \( \beta \in \partial s(u) \) and all \( u \in \text{dom } s \) such that \( \partial s(u) \neq \emptyset \); see Theorem 23.5 of [33] or Theorem A.4 of [34]. This generalizes to nondifferentiable functions the standard Legendre transform defined as

\[
s(u) = \beta u - \varphi(\beta), \quad \beta = s'(u).
\]

For an explanation of the difference between Legendre and Legendre-Fenchel transforms and the need in thermodynamics for the latter, see Sec. 5.2.3 of [29].

**B. Energy-temperature relation**

The thermodynamic equivalence of the canonical and microcanonical ensembles can be understood more physically by comparing the mean energies of the two ensembles in the thermodynamic limit. Since \( h_N \) is a random variable in the canonical ensemble, this ensemble and the microcanonical
ensemble, with its fixed mean energy $u$, cannot be equivalent for $N < \infty$. However, it is natural to expect the canonical measure of $h_N$ to concentrate in the thermodynamic limit around some equilibrium value $u_\beta$ of the mean energy, which can be related for a given $\beta$ to the mean energy $u$ of the microcanonical ensemble.

This reasoning is due to Gibbs [2] and can be found in almost all textbooks of statistical mechanics as the basis for stating that the canonical and microcanonical ensembles must become equivalent in the thermodynamic limit. To establish this reasoning as a rigorous result, we must determine the set of equilibrium values of $h_N$ in the canonical ensemble and see if they can indeed be related to the mean energy of the microcanonical ensemble [3, 6]. This is done in the next two results, which relate this problem to the concave points of $s$, and consequently the involutiveness of the Legendre-Fenchel transform between $s$ and $\varphi$.

**Proposition 3.** Under Assumptions A1-A2, $h_N$ satisfies the LDP in the canonical ensemble with respect to $P_{N,\beta}$ with rate function

$$J_\beta(u) = \beta u - s(u) - \varphi(\beta).$$

(25)

This result and its physical interpretation can be found in [35] and Example 5.5 of [29]. A rigorous proof is given next based on Varadhan’s Theorem applied to exponentially tilted measures; see Appendix B. For a similar result obtained for observables other than the mean energy, see Theorem 4.1 of [7].

**Proof.** The LDP and rate function (25) follow directly from Theorem 14 of Appendix B with the following substitutions: $-s(u)$ takes the role of $I(x)$, $P_{N,\beta}$ takes the role of $P_{n,F}$, and $F(h_N) = -\beta h_N$. Although the latter function is not bounded, we have $\varphi(\beta) < \infty$ by Assumption A1. Therefore, the result of this theorem applies and yields that $h_N$ satisfies the LDP with respect to $P_{N,\beta}$ with rate function

$$\beta u - s(u) - \inf_u \{\beta u - s(u)\} = \beta u - s(u) - \varphi(\beta).$$

(26)

Following the logarithmic notation introduced earlier, we express the LDP of Proposition 3 as

$$P_{N,\beta}\{h_N \in du\} \asymp e^{-NJ_\beta(u)} du$$

(27)

to emphasize the exponential concentration of the canonical measure of $h_N$ and the fact that the canonical equilibrium values of $h_N$ must correspond to the zeros of $J_\beta$. Let $\mathcal{U}_\beta$ denote the set of these equilibrium values obtained for a given inverse temperature $\beta$, that is,

$$\mathcal{U}_\beta = \{u \in \mathbb{R} : J_\beta(u) = 0\}.$$

(28)

Note that the minimizers of $J_\beta$ are necessarily in $\text{dom } s$. From the explicit form of this rate function, we obtain the following relation between the elements of $\mathcal{U}_\beta$ and the entropy:

**Proposition 4.** Assume A1-A2. Then $u \in \mathcal{U}_\beta$ if and only if $\beta \in \partial s(u)$.

**Proof.** We first prove the necessary part of this result. Let $u \in \text{dom } s$ and assume that $\beta \in \partial s(u)$. Then, by the definition of subdifferentials (see Appendix A), we have

$$s(v) \leq s(u) + \beta(v - u)$$

(29)

for all $v \in \mathbb{R}$. Equivalently,

$$\beta u - s(u) \leq \beta v - s(v),$$

(30)
FIG. 2. Left: Nonconcave entropy $s(u)$. Center: Associated free energy $\varphi(\beta)$ having a nondifferentiable point at $\beta_c$. Right: Equilibrium mean energy $u_\beta$ in the canonical ensemble as a function of $\beta$: as $\beta$ is varied continuously, $u_\beta$ skips over the nonconcave interval $(u_l, u_h)$, giving rise to a first-order phase transition in the canonical ensemble with specific latent heat $\Delta u = u_h - u_l$.

which implies from (25) that $u$ is a global minimum of $J_\beta(u)$. Therefore, $u \in U_\beta$.

For the sufficiency part, choose $u \in U_\beta$, so that $J_\beta(u) = 0$. Since $J_\beta(v) \geq 0$ for all $v \in \mathbb{R}$, we must have

$$\beta u - s(u) \leq \beta v - s(v) \quad (31)$$

for all $v$, which implies that $\beta \in \partial s(u)$ by definition of subdifferentials.

The complete physical interpretation of Proposition 4 is discussed in Sec. 4.2 [3], [36], and Example 5.9 of [29]. For the purpose of this paper, we mention only two particular cases of interest for physical applications:

1. If $s$ is strictly concave and differentiable at $u$, then $U_\beta = \{u\}$ for $\beta = s'(u)$, which means that $u$ is the unique equilibrium mean energy in the canonical ensemble at $\beta$. In this case, Gibbs's reasoning is valid: there is equivalence of ensembles in the expected physical way with the temperature-entropy relation $\beta = s'(u)$ arising from the (involutive) Legendre transform between $\varphi$ and $s$.

2. If $s$ is nonconcave at $u$, then $u \notin U_\beta$ for any $\beta \in \mathbb{R}$. In this case, illustrated in Fig. 2, Gibbs's reasoning does not work: there is nonequivalence of ensembles because there is no inverse temperature in the canonical ensemble that yields $u$ as the equilibrium mean energy in the canonical ensemble.

The second case also implies, as illustrated in Fig. 2, that the nonconcave region of $s$ is ‘skipped over’ by the canonical ensemble, and therefore that there must be a discontinuous or first-order phase transition in that ensemble. This relation between nonconcave entropies and canonical first-order phase transitions is completely general and provides a clear physical explanation of nonequivalent ensembles. For more precise results on this relation, see [36], Theorem 4.10 of [4] or Sec. 5.5 of [29]; for examples of long-range systems having nonconcave entropies, see [16].

IV. MACROSTATE EQUIVALENCE

We now discuss the equivalence of ensembles at the deeper level of equilibrium macrostates. Our previous discussion of the equilibrium values of $h_N$ in the canonical ensemble is already a form of macrostate equivalence relating the elements of $U_\beta$ to the control parameter $u$ of the microcanonical ensemble. In this section, we study this macrostate level in a more general way by comparing
the two sets $\mathcal{E}_\beta$ and $\mathcal{E}^u$ of equilibrium values of the macrostate $M_N$ obtained in the canonical and microcanonical ensembles.

The study of this equivalence level started historically with Lax [37] (see also [38–40]), who noted that expected values calculated in the microcanonical ensemble were not always identical to those calculated in the canonical ensemble. Subsequently, the problem attracted little attention, despite its obvious physical importance, until it was studied in a general way by Ellis, Haven and Turkington [4] following previous results by Eyink and Spohn [41]. Other works (see [42–48]) have considered the equivalence of ensembles at the level of a function macrostate known in large deviation theory as the empirical process [26–28].

