Mind the Gap:
Boltzmannian versus Gibbsian Equilibrium

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Abstract

There are two main theoretical frameworks in statistical mechanics, one associated with Boltzmann and the other with Gibbs. Despite their well-known differences, there is a prevailing view that equilibrium values calculated in both frameworks coincide. We show that this is wrong. There are important cases where the Boltzmannian and Gibbsian equilibrium concepts yield different outcomes. Furthermore, the conditions under which equilibria exists are different for Gibbsian and Boltzmannian statistical mechanics. There are, however, special circumstances under which it is true that the equilibrium values coincide. We prove a new theorem providing sufficient conditions for this to be the case.

1 Introduction

There are two main theoretical frameworks in statistical mechanics (SM), one associated with Boltzmann and the other with Gibbs. One of the crucial differences is the characterisation of equilibrium. While in the Boltzmannian framework equilibrium corresponds to the largest macro-region, the Gibbsian framework associates equilibrium with the stationary probability distribution of maximum entropy. The Boltzmannian picture is usually accepted as correct when it comes to answering foundational questions, in particular in connection with the approach to equilibrium. At the same time the Gibbsian framework is dismissed as 'thoroughly misguided' (Goldstein 2001, 39) and stands accused of introducing theoretical instruments that we 'neither have nor [...] need' (Lebowitz 1993, 38). Yet, the Gibbsian framework is the undisputed workhorse of the practitioner.

This would be not be particularly worrisome if the two formalisms were equivalent or inter-translatable as, for instance, the Schrödinger and the Heisenberg picture in quantum mechanics. But they are not. Not only do they disagree on how equilibrium is conceptualised; they do not even study the same entities. While the Boltzmannian framework investigates individual systems, the object of study in the Gibbs approach are ensembles, and there is no obvious way to translate results from one framework into the other. This creates an awkward situation: how can we think that the Boltzmannian framework gives the right foundational account of SM and at the same time rely on the Gibbsian framework for calculations if the two accounts are in fact at odds with each other?

A common response is to play down the severity of the problem with the argument that the two frameworks lead to the same results. One can, so the argument goes, use the Gibbs formalism as effective tool for the calculation of equilibrium values of a wide spectrum of

physical quantities, because these coincide with the values that would come out of the Boltzmann machinery if one was able to make the calculations. However, the reasoning behind this assertion remains unclear. Either it is simply asserted as an obvious truism (Davey 2016 and Wallace quoted in Werndl and Frigg (forthcoming*c*)), or arguments are given only for special cases (Lavis 2005 and Malament and Zabell 1980). So the claim that Gibbsian and Boltzmannian equilibrium values generally coincide has the status of an article of faith. Faith need not be wrong, but it can be. The project for this paper is to investigate whether the purported equivalence of results really holds.

Our answer is negative. If understood as a general proposition, the claim is provably wrong. After briefly introducing the Boltzmannian and the Gibbsian notions of equilibrium (Section 2) we present two examples in which Boltzmannian and Gibbsian equilibrium values come apart: the baker's gas (Section 3) and the Ising model (Section 4). The differences between the two frameworks have gone unnoticed partly because Boltzmannian and Gibbsian calculations are seldom carried out on the *same* systems. We make a first step towards rectifying this situation by discussing our examples from both theoretical vantage points, which makes visible how the two frameworks differ. Things get worse still. Not only do equilibrium values fail to coincide; equilibria don't necessarily exist under the same conditions. There are systems that have a Boltzmannian equilibrium but fail to have a Gibbsian equilibrium and vice versa (Section 5). This raises the question whether there is even a grain of truth in common wisdom, and the good news is that there is. We prove a new theorem establishing that under certain special circumstances the results of the two formalisms indeed coincide (Section 6). We describe these circumstances in some detail and give examples. We end by offering some conclusions (Section 7).

2 Equilibrium in Gibbs and Boltzmann

In this section we briefly introduce the Boltzmannian and the Gibbsian notions of equilibrium (for details see Uffink, 2007; Frigg, 2008). Throughout the paper we consider systems with a phase space X. Let μ_X denote the probability measure on X. Further, let $T_t(x)$ denote the state of the system after t time units that starts in x. The dynamics T_t is usually deterministic. Sometimes, for instance in the Ising model, dynamics are considered that are stochastic processes $\{Z_t\}$. For ease of presentation we state general definitions and results for the deterministic case; but all definitions have stochastic equivalents and the results equally also hold in the stochastic case (see Werndl and Frigg (forthcoming*a*) for a discussion of stochastic systems).