In this section, we show that ensemble equivalence holds at the level of general systems and macrostates under the same conditions as thermodynamic equivalence. The presentation follows the results announced in [8], which generalize those of [4] to any classical $N$-body systems and macrostates $M_N$ under the following assumptions:

**Assumptions (Existence of equilibrium macrostates).**

(A3) $M_N$ satisfies the LDP with respect to the canonical measure $P_{N,\beta}$ with rate function $I_\beta$ for all $\beta \in \text{dom } \varphi$;

(A4) $M_N$ satisfies the LDP with respect to the microcanonical measure $P_N^u$ with rate function $I^u$ for all $u \in \text{dom } s$.

These assumptions, which also require A1-A2, are obviously weak: they are there only to make sure that $\mathcal{E}_\beta$ and $\mathcal{E}^u$ exist, are non-empty (by lower semicontinuity of rate functions), and so can be compared. The problem of identifying classes of Hamiltonians for which these assumptions are verified is a much more difficult problem, which we do not address here. For long-range systems, this is a completely open problem.

### A. Canonical ensemble as a mixture of microcanonical ensembles

The microcanonical and canonical ensembles are based on two obviously different probability measures on $\Lambda_N$: the former assigns a non-zero measure to microstates of a given energy, whereas the latter assigns a non-zero measure to all $\omega \in \Lambda_N$. However, the two are fundamentally related, in that the canonical ensemble can be expressed as a probabilistic mixture of microcanonical ensembles. This observation is the key insight needed to obtain general results about macrostate equivalence.

To explain what we mean by a mixture of ensembles, consider the canonical probability measure $P_{N,\beta}(d\omega)$ defined in (1). Since this measure depends only the product $\beta H_N(\omega)$, it is clear that all microstates having the same energy have the same probability. As a result, the conditional probability measure $P_{N,\beta}(d\omega|h_N \in u)$ obtained by conditioning $P_{N,\beta}(d\omega)$ on the set of microstates such that $h_N(\omega) \in u$ must be uniform over that constrained set of microstates. This is obvious from the definition of $P_{N,\beta}$:

$$P_{N,\beta}(d\omega|h_N \in du) = \frac{P_{N,\beta}(d\omega, h_N \in du)}{P_{N,\beta}(h_N \in du)} = \frac{e^{-\beta N u}}{Z_N(\beta) P_{N,\beta}(h_N \in du)} dP_N(\omega),$$

which is proportional to $P_N^u(d\omega)$, as defined in (8). Since both probability measures must be normalized, we must then have

$$P_{N,\beta}(d\omega|h_N \in du) = P^u_N(d\omega)$$

(33)
for all $\omega \in \Lambda_N$. Incidentally, normalizing (32) explicitly yields
\[ P_{N,\beta}\{h_N \in du\} = \frac{e^{-\beta N u}}{Z_N(\beta)} P_N\{h_N \in du\} \] (34)
which is the basis of Proposition 3.

With the basic equality (33), it now follows from Bayes’ Theorem,
\[ P_{N,\beta}(d\omega) = \int \nabla P_{N,\beta}\{d\omega| h_N = u\} P_{N,\beta}\{h_N \in du\}, \] (35)
that
\[ P_{N,\beta}(d\omega) = \int \nabla P^u_N(d\omega) P_{N,\beta}\{h_N \in du\}. \] (36)
Extending this result to an arbitrary macrostate $M_N$ then yields
\[ P_{N,\beta}\{M_N \in A\} = \int \nabla P^u_N\{M_N \in A\} P_{N,\beta}\{h_N \in du\} \] (37)
for any measurable set $A$. Hence, we see that the canonical measure on both $\Lambda_N$ and $\mathcal{M}$ is a superposition of microcanonical measures weighted by the canonical mean energy distribution $P_{N,\beta}(du) = P_{N,\beta}\{h_N \in du\}$. It is this superposition, which is exact for any $N < \infty$, that we refer to as a probabilistic mixture of microcanonical ensembles.

In what follows, we use this result to relate the equilibrium states of the microcanonical ensembles to those of the canonical ensemble. Already, it should be clear that (37) implies a link between the different LDPs of these ensembles: we know from Proposition 3 that $P_{N,\beta}(du)$ satisfies the LDP with rate function $J(\beta)$, whereas $P_{N,\beta}\{M_N \in A\}$ and $P^u_N\{M_N \in A\}$ both satisfy the LDP by assumption. Exploiting the exponential form of these LDPs in the mixture integral (37), we then obtain the following result:

**Proposition 5.** Under Assumptions A1-A4,
\[ I(\beta) = \inf_{m \in \mathcal{M}} \{I^u(m) + J(\beta)(u)\} \] (38)
for any $m \in \mathcal{M}$ and $\beta \in \text{dom } \varphi$. The minimizers in this formula are necessarily in $\text{dom } s$.

This result was announced in [8] together with a formal proof giving the basic ideas behind it. A rigorous proof, which follows again from Varadhan’s Theorem, is presented next.

**Proof.** Considering for the set $A$ an infinitesimal interval or ball $dm$ in the probabilistic mixture (37) gives
\[ P_{N,\beta}\{M_N \in dm\} = \int \nabla P^u_N\{M_N \in dm\} P_{N,\beta}(du). \] (39)
By assumption, $M_N$ satisfies the LDP in the microcanonical ensemble with rate function $I^u$, while $h_N$ satisfies the LDP in the canonical ensemble with rate function $J(\beta)$. The product $P^u_N\{M_N \in dm\} P_{N,\beta}(du)$ must therefore satisfies the LDP with rate function $I^u + J(\beta)$. Applying Varadhan’s Theorem with $F = 0$, which is equivalent to the Laplace principle [49], we then obtain
\[ \lim_{N \to \infty} -\frac{1}{N} \ln \int \nabla P^u_N\{M_N \in dm\} P_{N,\beta}(du) = \inf_{\mathcal{M}} \{I^u(m) + J(\beta)(u)\}. \] (40)
This function must correspond to the rate function $I(\beta)$ of $P_{N,\beta}(dm)$ since rate functions are unique; see [26]. Moreover, the infimum over $\mathbb{R}$ can be restricted to $\text{dom } s$, since $I^u$ and $J(\beta)$ are by assumption infinite outside $\text{dom } s$. \qed
The minimization problem of Proposition 5 relates the fluctuations of the canonical and microcanonical ensembles. The result is interesting physically as it shows that these fluctuations strongly depend on the system and macrostate considered, and cannot be the same in general.\(^5\) For this reason, one cannot speak of the equivalence of ensembles in terms of macrostate fluctuations – only in terms of their equilibrium macrostates.

**B. Equivalence results**

Since rate functions are nonnegative, \(I_\beta(m)\) vanishes if and only if both \(I^u(m)\) and \(J_\beta(u)\) vanish in (38). This implies that the equilibrium values of \(M_N\) in the canonical ensemble must correspond to the equilibrium values of \(M_N\) in the microcanonical ensemble for all mean energies realized at equilibrium in the canonical ensemble. This is stated in the next result.

**Proposition 6.** Under Assumptions A1-A4:

\[
\mathcal{E}_\beta = \bigcup_{u \in \mathcal{U}_\beta} \mathcal{E}^u. \tag{41}
\]

Proof. Take \(m \in \mathcal{E}_\beta\). Then \(I_\beta(m) = 0\) by definition of \(\mathcal{E}_\beta\), so that, by Proposition 5,

\[
0 = \inf_u \{I^u(m_\beta) + J_\beta(u)\}. \tag{42}
\]

Since rate function are nonnegative, this implies that there exists \(u \in \text{dom } s\) such that \(I^u(m) = 0\), implying \(m \in \mathcal{E}^u\), and \(J_\beta(u) = 0\), implying \(u \in \mathcal{U}_\beta\). As this is true for all elements of \(\mathcal{E}_\beta\), we obtain

\[
\mathcal{E}_\beta \subseteq \bigcup_{u \in \mathcal{U}_\beta} \mathcal{E}^u = \mathcal{E}\mathcal{U}_\beta. \tag{43}
\]

We now prove the reverse inclusion. Consider \(u \in \mathcal{E}_\beta\) for which \(J_\beta(u) = 0\) and \(m \in \mathcal{E}^u\) for which \(I^u(m) = 0\). Then the result of Proposition 5 gives \(I_\beta(m) = 0\), so that \(m \in \mathcal{E}_\beta\). As this is true for all \(m \in \mathcal{E}^u\) with \(u \in \mathcal{U}_\beta\), we obtain

\[
\bigcup_{u \in \mathcal{U}_\beta} \mathcal{E}^u \subseteq \mathcal{E}_\beta. \tag{44}
\]

Therefore, the two sides are equal.

The covering result (41) shows that the canonical equilibrium macrostates are always realized in the microcanonical ensemble for some value(s) of \(h_N\). To determine when the converse is true, that is, when \(\mathcal{E}^u\) coincides with \(\mathcal{E}_\beta\) for some \(\beta\), we next use Proposition 4 to determine whether \(\mathcal{U}_\beta\) has one element, many elements, or is empty. This leads us to the following result about macrostate equivalence, which is the main result of this section.

**Theorem 7 (Macrostate equivalence).** Assume A1-A4. Then

(a) Strict equivalence: If \(s\) is strictly concave at \(u\), then \(\mathcal{E}^u = \mathcal{E}_\beta\) for some \(\beta \in \mathbb{R}\);

(b) Nonequivalence: If \(s\) is nonconcave at \(u\), then \(\mathcal{E}^u \neq \mathcal{E}_\beta\) for all \(\beta \in \mathbb{R}\);

(c) Partial equivalence: If \(s\) is concave but not strictly concave at \(u\), then \(\mathcal{E}^u \subseteq \mathcal{E}_\beta\).

\(^5\) Consider the obvious example of the mean energy \(h_N\), which does not fluctuate in the microcanonical ensemble but does in the canonical ensemble.
Proof. Case (a): This follows from the result stated after Proposition 4 that, if \( s \) is strictly concave at \( u \), then \( \mathcal{U}_\beta \) is the singleton set \( \{ u \} \) for \( \beta \in \partial s(u) \). From the covering result (41), we then obtain \( \mathcal{E}_\beta = \mathcal{E}^u \) for all \( \beta \in \partial s(u) \).

Case (b): The assumption that \( s \) is nonconcave at \( u \) implies also from Proposition 4 that \( u \notin \mathcal{U}_\beta \) for all \( \beta \in \mathbb{R} \). Let \( m^u \in \mathcal{E}^u \) and assume that \( m^u \in \mathcal{E}_\beta \) for some \( \beta \in \mathbb{R} \). Then using (41), or equivalently the relation (38), we must have \( u \in \mathcal{U}_\beta \), which contradicts the result that \( u \notin \mathcal{U}_\beta \). Since this contradiction is reached for any \( m^u \in \mathcal{E}^u \) and any \( \beta \in \mathbb{R} \), we conclude that \( \mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset \) for all \( \beta \in \mathbb{R} \), a result which we write as \( \mathcal{E}^u \neq \mathcal{E}_\beta \) for all \( \beta \).

Case (c): If \( s \) is concave at \( u \) but non-strictly concave, then \( u \in \mathcal{U}_\beta \) for \( \beta \in \partial s(u) \), but \( \mathcal{U}_\beta \) is no longer a singleton: by definition of non-strict concave points, there must exist at least one \( v \neq u \) for which \( \beta \in \partial s(v) \) and so for which \( v \in \mathcal{U}_\beta \). In this case, the covering result (41) involves at least two sets, which implies that \( \mathcal{E}^u \subseteq \mathcal{E}_\beta \) in general. If, as in most systems, \( \mathcal{E}^u \neq \mathcal{E}^u \), then this inclusion is strengthened to \( \mathcal{E}^u \subseteq \mathcal{E}_\beta \), that is, \( \mathcal{E}^u \) is a proper subset of \( \mathcal{E}_\beta \).

Cases (a) and (b) have clear interpretations in terms of Gibbs’s reasoning [3]. In case (a), the microcanonical and canonical ensemble are equivalent at the macrostate level because the mean energy of the latter ensemble is concentrated on a single value corresponding to \( u \) for \( \beta \in \partial s(u) \). For \( s(u) \) differentiable, \( \beta \) and \( u \) are then related by the standard thermodynamic relation \( \beta = s'(u) \), as already mentioned after Proposition 4. In case (b), we have nonequivalence because \( u \) is never realized in the canonical ensemble as an equilibrium mean energy, so that the set \( \mathcal{E}^u \), which can be realized in the microcanonical ensemble by fixing \( h_N = u \), cannot be realized in the canonical ensemble by varying \( \beta \) instead.

Case (c) is more subtle: it corresponds to the case where \( \mathcal{U}_\beta \) has more than one element, and so to a case where the canonical ensemble has many coexisting equilibrium mean energies, giving rise at the macrostate level to many coexisting equilibrium macrostates, called phases in statistical mechanics. The next result, which follows from the theorem above, shows that this case naturally arises whenever \( s(u) \) is nonconcave or has some linear parts.

**Corollary 8.** If \( s(u) \) is nonconcave or is non-strictly concave, then there exists \( \beta_c \in \mathbb{R} \) such that \( \mathcal{E}_{\beta_c} \) is composed of two or more microcanonical sets \( \mathcal{E}^u \) with \( u \in \mathcal{U}_{\beta_c} \), i.e., \( \mathcal{E}_{\beta_c} = \mathcal{E}^u \cup \mathcal{E}^u' \cup \cdots \), with \( u, u', \ldots \in \mathcal{U}_{\beta_c} \).

Figure 2 illustrates the case, commonly encountered in long-range systems, in which two phases appear at some critical inverse temperature \( \beta_c \) due to the nonconcavity of \( s(u) \) over some interval \( (u_l, u_h) \), leading to \( \mathcal{U}_{\beta_c} = \{ u_l, u_h \} \) and \( \mathcal{E}_{\beta_c} = \mathcal{E}^u \cup \mathcal{E}^h \). The relation between the nonconcave region of \( s(u) \) and the nondifferentiability of \( \varphi(\beta) \) is illustrated in Fig. 2. If \( s \) has a linear or affine parts over \( (u_l, u_h) \), then a similar physical interpretation involving a first-order phase transition also applies, but with discrete phases replaced by a continuum of phases [29].

**C. Remarks**

Proposition 6 and Theorem 7 above are generalizations of two results obtained in [4]. Here we have derived these results by assuming that \( \mathcal{E}_\beta \) and \( \mathcal{E}^u \) exist and have used the idea of probabilistic mixture of microcanonical ensembles to relate these sets. In [4], Ellis, Haven, Turkington use a different approach: they explicitly construct the rate functions \( I_\beta \) and \( I^u \) and then relate with these \( \mathcal{E}_\beta \) and \( \mathcal{E}^u \). In doing so, they assume the following:

1. There exists a function \( \tilde{h} : \mathcal{M} \to \mathbb{R} \) such that

\[
\lim_{N \to \infty} \left| h_N(\omega) - \tilde{h}(M_N(\omega)) \right| = 0
\] (45)
uniformly over all $\omega \in \Lambda_N$. In this case, we say that $h_N$ admits an energy representation function in terms of $M_N$.