In *Gibbsian SM* the object of study is an *ensemble*, an infinite collection of independent systems that are all governed by the same equations but are in different states. The ensemble is described by a probability density $\rho(x, t)$, $x \in X$, reflecting the probability of finding the state of a system chosen at random from the ensemble in a certain part of X at time t. Physical observables are associated with real valued functions $f : X \times t \to \mathbb{R}$. The *phase average* of such a function is:

$$\bar{f}(t) = \int_X f(x, t)\rho(x, t)dx. \tag{1}$$

According to the standard understanding of the formalism, phase averages are observed in experiments. The Gibbs entropy of a distribution is

$$S_G[\rho] = -k \int_X \rho(x, t) \log[\rho(x, t)]dx, \tag{2}$$

where k is Boltzmann's constant. A distribution $\rho(x, t)$ is stationary if it does not depend on

time: $\rho(x,t) = \rho(x)$ for all t. In Gibbsian SM equilibrium is the property of an ensemble. The ensemble is in equilibrium if the distribution is stationary and has maximum entropy given the constraints imposed on the system. The most common equilibrium distributions are the microcanonical, canonical and grand-canonical distributions (Uffink 2007).

It is customary to begin a presentation of *Boltzmannian SM* with the combinatorial argument. However, it is now recognised that combinatorial considerations do not provide a good general definition of Boltzmannian equilibrium (Uffink 2007) and we therefore work with our own alternative definition (Werndl and Frigg 2015a, 2015b).[1] Consider the same dynamical system as above and assume that the measure μ_X is stationary. At the macro level the system is characterised by a set of *macro-variables* $\{v_1, ..., v_l\}$ ($l \in \mathbb{N}$). They are measurable functions $v_i : X \to \mathbb{R}$, associating a value with each $x \in X$. We use capital letters V_i to denote the values of v_i. A particular set of values $\{V_1, ..., V_l\}$ defines a macro-state $M_{V_1,...,V_l}$. The region of phase space corresponding to the macro-state $M_{V_1,...,V_l}$, its *macro-region*, is denoted by $Z_{M_{V_1,...,V_l}}$.

The equilibrium macro-state is defined as the state in which a system spends most of its time. Let LF_R be the fraction of time a system spends in region $R \in X$ in the long run:

$$LF_R(x) = \lim_{t\to\infty} \frac{1}{t} \int_0^t 1_A(T_\tau(x))d\tau, \tag{3}$$

where $1_A(x)$ is the characteristic function of R: $1_A(x) = 1$ for $x \in R$ and 0 otherwise. The notion of 'most' can be read in two different ways, leading to two different notions of equilibrium. The first introduces a lower bound of $1/2$ for the fraction of time spent in equilibrium, leading to the notion of an α-ε-equilibrium:

[1]Combinatorial considerations are of course still useful to construct macro-states, and we rely on them below.

> Let α be a real number in the interval $(\frac{1}{2}, 1]$, and let ε be a very small positive real number.[2] If there is a macro-state $M_{V_1^*,\ldots,V_l^*}$ satisfying the following condition, then it is the α-ε-equilibrium state of S: There exists a set $Y \subseteq X$ such that $\mu_X(Y) \geq 1 - \varepsilon$, and all initial states $x \in Y$ satisfy $LF_{X_{M_{V_1^*,\ldots,V_l^*}}}(x) \geq \alpha$.

The second reading takes 'most' to refer to the fact that the system spends more time in equilibrium than in any other state (this can be less that 50% of its time). This provides the γ-ε-equilibrium:

> Let γ be a real number in $(0, 1]$ and let ε be a small positive real number ($\varepsilon < \gamma$). If there is a macro-state $M_{V_1^*,\ldots,V_l^*}$ satisfying the following condition, it is the γ-ε equilibrium state of S: There exists a set $Y \subseteq X$ such that $\mu_X(Y) \geq 1 - \varepsilon$ and for all initial conditions $x \in Y$: $LF_{Z_{M_{V_1^*,\ldots,V_l^*}}}(x) \geq LF_{Z_M}(x) + \gamma$ for all macro-states $M \neq M_{V_1^*,\ldots,V_l^*}$.