2. $M_N$ satisfies the LDP with respect to the prior measure $P_N$.

The explicit expressions of $I_\beta$ and $I^u$ obtained under these assumptions can be found in Theorem 2.4 and Theorem 3.2 of [4], respectively. In terms of $h$, our Theorem 6 then corresponds to Theorem 4.10 of [4], which has the form

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

while our Theorem 7 corresponds essentially to Theorem 4.4 of [4]. The difference between the two sets of results is that $\mathcal{U}_\beta$ is replaced by $\tilde{h}(\mathcal{E}_\beta)$.

It can be shown using the so-called contraction principle of large deviation theory that if $\tilde{h}$ exists, then $\mathcal{U}_\beta = \tilde{h}(\mathcal{E}_\beta)$ and the covering results of (41) and (46) are equivalent. What we have shown here is that (41) does not rely on the existence $\tilde{h}$ and $I$ to hold. Consequently, the existence of these functions is a sufficient but not a necessary condition for macrostate equivalence to be directly related to thermodynamic equivalence. This relationship is only based on the existence of thermodynamic functions and equilibrium macrostates and is, as such, a general result of statistical mechanics.

This generalization is important as there are many physical systems and observables of interest that do not admit an energy representation function. An obvious example is the magnetization of spin systems which can be used to construct $\tilde{h}$ only for non-interacting and mean-field models. Similarly, the empirical measure can be used as a ‘representation’ macrostate only for non-interacting models, mean-field models, and some long-range systems (see [4, 16, 41] for examples) which, crucially, do not include gravitational systems.

For other models, the only macrostates for which $\tilde{h}$ exists in general is the infinite-dimensional empirical process, whose large deviations are known from the so-called level-3 LDP involving the relative entropy; see [26–28] for details. For 1D systems with nearest-neighbor interactions, one can contract the empirical process down to the pair empirical measure to obtain $\tilde{h}$ [50], but this is not possible for short-range systems defined on higher-dimensional lattices, such as the 2D Ising model.

V. MEASURE EQUIVALENCE

The last level of ensemble equivalence that we discuss is concerned with the thermodynamic-limit convergence of $P_{N,\beta}(d\omega)$ and $P_N^u(d\omega)$ at the microstate level. This equivalence is suggested mathematically by the fact that macrostate equivalence implies in the strict concave case the mean convergence equality

$$\lim_{N \to \infty} E_{P_{N,\beta}}[M_N] = \lim_{N \to \infty} E_{P_N^u}[M_N]$$

for any macrostate satisfying Assumptions A1-A4. Falling to have $P_{N,\beta} = P_N^u$, this suggests that $P_{N,\beta}$ must get close to $P_N^u$ as $N \to \infty$ relative to a scale or ‘metric’ that ‘sees’ a difference between these measures only when its affects their large deviation concentration.

In this section, we consider two such ‘metrics’, the specific relative entropy and specific action, and show that measure equivalence holds in both cases when $s(u)$ is concave, and thus when there is thermodynamic and macrostate equivalence. Our results for the specific relative entropy recover previous results obtained by Lewis, Pfister and Sullivan [5–7]. New and stronger results are obtained for the specific action, which point interestingly to a general form of the asymptotic equipartition property studied in information theory and the theory of ergodic processes.
A. Relative entropy

Let \( P \) and \( Q \) be two probability measures defined on a space \( \mathcal{X} \), and assume that \( P \) is absolutely continuous with respect to \( Q \) (denoted by \( P \ll Q \)). The relative entropy of \( P \) with respect to \( Q \) is defined as

\[
D(P||Q) = \int_{\mathcal{X}} dP(\omega) \ln \frac{dP}{dQ}(\omega),
\]

where \( dP/dQ \) denotes the Radon-Nikodym derivative of \( P \) with respect to \( Q \). The relative entropy is also called the information gain [5–7], the information divergence [51–53] or Kullback-Leibler distance [31]. Strictly speaking, \( D(P||Q) \) is not a distance, since it is not symmetric and does not satisfy the triangle inequality. However, \( D(P||Q) \geq 0 \) with equality if and only if \( P = Q \) almost everywhere. Therefore, it can be interpreted as a generalized metric inducing a well-defined topology on the space of distributions. Moreover, it is known that \( D(P||Q) \) is an upper bound on the total variation norm:

\[
d_{TV}(P,Q) = \frac{1}{2} \int_{\mathcal{X}} |dQ - dP| \leq \sqrt{D(P||Q)}; \tag{49}
\]

see, e.g., Proposition 10.3 of [7].

For the microcanonical and canonical ensembles, we have \( P^u_N \ll P_{N,\beta} \) but \( P_{N,\beta} \not\ll P^u_N \), since \( P^u_N \) is a restriction of \( P_{N,\beta} \), so that the correct relative entropy to consider is

\[
D(P^u_N||P_{N,\beta}) = \int_{\Lambda_N} dP^u_N(\omega) \ln \frac{dP^u_N}{dP_{N,\beta}}(\omega). \tag{50}
\]

From this, we define the specific relative entropy by the limit

\[
d^u_\beta = \lim_{N \to \infty} \frac{1}{N} D(P^u_N||P_{N,\beta}). \tag{51}
\]

This quantity, when it exists, is also called the relative entropy rate, the specific information gain [5–7] or divergence rate [54]. We use it next to give a first definition of measure equivalence found in [5–7].

**Definition 9 (Measure equivalence I).** The canonical and microcanonical ensembles are said to be equivalent at the measure level, in the specific relative entropy sense, if \( d^u_\beta = 0 \).

Lewis, Pfister and Sullivan [5–7] use a different terminology borrowed from the work of Csiszár [51–53] on conditional limit theorems: they say that \( P^u_N \) and \( P_{N,\beta} \) are asymptotically information-divergence null, or I-null for short, when \( d^u_\beta = 0 \). It is clear from this definition that \( d^u_\beta = 0 \) does not imply \( P^u_N(\omega) = P_{N,\beta}(\omega) \) for almost all \( \omega \in \Lambda_N \); it only implies that \( D(P^u_N||P_{N,\beta}) \) grows slower than \( N \), and consequently that the total variation \( d_{TV}(P^u_N,P_{N,\beta}) \) grows slower than \( \sqrt{N} \) as \( N \to \infty \). This, as shown next, is a necessary and sufficient condition for measure equivalence to coincide with thermodynamic and macrostate equivalence.

**Theorem 10 (Measure equivalence I).** Under Assumptions A1-A4, \( d^u_\beta = 0 \) if and only if \( \beta \in \partial s(u) \). Therefore, except possibly at boundary points of \( \text{dom} s \), measure equivalence holds in the specific relative entropy sense if and only if thermodynamic equivalence holds.

**Proof.** The result follows simply by writing the explicit expression of the Radon-Nikodym derivative of \( P^u_N \) with respect to \( P_{N,\beta} \):

\[
\frac{dP^u_N}{dP_{N,\beta}}(\omega) = \frac{e^{N\beta h_N(\omega)}Z_N(\beta)}{P_N\{h_N \in du\}} 1_{du}(h_N(\omega)). \tag{52}
\]
Inserting this expression into $D(P^u_N||P_{N,\beta})$ and taking the trivial expectation with respect to $P^u_N$ yields

$$d^u_\beta = \beta u - s(u) - \varphi(\beta) = J_\beta(u), \quad (53)$$

where we have also used the limits (16) and (18) defining $\varphi(\beta)$ and $s(u)$, respectively. From this result, the statement of the theorem then follows using Proposition 4 relating the zeros of the canonical rate function $J_\beta(u)$ and the concave points of the microcanonical entropy $s(u)$.

Part of this theorem can be found in Theorem 5.1 (see also Lemma 5.1) of [6] and is applied in that work to lattice spin systems, including the mean-field Curie-Weiss model and the 2D Ising model. For related results obtained in the context of 1D and 2D lattice gases, see [42–44]. Finally, for an application to the nonequilibrium zero-range process, see [55].

**B. Radon-Nikodym derivative**

We now consider the random variable

$$R^u_{N,\beta}(\omega) = \frac{1}{N} \ln \frac{dP^u_N}{dP_{N,\beta}}(\omega), \quad (54)$$

which depends on the two parameters $\beta$ and $u$. We call this random variable the *specific action* following the definition of a similar quantity for Markov processes [29].

The result proved in Theorem 10 is about the convergence in mean of $R^u_{N,\beta}$ with respect to $P^u_N$. Here we prove a stronger convergence for $R^u_{N,\beta}$ using convergence in probability with respect to both $P^u_N$ and $P_{N,\beta}$, which expresses the concentration of this random variable with respect to both measures. This is basis of our second definition of measure equivalence stated next, which implies the previous one based on the specific relative entropy.

**Definition 11 (Measure equivalence II).** The canonical and microcanonical ensembles are said to be equivalent at the measure level, in the specific action sense, if

$$\lim_{N \to \infty} R^u_{N,\beta}(\omega) = 0 \quad (55)$$

almost everywhere with respect to both $P^u_N$ and $P_{N,\beta}$.

This definition can be expressed differently by saying that the two ensembles are equivalent at the measure level if $P^u_N$ and $P_{N,\beta}$ are logarithmically equivalent almost everywhere with respect to these measures, that is, $P^u_N(d\omega) \asymp P_{N,\beta}(d\omega)$ or, equivalently,

$$\frac{dP^u_N}{dP_{N,\beta}}(\omega) \asymp 1 \quad (56)$$

almost everywhere with respect to $P^u_N$ and $P_{N,\beta}$. This is a natural definition given that the logarithmic equivalence is the defining scale of large deviation theory in general, and thermodynamic LDPs in particular. Our final result shows that this definition is also related to the concavity of the entropy, which means that it relates physically to all the definitions of equivalence studied before. The probabilistic interpretation of this new result, which can actually be extended to general measures beyond the microcanonical and canonical ensembles, is discussed in the next subsection.

**Theorem 12 (Measure equivalence II).** Assume A1-A4. Then

---

6 H. Touchette. In preparation
(a) Strict equivalence: If \( s \) is strictly concave at \( u \), then measure equivalence holds in the specific action sense for all \( \beta \in \partial s(u) \);

(b) Nonequivalence: If \( s \) is nonconcave at \( u \), then measure equivalence does not hold in the specific action sense for any \( \beta \in \mathbb{R} \);

(c) Partial equivalence: If \( s \) is concave at \( u \) but not strictly concave, then

\[
\lim_{N \to \infty} R_{N,\beta}^u(\omega) = 0
\]

\( P_N^u \)-almost everywhere for all \( \beta \in \partial s(u) \), but the same limit is in general undefined with respect to \( P_{N,\beta} \).

**Proof.** Recall that \( R_{N,\beta}^u \) is a random variable that depends on the two parameters \( \beta \in \text{dom } \varphi \) and \( u \in \text{dom } s \). From the explicit expression of the Radon-Nikodym derivative found in (52), we have in fact

\[
r_{\beta}^u(\omega) = \lim_{N \to \infty} \frac{1}{N} \ln \frac{dP_N^u}{dP_N(\omega)} = \begin{cases} J(\beta(u)) & h_N(\omega) \in du \\ -\infty & \text{otherwise.} \end{cases}
\]

(58)

Thus the limit \( r_{\beta}^u(\omega) \) is also a random variable, and since it depends only on \( h_N(\omega) \), it inherits by the contraction principle the LDP of \( h_N \) with respect to \( P_N^u \) or \( P_{N,\beta} \), which means that we can describe its concentration in terms of these LDPs.

To prove the different cases of the theorem in a complete way, we will distinguish between the parameters \( u \) and \( \beta \) of \( r_{\beta}^u \) and those of the microcanonical and canonical ensemble, which we denote instead by \( u' \in \text{dom } s \) and \( \beta' \in \text{dom } \varphi \), respectively. Thus, we want to study the concentration of \( r_{\beta}^u \) with respect to \( P_{N}^{u'} \) and \( P_{N,\beta'} \).

We begin with the microcanonical ensemble. Clearly, \( h_N(\omega) \in du' \) with probability 1 with respect to \( P_{N}^{u'} \), so that

\[
r_{\beta}^u(\omega) = \begin{cases} J(\beta(u)) & u' = u \\ -\infty & \text{otherwise} \end{cases}
\]

(59)

for all \( \omega \) relative to \( P_{N}^{u'} \). Moreover, we know from Proposition 4 that \( J(\beta(u)) \) = 0 if and only if \( \beta \in \partial s(u) \). Therefore, \( r_{\beta}^u \) = 0 relative to \( P_{N}^{u'} \) if \( \beta \in \partial s(u) \) and \( r_{\beta}^u \neq 0 \) otherwise, proving the microcanonical half of the theorem.

For the canonical ensemble, the concentration is more involved and must be treated following the three different cases considered:

(a) \( s \) is strictly concave at \( u \): In this case, we know by Proposition 4 that \( J(\beta(u)) \) = 0 and \( U_{\beta} = \{ u \} \) for all \( \beta \in \partial s(u) \). This means that \( u \) is the unique equilibrium value of \( h_N \) with respect to \( P_{N,\beta} \), so that

\[
\lim_{N \to \infty} P_{N,\beta}\{ h_N \in du \} = 1.
\]

(60)

Thus, although \( r_{\beta}^u(\omega) \) diverges for \( \omega \) such that \( h_N \notin du \), these microstates have zero measure with respect to \( P_{N,\beta} \), so that \( r_{\beta}^u = 0 \) almost everywhere with respect to \( P_{N,\beta} \). This also holds with respect to \( P_{N,\beta'} \) if \( \beta' \in \partial s(u) \) and \( \beta \in \partial s(u) \) but \( \beta' \neq \beta \) because in that case \( h_N \) still concentrates on \( u \) with respect to \( P_{N,\beta'} \). However, if \( \beta' \notin \partial s(u) \), then \( h_N \) will not concentrate on \( u \), implying \( r_{\beta}^u(\omega) = -\infty \).
(b) \( s \) is nonconcave at \( u \): In this case, we also know from Proposition 4 that \( u \notin \mathcal{U}_\beta \) for all \( \beta \in \mathbb{R} \), so that \( J_\beta(u) > 0 \) for all \( \beta \in \mathbb{R} \). This directly implies \( r_\beta^u \neq 0 \) with respect to \( P_{N,\beta'} \) with any \( \beta' \in \mathbb{R} \) including \( \beta' = \beta \). To be more precise, we must have in fact \( r_\beta^u(\omega) = -\infty \) almost surely with respect to \( P_{N,\beta'} \) for any \( \beta' \in \mathbb{R} \), since \( h_N \) does not concentrate on \( u \) for any \( \beta' \in \mathbb{R} \).