It is obvious that on both notions of equilibrium the value associated with the equilibrium macro-state is the observed value in equilibrium. It can be proven that equilibrium states *thus defined* are the largest states in the system in the following sense: their measure is larger than $\alpha(1 - \varepsilon) > 1/2$ for an α-ε-equilibrium and their measure is $\gamma - \varepsilon$ larger than the measure of any other macro-region for a γ-ε-equilibrium.[3]

[2] We assume that $(1 - \alpha)\varepsilon > 1/2$.

[3] Proofs for the deterministic case are given in Werndl and Frigg (2015b) and for the stochastic case in Werndl and Frigg (forthcoming*a*). The problem of the existence of such equilibrium states is discussed in Werndl and Frigg (forthcoming*b*).

3 Example 1: The Baker's Gas

The baker's gas consists of N identical particles that evolve independently according to the baker's transformation (Lavis 2005). Its micro-states are of the form $x = (b_1, c_1, \ldots, b_N, c_N)$, where $b_i \in [0, 1]$ is the momentum and $c_i \in [0, 1]$ is the position coordinate of the i-th particle. The system's phase space therefore is $X = [0, 1]^{2N}$, which is endowed with the uniform probability measure μ_X (the $2N$-dimensional Lebesgue measure). Time is discrete and the evolution to the next time step is given by applying the baker's transformation to each coordinate: $x = (\ldots b_i, c_i \ldots)$ evolves into $\Lambda(x) = (\ldots \theta(b_i, c_i) \ldots)$, where

$$\theta(b_i, c_i) = 2b_i, \frac{c_i}{2} \text{ if } 0 \leq b_i \leq \frac{1}{2} \text{ and } 2b_i - 1, \frac{c_i + 1}{2} \text{ otherwise.} \tag{4}$$

Let us begin with the *Boltzmannian treatment* of the baker's gas. Here μ_X is the stationary measure. We now use combinatorial considerations to construct the system's macro-state. Consider a partition of the unit square (the phase space for one particle) into cells of equal size $\delta\omega$ whose dividing lines run parallel to the position and momentum axes. This results in a finite partition $\Omega_{bg} := \{\omega_1^{bg}, ..., \omega_k^{bg}\}$, $k \in \mathbb{N}$. The coarse-grained micro-state of a particle is the cell in which a particle's state lies. An *arrangement* is given by a specification of the coarse-grained micro-states of all the particles. A *distribution* is a specification of how many particles' states lie in a given cell. Consider the distribution $D_{bg} = (N_1, N_2, \ldots, N_k)$, where N_i is the number of particles in cell ω_i. The number $G(D_{bg})$ of arrangements that lead to the same distribution D_{bg} is $G(D_{bg}) = N! \,/\, N_1!N_2! \ldots, N_k!$.

One can now define a partition on X by grouping together in one cell all points that have the same distribution. It is easy to see that the cell X_u corresponding to the uniform distribution (i.e

where $N_i = N/k$)[4] is larger than any other cell. We now introduce a macro-variable V as follows: $V(x) = 0$ for $x \in X_u$ and for all other cells of the partition $V(x)$ takes values between 10^6 and 10^8 so that no two cells have the same value. The baker's gas is ergodic (Lavis 2005), and hence spends more time in X_u than in any other cell. Therefore the long run fraction of time for which the value of V is 0 is larger than the long run fraction for any other value. Thus the macro-state defined by $V = 0$ is a γ-0-equilibrium, and $V = 0$ is the Boltzmannian equilibrium value.[5]

Let us now turn to the *Gibbsian treatment* of the baker's gas. The stationary maximum entropy distribution is the uniform distribution $\rho(x) = 1$. The phase space average $\bar{V}$ for the macro-variable V will be greater than $(1\text{-}\mu_X(X_u)) \times 10^6$. Lavis (2005) has shown that $\mu_X(X_u) \approx 0.47$ (for large N), and hence $0.53 \times 10^6 = 530000$ is a lower bound for $\bar{V}$.

So we find Boltzmannian and Gibbsian equilibrium values that are very different! The macro-variable of this system is admittedly contrived and so one might argue that the problem does not arise in practice. The grain of truth in this remark is that much depends on the choice of the macro-variable and for sufficiently restrictive classes of macro-variables the problem can indeed be avoided (see Section 6 for a characterisation of such classes). However, there are real physical systems that do *not* fall into these classes. Thus the relevant contrast is not between 'mathematical contrivance' and 'sensible physics'. The example we discuss in the next section is a case in point.

[4]We assume that $N = k \times r$ for some $r \in \mathbb{N}$.