(c) \( s \) is non-strictly concave at \( u \): In this case, Proposition 4 implies that \( J_\beta(u) = 0 \) for \( \beta \in \partial s(u) \); however, although \( u \in \mathcal{U}_\beta \), \( u \) is not the only element of \( \mathcal{U}_\beta \), which means that the concentration point of \( h_N \) with respect to \( P_{N,\beta'} \) with \( \beta' = \beta \) is in general unknown: it can be \( u \), in which case \( r_\beta^u(\omega) = 0 \) as (a), or it can be a different mean energy value, in which case \( r_\beta^u(\omega) = -\infty \) as in (b).

The indefinite result in the last case is a consequence again of the phase coexistence arising when \( s(u) \) is non-strictly concave. If we make the additional assumption that \( u \in \mathcal{U}_\beta \) is a concentration point of \( h_N \) with respect to \( P_{N,\beta} \), as discussed in Subsection II D, then we recover measure equivalence as in case (a). Consequently, under this additional condition, measure equivalence holds in the specific action sense if and only if \( s(u) \) is concave (strictly or non-strictly) and, therefore, if and only if macrostate and thermodynamic equivalence holds (except possibly at boundary points of dom \( s \)).

\[
\text{C. Remarks}
\]

The roles of \( P_{N,\beta} \) and \( P_N^u \) can be reversed in all the results of this section to study the convergence of \( dP_{N,\beta}/dP_N^u \) instead of \( dP_N^u/dP_{N,\beta} \). Indeed, although the former Radon-Nikodym derivative diverges for some \( \omega \in \Lambda_N \) because \( P_N^u \gg P_{N,\beta} \), these divergencies happen to be exactly cancelled when measure equivalence holds by the fact that \( P_{N,\beta} \) concentrates towards \( P_N^u \) in the thermodynamic limit, which implies that these divergencies have zero measure in the canonical ensemble. From this, one can re-derive results similar to Theorems 10 and 12 with \( P_{N,\beta} \) and \( P_N^u \) interchanged in the definitions of the relative entropy and Radon-Nikodym derivative.

The same equivalence results can be obtained, interestingly, not by calculating the explicit expression of the Radon-Nikodym derivative entering in both the relative entropy and the specific action, as done above, but by appealing to the macrostate level of equivalence and the probabilistic mixture of microcanonical ensembles. In fact, there are three other ways whereby these results can be obtained from the macrostate level.

The first simply follows by noticing that the specific action \( R_{N,\beta} \) defined in (54) is a macrostate for which our results of Sec. IV apply. The LDP of this macrostate with respect to \( P_N^u \) is trivial, while its LDP with respect to \( P_{N,\beta} \) follows by contraction from the LDP of \( h_N \) in the canonical ensemble, as mentioned in the proof of Theorem 12. With these LDPs, we can then apply Theorem 7 to obtain Theorem 12, which clearly demonstrates that measure equivalence is directly related to macrostate equivalence.

The second way follows by considering the empirical process, mentioned before, and by proving that the equilibrium points of this particular macrostate converge to the ensemble measures in the thermodynamic limit. This approach is followed in [42–48] and is also used for proving the equivalence of Gibbs measures (or Gibbs random fields) and translationally invariant measures in the thermodynamic or infinite-volume limit [56–58].

Finally, measure equivalence can be understood by considering the integral (36), which expresses the mixture of microcanonical ensembles at the microstate level. Because of the LDP of \( h_N \) with respect to \( P_{N,\beta} \), this integral is a Laplace integral that concentrates in an exponential way as \( N \to \infty \) on the set \( \mathcal{U}_\beta \) of canonical equilibrium values of \( h_N \), as explain before. In the particular
case where $U\beta$ is a singleton $\{u\beta\}$, we can then approximate this integral on the exponential scale to formally write

$$P_{N,\beta}(d\omega) \propto P_{u\beta}^N(d\omega),$$  \hspace{0.5cm} (61)

which recovers our definition of measure equivalence based on the specific action and the logarithmic equivalence. This means in terms of microstates that, although $P_{N,\beta}(d\omega)$ varies in general from one microstate to another according to their energy, most microstates with respect to $P_{N,\beta}$ are roughly equiprobable, as in the microcanonical ensemble, because most of these microstates have a constant energy $u\beta$ with respect to $P_{N,\beta}$.

In information theory, this equiprobability property of random sequences (here microstates) is called the asymptotic equipartition property (AEP) and the set of sequences (viz., microstates) having this property is called the typical or typicality set [31]. In the standard case where the prior $P_N$ is chosen to be uniform, this property is translated as follows. Let $\Lambda_{N,u}$ denote the subset of microstates having a mean energy $h_N(\omega)$ close to $u$, that is,

$$\Lambda_{N,u} = \{\omega \in \Lambda_N : h_N(\omega) \in du\}. \hspace{0.5cm} (62)$$

Then assuming strict equivalence, we have

$$P_{N,\beta}\{h_N \in du\beta\} = P_{N,\beta}\{\Lambda_{N,u\beta}\} \propto 1, \hspace{0.5cm} (63)$$

for some unique $u\beta$, which means that $\Lambda_{N,u\beta}$ is typical in the canonical ensemble. Moreover, since all microstates $\omega$ such that $H_N(\omega) = Nu\beta + o(N)$ eventually falls in $\Lambda_{N,u\beta}$ in the thermodynamic limit, they must be asymptotically equiprobable,

$$P_{N,\beta}(d\omega) \propto e^{-\frac{\beta Nu\beta}{Z_N(\beta)}}, \hspace{0.5cm} (64)$$

which implies that the volume of these microstates must approximately be given by

$$|\Lambda_{N,u\beta}| \propto e^{\frac{\beta Nu\beta}{Z_N(\beta)}}. \hspace{0.5cm} (65)$$

This general form of AEP follows from our results for any $N$-particle system satisfying assumptions A1-A2, that is, any system with a well-defined thermodynamic-limit free energy and entropy.

VI. OTHER ENSEMBLES

As mentioned in the introduction, our discussion of ensemble equivalence centered on the canonical and microcanonical ensembles to be specific and to simplify the notations. In this section, we briefly discuss how these results are generalized to ensembles other than the canonical and microcanonical. By way of example, we start with the equivalence of the canonical and grand-canonical ensembles, and then point out how more general dual ensembles can be treated, following results of [4]. We discuss finally the case of ensembles defined on random paths of stochastic processes rather than static (spatial) configurations.

A. Canonical and grand-canonical ensembles

Denote by $H_V$ the energy of a system with volume $V$ and by $N_V$ its particle number. The grand-canonical ensemble associated with this system is defined by the probability measure

$$P_{V,\beta,\mu}(d\omega) = \frac{e^{-\beta(H_V(\omega)-\mu N_V(\omega))}}{Z_V(\beta,\mu)} P_V(d\omega), \hspace{0.5cm} (66)$$
where
\[
Z_V(\beta, \mu) = \int_{\Lambda_V} e^{-\beta (H_V(\omega) - \mu N_V(\omega))} P_V(d\omega)
\]  
(67)
is the grand-canonical partition function and \( P_V(d\omega) \) is the prior measure on the space \( \Lambda_V \) of microstates at volume \( V \). This ensembles extends, as is well known, the canonical ensemble by allowing fluctuations of the particle number \( N_V(\omega) \) in a system of fixed volume \( V \). In terms of the particle density \( r_V(\omega) = N_V(\omega)/V \), the canonical ensemble with fixed density \( r_V = \rho \) is then defined as
\[
P_{\rho V, \beta}(d\omega) = \frac{e^{-\beta H_V(\omega)}}{W_{\rho V}(\beta)} 1_{dp}(r_N(\omega)) P_V(d\omega),
\]  
(68)where \( Z_{\rho V}(\beta) \) is a normalization factor given by
\[
Z_{\rho V}(\beta) = \int_{\Lambda_N} e^{-\beta H_V(\omega)} 1_{dp}(r_N(\omega)) P_V(d\omega) = E_{P_V} \left[ e^{-\beta H_V} 1_{dp}(r_N) \right]
\]  
(69)and, as before, \( dp \) is some infinitesimal interval centered at \( \rho \). The superscripts and subscripts in these expressions follow the notations of [4] and denote either a microcanonical-like constraint (superscript \( \rho \)) or a canonical-like exponential (subscript \( \mu \)) involving a Lagrange parameter conjugated to the constraint.