[5]It is not an α-ε-equilibrium because the equilibrium macroregion takes up less than half of the phase space for large N (Lavis 2005).

4 Example 2: The Ising Model

The two-dimensional Ising model is an important system in SM. We here consider a version of the model with nearest neighbour interactions in the absence of an external field. Despite being only two-dimensional, this model provides a realistic description of crystals such as K_2NF_4 and RB_2MnF_4, which have strong horizontal and weak vertical interactions (Baxter 1982).

Consider a regular two-dimensional lattice with N grid points. The lattice is assumed to lie on a two dimensional torus so that every grid point has exactly four nearest neighbours (allowing us to neglect border effects). At every grid point there is a spin pointing either up ($\sigma = 1$) or down ($\sigma = -1$). The system's micro-state is given by

$$\sigma = \{\sigma_1, \ldots, \sigma_N\}, \tag{5}$$

and its Hamiltonian is:

$$H(\sigma) = -J \sum_{nn} \sigma_i \sigma_j. \tag{6}$$

The sum is over all nearest-neighbour pairs and the constant $J \geq 0$ is the energy associated with the nearest-neighbour interaction (Baxter 1982).

We treat the model stochastically and hence we first introduce probabilities. The probability distribution has the *form* of a Gibbsian distribution, but it is important to emphasise that at this point this is nothing more than a formal definition that is neither Gibbsian nor Boltzmannian. We begin with the partition function:

$$Z = \sum_{\sigma} e^{-\beta H(\sigma)}. \tag{7}$$

The sum is taken over all possible configurations σ of the model and $\beta = 1/kT$ is a constant, where T is the temperature and k is Boltzmann's constant. The probability of finding the system in a certain configuration σ is given by the canonical distribution:

$$P(\sigma) = \frac{e^{-\beta H(\sigma)}}{Z}. \tag{8}$$

For large values of β (low temperature), the probabilities of the lower energy states are dominant. For small values of β (high temperature) the probability distribution is flattened out and all configurations are more or less equally likely (Baxter 1982; Cipra 1987).

The *Boltzmannian treatment* is as follows. The probability $P(\sigma)$ is the stationary measure which defines the dynamics of the stochastic dynamical system of Section 2. It can be shown that this dynamics is in fact an irreducible Markov chain, the stochastic equivalent to ergodicity (Berger 2001). As the relevant macro-variable we choose the *internal energy*:

$$E(\sigma) = \sum_{n,n} -J\sigma_i\sigma_j, \tag{9}$$

where the sum is over all nearest-neighbour interactions. Let $\bar{\sigma}$ be the micro-state for which $\sigma_i = 1$ for all i, and let $\hat{\sigma}$ be the micro-state for which $\sigma_j = -1$ for all j. $A := \{\bar{\sigma}, \hat{\sigma}\}$ is then the macro-state for which the internal energy has value $E = -2JN$ (because there are $2N$ nearest-neighbour pairs for a quadratic lattice with N sites for $N \geq 9$). As noted above, the higher β the larger the probabilities of the lower energy states. Since the dynamics is irreducible, for large enough β the system spends most of its time in A. Hence A is a Boltzmannian γ-0-equilibrium and the value of the internal energy in equilibrium is $-2JN$.

Let us now turn to the *Gibbsian treatment*. Here $P(\sigma)$ is the stationary measure of maximum entropy. As above the value of E is lowest for $\bar{\sigma}$ and $\hat{\sigma}$, namely $-2JN$. Since all other micro-states have higher energy, the Gibbsian phase average of E over all micro-states is higher than $-2JN$ (Baxter 1982; Cipra 1987; Sekular 2015).

It follows that the equilibrium value of the internal energy in a Boltzmann equilibrium ($-2JN$) is lower than in Gibbsian equilibrium. This difference arises because the macro-variable takes the lowest value in the largest macro-region and a higher value in all other macroregions.