Comparing these ensembles with the definitions of the original canonical and microcanonical ensembles, it is easy to see that the grand-canonical ensemble conditioned on a fixed value of the particle density \( r_V = \rho \) is equivalent to the canonical ensemble, which means that the former is a probabilistic mixture of the latter, with \( r_N \) playing the role of the ‘mixing’ random variable. Following our discussion of macrostate equivalence, the probability measure of \( r_N \) that determines this mixture is the one obtained in the non-constrained ensemble, that is, the grand-canonical ensemble. Assuming that this measure satisfies the LDP,
\[
P_{\rho V, \beta, \mu} \{ r_N \in dp \} \asymp e^{-V J_{\rho V, \beta, \mu}(\rho)}
\]  
(70)in the thermodynamic limit \( V \to \infty \) with \( \rho = r_V/V \) constant, we find from the probabilistic mixture that the rate function \( J_{\beta, \mu}(\rho) \) is given by
\[
J_{\beta, \mu}(\rho) = -\beta \mu \rho - s_\beta(\rho) - \varphi(\beta, \mu)
\]  
(71)where
\[
\varphi(\beta, \mu) = \lim_{V \to \infty} \frac{1}{V} \ln Z_V(\beta, \mu)
\]  
(72)is the grand-canonical free energy, or grand potential, and
\[
s_\beta(\rho) = \lim_{V \to \infty} \frac{1}{V} \ln Z_{\rho V}(\beta)
\]  
(73)is the thermodynamic potential associated with the canonical ensemble with fixed Lagrange parameter \( \beta \) and fixed constraint \( \rho \). The grand-canonical potential \( \varphi(\beta, \mu) \) obviously plays the role of \( \varphi(\beta) \) while \( s_\beta(\rho) \) takes the role of \( s(u) \). Therefore, what determines the equivalence of the grand-canonical and canonical ensemble, with respect to \( r_N \), is the concavity of \( s_\beta(\rho) \) as a function of \( \rho \). In other words, all our results involving \( s(u) \) generalize to these ensembles by considering \( s_\beta(\rho) \) instead.
To see this more clearly, rewrite the grand-canonical and canonical measures as

\[ P_{V,\beta,\mu}(d\omega) = \frac{e^{-\gamma VrV(\omega)}}{Z_V(\beta, \mu)} Q_{V,\beta}(d\omega), \tag{74} \]

and

\[ P_{V,\rho}(d\omega) = \frac{1}{d\rho(\rho)} W_{V}(\beta) P_{V}(d\omega), \tag{75} \]

respectively, by defining \( \gamma = -\beta \mu \) and the positive but non-normalized measure

\[ Q_{V,\beta}(d\omega) = e^{-\beta H_V(\omega)} P_V(d\omega). \tag{76} \]

Then these ensembles take the same form as the canonical and microcanonical ensembles, respectively, but with the prior measure \( P_N \) replaced by \( Q_{V,\beta} \). Moreover, \( h_N \) is replaced by \( r_N \) while \( N \) is replaced by \( V \). As a result, the entropy function \( s(u) \) defined in (18) which determines equivalence between the canonical and microcanonical ensembles must now be defined for \( r_N \) with respect to \( Q_{V,\beta} \), which leads us to \( s_\beta(\rho) \) as defined in (73).

For applications of these ideas to the case of two constraints involving the energy and magnetization, see [59]; for an application to the zero-range process with a single particle density constraint, see [55].

B. Mixed ensembles

More general ensembles involving more than one constraints can be treated along the lines just discussed or, more completely, by following Sec. 5 of Ellis, Haven and Turkington [4] who refer to these ensemble as ‘mixed ensembles’. Here we briefly summarize the changes that need to be taken into account following the notations of [4]. In terms of definitions, the changes are as follows:

- Write all the conserved quantities \( h_{N,1}, \ldots, h_{N,\sigma} \) considered in the model as a vector \( h_N = (h_{N,1}, \ldots, h_{N,\sigma}) \), referred to as the generalized Hamiltonian.
- Denote the quantities to be treated canonically as \( h_{1,N} \) and those to be treated microcanonically (as constraints) as \( h_{2,N} \). Then write \( h_N = (h_{1,N}, h_{2,N}) \).
- Associate a vector \( \beta = (\beta_1, \ldots, \beta_\sigma) \) of Lagrange parameters to \( h_N \) and denote the restriction of that vector associated with the canonical part \( h_{1,N} \) by \( \beta_1 \).
- Define the full canonical ensemble for \( h_N \) as

\[ P_{N,\beta}(d\omega) = \frac{e^{-N\langle \beta, h_N(\omega) \rangle}}{Z_N(\beta)} P_N(d\omega) \tag{77} \]

where \( \langle \beta, h_N \rangle = \sum_{i=1}^{\sigma} \beta_i h_{N,i} \) is the normal scalar product.
- Define the mixed ensemble for \( h_{1,N} \) canonical and \( h_{2,N} \) microcanonical as

\[ P_{N,\beta_1}^{u_2}(d\omega) = \frac{e^{-N\langle \beta_1, h_{1,N}^{\beta_1}(\omega) \rangle}}{Z_N^{u_2}(\beta_1)} \mathbf{1}_{du_2}(h_{2,N}(\omega)) P_N(d\omega) \tag{78} \]

The equivalence of these two types of ensembles is determined using the same results as before with the following changes:
• The real parameter $\beta$ is now a vector in $\mathbb{R}^\sigma$.
• The real parameter $u$ is replaced by the vector $u^2$.
• $\varphi(\beta)$ is still defined from $Z_N(\beta)$ with $\beta$ now a vector.
• $s(u)$ is replaced by the thermodynamic potential $s_{\beta_1}(u^2)$ of the mixed ensemble:

$$s_{\beta_1}(u^2) = \lim_{N \to \infty} \frac{1}{N} \ln Z_N^2(\beta_1).$$

(79)
• The product $\beta u$ in the Legendre-Fenchel transform is replaced by the scalar product $\langle \beta_2, u^2 \rangle$.
• Supporting lines must be replaced by supporting planes or hyperplanes; see [4].
• Concave points of vector functions have supporting hyperplanes in their domain except possibly at relative boundary points, that is, points on the boundary of the relative interior of their domain; see also [4].

The first change concerning $s(u)$ should be clear from our discussion of the grand-canonical and canonical case; for more details, see Sec. 5 of [4]

C. Nonequilibrium path ensembles

The physical interpretation of $P_{N,\beta}$, $P_N^m$ and the Hamiltonian function $H_N$ entering in both measures is not important for establishing that these two measures are equivalent in the thermodynamic limit. Clearly, this equivalence is a general relation between a measure conditioned on some event (microcanonical) and a different measure obtained by replacing this conditioning with an exponential factor involving a Lagrange parameter dual to the constraint (canonical). Mathematically, we say that equivalence is between a conditioning and a tilting of the same measure [7].