The differences between the equilibrium values is *not* negligible. By way of illustration consider the case of a two-dimensional lattice with four grid-points: $\sigma = (\sigma_1, \sigma_2, \sigma_3, \sigma_4)$ where (σ_1, σ_2) constitute the first row and (σ_3, σ_4) constitute the second row. Let $\beta = 1/2$ and $J = 1$. There are four nearest-neighbour pairs. The Boltzmannian equilibrium macro-state is $\{(1,1,1,1),(-1,-1,-1,-1)\}$, and the equilibrium value is -4. The value obtained by phase space averaging can be obtained as follows. There are two states which have energy -4 and whose probability is $e^{4/2}/Z \approx 7.389/Z$: $(1,1,1,1),(-1,-1,-1,-1)$. There are twelve states which have energy 0 and whose probability is $e^{0/2}/Z = 1/Z$: $(-1,1,1,1)$, $(1,-1,1,1)$, $(1,1,-1,1)$, $(1,1,1,-1)$, $(-1,-1,-1,1)$, $(-1,-1,1,-1)$, $(-1,1,-1,-1)$, $(1,-1,-1,-1)$, $(1,1,-1,-1)$, $(-1,-1,1,1)$, $(1,-1,1,-1)$, $(-1,1,-1,1)$. Finally, there there are two states which have energy 4 and whose probability is $e^{-4/2}/Z \approx 0.1353/Z$: $(-1,1,-1,1)$, $(1,-1,1,-1)$. Hence the phase average is:

$$\frac{-4 \times 2 \times 7.389 + 0 \times 12 \times 1 + 4 \times 2 \times 0.1353}{2 \times 7.389 + 12 \times 1 + 2 \times 0.1353} = -2.1454 \tag{10}$$

So the Gibbsian equilibrium value (-2.1454) is almost half of the Boltzmannian equilibrium value (-4).

Nothing depends on the choice $N = 4$. It remains the case for large N that Gibbsian phase averages will be *different* from the Boltzmannian equilibrium values. Indeed this situation remains unchanged even in the limit $N \to \infty$, where one also finds that the Boltzmannian and Gibbsian values differ.[6]

5 Existence Under Different Conditions

We have shown that Gibbsian and Boltzmannin equilibrium values fail to coincide. And things get worse: there are systems that have a Boltzmannian equilibrium but fail to have a Gibbsian equilibrium and vice versa.

5.1 Gibbs does not imply Boltzmann

Consider the baker's gas (Section 3) with an even number of particles with one macro-variable V indicating whether there are more particles on the left side of the container than on the right side: V assumes value 1 if there are more particles on the left and it assumes value 0 if there are more particles on the right. The corresponding macro states are M_1 and M_0. Both macro-regions have the same measure, namely $1/2$. The dynamics is ergodic and therefore the system spends half of the time in M_0 and half of the time in M_1. For this reason the system has no Boltzmannian equilibrium (neither of the α-ε nor of the γ-ε kind). However, there exists a

[6]More specifically, one finds that for arbitrary large N the macro-value closest to the value obtained by Gibbs phase space averaging will always be *different* to the macro-value representing the Boltzmannian equilibrium.

Gibbs equilibrium: the uniform measure μ_B is the stationary distribution of maximum entropy.

The Ising Model (Section 4) provides another example. Consider again the above example with four sites and assume $\beta = 0$.[7] Suppose that there are two macro-states: (i) one where all the molecules point upwards, all the molecules point downwards or there are an equal number of molecules that point upwards and downwards (eight micro-states in total), and (ii) where this is not the case (again eight micro-states in total). The usual dynamics considered for the Ising models are irreducible Markov chains. Recall that irreducibility is the stochastic equivalent to ergodicity, and hence, as in the previous example, there is no Boltzmannian equilibrium because both macro-regions have the same measure $1/2$. However, a Gibbsian equilibrium exists. The probability P is the canonical distribution, which is the stationary distribution of maximum entropy.

5.2 Boltzmann does not imply Gibbs

Boltzmannian equilibrium is defined for systems with a stationary measure μ_X, and so there always exists at least one stationary distribution. Nevertheless, a stationary distribution of maximum entropy need not exist, as the following example shows.

Consider a system with phase space $[0, 2] \times [0, 1]$. The dynamics T_t of the system consists of two 'copies' of the baker's gas in the following sense: the restriction of T_t to $[0, 1] \times [0, 1]$ is the standard baker's transformation (see Section 3) and the restriction of T_t to $(1, 2] \times [0, 1]$ is the baker's transformation with the position coordinate shifted by one unit to the right. The

[7]This corresponds to an infinite temperature, which is often considered as an approximation to very high temperatures (e.g. Baxter 1982). We work with $\beta = 0$ for reasons of simplicity; similar examples could be given for low but non-zero values of β.

measure of the system is $1/3 \times 1_{[0,1]\times[0,1]} + 2/3 \times 1_{(1,2]\times[0,1]}$, where 1_A is the characteristic function of A. Since the baker's system is ergodic, clearly, the phase space consists of two components ($[0, 1] \times [0, 1]$ and $(1, 2] \times [0, 1]$), restricted to each of which the dynamics is ergodic. Suppose that the macro-variable takes the value 0 if the position coordinate is in $[1/4, 7/4]$, 100 if the position coordinate is in $[0, 1/4)$, -100 if the position coordinate is in $(7/4, 2]$. Clearly, there exists a Boltzmannian equilibrium. The value 0 corresponds to an 0.75-0-equilibrium: since the system is ergodic on each component and the 0 macro-state takes up three-quarters on each component, three quarters of the time the system takes the value 0.