This general perspective on equivalence can be used to replace macrostate-based constraints and large deviation (or rare event) conditionings in Monte Carlo or molecular simulations, which are often hard to deal with, by modified sampling schemes based on exponentially-tilted measures. It can also be used to establish the equivalence of microcanonical and canonical-like probability measures defined in the context of nonequilibrium systems.

To illustrate this case, consider a measure $P_T(d\omega)$ on the space $\Lambda_T$ of trajectories $\omega = \{\omega_t\}_{t=0}^T$ of a continuous-time Markov process evolving over the time span $[0, T]$. This probability plays the role of the prior $P_N$ used to define the microcanonical and canonical ensembles. For a macrostate or observable $A_T$, which is in general a functional of $\omega$, we define the microcanonical ensemble as

$$P_T^m(d\omega) = P_T\{d\omega | A_T \in da\}$$

(80)

and the canonical ensemble as

$$P_{T,k}(d\omega) = \frac{e^{kTA_T(\omega)}}{W_T(k)} P_T(d\omega)$$

(81)

where $k \in \mathbb{R}$ and

$$W_T(k) = E_{P_T}[e^{kTA_T}]$$

(82)

From these definitions, we see that the parameter $k$ plays the role of (minus) an inverse temperature and that the time $T$ plays the role of the particle number $N$, so that the thermodynamic limit is
now $T \to \infty$ with $A_T$ finite. In this limit, all our equivalence results holds for $P^n_T$ and $P_{T,k}$ under assumptions similar to A1-A4. In particular, assuming that $A_T$ satisfies the LDP with respect to $P_T$ with rate function $I(a)$, then $P^n_T$ and $P_{T,k}$ are equivalent in the specific action sense if $I$ is convex at $a$.\(^7\) In this case, we also have macrostate equivalence, which means that $P^n_T$ and $P_{T,k}$ have the same stationary properties.

This equivalence of path measures was discussed recently in [60] (see also references cited therein). An interesting open problem in this context is to find examples of stochastic processes and observables characterized by nonconvex rate functions for which the microcanonical and canonical path measures are not equivalent.

Appendix A: Concavity of the entropy

Let $s : \mathbb{R} \to \mathbb{R} \cup \{ -\infty \}$ be a real function with domain $\text{dom} \ s$, and consider the inequality

$$s(v) \leq s(u) + \beta(v-u), \quad v \in \mathbb{R}. \quad (A1)$$

The set of all $\beta \in \mathbb{R}$ for which this inequality satisfied is called the subdifferential set or simply the subdifferential of $s$ at $u$ and is denoted by $\partial s(u)$. The interpretation of this inequality is shown in Fig. 1: if it is possible to draw a line passing through the graph of $s(u)$ which is everywhere above $s$, then $\partial s(u) \neq \emptyset$. In this case, we also say that $s$ admits a supporting line at $u$, which is unique if $s$ is differentiable at $u$. If $\partial s(u) = \emptyset$, then $s$ admits no supporting line at $u$.

It is easy to see geometrically that nonconcave points of $s$ do not admit supporting lines, while concave points have supporting lines, except possibly if they lie on the boundary of $\text{dom} \ s$; see Sec. 24 of [33] or Appendix A of [34]. The reason for possibly excluding boundary points arises because $s(u)$ may have diverging ‘slopes’ where $\partial s(u)$ is not defined, as in the following example adapted from [33, p. 215]:

$$s(u) = \begin{cases} \sqrt{1-x^2} & |x| \leq 1 \\ -\infty & \text{otherwise.} \end{cases} \quad (A2)$$

In this case, $s(u) = s^{**}(u)$ for all $u \in \text{dom} \ s = [-1,1]$, so that $s$ is a concave function, but it has supporting lines only over $(-1,1) = \text{int}(\text{dom} \ s)$, since $s'(u)$ diverges as $u \to \pm 1$ from within its domain. All cases of concave points with no supporting lines are of this type, since it can be proved in $\mathbb{R}$ that

$$\text{int}(\text{dom} \ s) \subseteq \text{dom} \ \partial s \subseteq \text{dom} \ s; \quad (A3)$$

see again Sec. 24 of [33] or Appendix A of [34].

With this proviso on boundary points, $s$ is often defined to be strictly concave at $u$ if it admits supporting lines at $u$ that do not touch other points of its graph. If $s$ has a supporting line at $u$ touching other points of its graph, then $s$ is said to be non-strictly concave at $s$. Finally, if $s$ admits no supporting line at $u$, then $s$ is said to be nonconcave at $u$. These definitions are also illustrated in Fig. 1. For generalizations of these definitions to $\mathbb{R}^d$ in terms of supporting hyperplanes, see [33] and Appendix A of [34].

Appendix B: Varadhan’s Theorem and the Laplace principle

We recall in this section two important results about Laplace approximations of exponential integrals in general spaces. In the following, $\{a_n\}_{n=1}^{\infty}$ is an increasing sequence such that $a_n \to \infty$ when $n \to \infty$.

\(^7\) Convexity is used instead of concavity because $I$ is defined as a rate function rather than an entropy function.
When $n \to \infty$. Moreover, $\{P_n\}_{n=1}^\infty$ is a sequence of probability measures defined on a (Polish) space $\mathcal{X}$. In this paper, $N$ takes the role of $a_n$ and $n$.

**Theorem 13 (Varadhan, 1966 [32]).** Assume that $P_n(dx)$ satisfies the LDP with speed $a_n$ and rate function $I$ on $\mathcal{X}$. Let $F$ be a continuous function.

(a) (Bounded case) Assume that $\sup_x F(x) < \infty$. Then

$$\lim_{n \to \infty} \frac{1}{a_n} \ln \int_{\mathcal{X}} e^{a_n F(x)} P_n(dx) = \sup_{x \in \mathcal{X}} \{F(x) - I(x)\} < \infty. \quad (B1)$$

(b) (Unbounded case) Assume that $F$ satisfies

$$\lim_{L \to \infty} \lim_{n \to \infty} \frac{1}{a_n} \ln \int_{\{F \geq L\}} e^{a_n F(x)} P_n(dx) = -\infty \quad (B2)$$

Then the result of (a) holds and is finite. In particular, if $F$ is bounded above on the support of $P_n$, then (a) holds.

For a proof of this result, see the Appendix B of [26] or Theorem 4.3.1 in [30]. For historical notes on this result, see Sec. 3.7 of [29].

Consider now the *exponentially tilted* probability measure

$$P_{n,F}(dx) = \frac{e^{a_n F(x)} P_n(dx)}{W_{n,F}}, \quad (B3)$$

where

$$W_{n,F} = \int_{\mathcal{X}} e^{a_n F(x)} P_n(dx) = E_P[e^{a_n F(X)}]. \quad (B4)$$

This is also known as the *exponential family* or *Esscher transform* of $P_n$.

**Theorem 14 (LDP for tilted measures).** Assume that $W_{n,F} < \infty$. Then $P_{n,F}$ satisfies the LDP with speed $a_n$ and rate function

$$I_F(x) = I(x) - F(x) + \lambda_F, \quad (B5)$$

where

$$\lambda_F = \lim_{n \to \infty} \frac{1}{a_n} \ln W_{n,F}. \quad (B6)$$

A proof of this result can be found in Theorem 11.7.2 of [26] or by combining Proposition 3.4 and Theorem 9.1 of [27]. A thermodynamic version of this result also appears in Theorem 4.1 of [7].

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