Yet suppose that the class of distributions of interest are all densities over $[0, 2] \times [0, 1]$ of the form $\alpha 1_{[0,1]\times[0,1]} + \beta 1_{(1,2]\times[0,1]}$ where $\alpha, \beta \geq 0$, $\alpha + \beta = 1$ and the uniform distribution (the case $\alpha = \beta = 1/2$) is excluded. Then there is no Gibbsian equilibrium. It is clear that all distributions are stationary (because μ_B of the baker's gas is stationary), but by construction, there is no distribution of maximum entropy: the closer α and β are to $1/2$, the higher the entropy (2). Yet there is no maximum since the uniform distribution ($\alpha = \beta = 1/2$) is not among the class of distributions under consideration.

6 When Boltzmann and Gibbs Agree

This section focuses on special cases where the Boltzmannian and Gibbsian calcuations agree. We first consider the main case discussed in the literature. Then we present a new theorem specifying a set of conditions under which Boltzmannian and Gibbsian values coincide. We show that many standard examples satisfy these conditions and that they fail in the cases discussed in previous sections.

Suppose that the relevant observable is such that it takes the value of the phase average

nearly everywhere on phase space. Furthermore assume that a Boltzmannian equilibrium exists. In such a situation it will be the case that the value of the observable in the Boltzmannian equilibrium macro-state is equal to the phase average. The question is under what circumstances something like this is the case. One such situation is described by Khinchin (1949). He argued that phase functions have to satisfy strong symmetry requirements and therefore ought to have small dispersion for systems with a large number of constituents (we refer to this as the 'Khinchin condition'). This, or something like it, is often taken to be an explanation of why calculations in both framworks coincide (Davey 2015; Malament and Zabell 1980; Wallace quoted in Werndl and Frigg forthcoming*c*).

This is correct, but the question is how far it goes. The point to note is that the conditions not only rule out artificial examples, but also realistic physical models. Examples of systems with macro-variables that do not satisfy the Khinchin condition include the Ising model with the internal energy or the magnetisation as macro-variable, the six-vertex model with the internal energy or the polarization as macro-variable (cf. Baxter 1982), and the KAC-ring with the standard macrostate structure of the number of black and white balls.

So we need other conditions next to the Khinchin condition. Let us look at a situation in which a system has both a Boltzmann and a Gibbs equilibrium. In this case the following theorem provides sufficient conditions for the equilibrium values of both equilibria to coincide:

> **Equilibrium Equivalence Theorem (EET)**. Suppose that the system (X, T_t, μ_X) is composed of $N \geq 1$ constituents. That is, the state $x \in X$ is given by the N coordinates $x = (x_1, \ldots, x_N)$; $X = X_1 \times X_2 \ldots \times X_N$, where $X_i = X_{oc}$ for all $1 \leq i \leq N$ (X_{oc} is the one-constituent space). Let μ_X be the product measure

> $\mu_{X_1} \times \mu_{X_2} \ldots \times \mu_{X_N}$, where $\mu_{X_i} = \mu_{X_{oc}}$ is the measure on X_{oc}. Suppose that an observable κ is defined on the one-particle space X_{oc} and takes the values $\kappa_1, \ldots, \kappa_k$ with equal probability $1/k$, $k \leq N$.[8] Suppose that the macro-variable K is the sum of the one-component observable, i.e. $K(x) = \sum_{i=1}^{N} \kappa(x_i)$. Then the value corresponding to the largest macro-region as well as the value obtained by phase space averaging is $\frac{N}{k}(\kappa_1 + \kappa_2 + \ldots \kappa_k)$.

The proof is stated in full in the Appendix; an intuitive sketch is as follows. Because the observable on the one-constituent space takes the values $\{\kappa_1, \ldots, \kappa_k\}$ with equal probability, combinatorial considerations show that the *Boltzmannian equilibrium macro-region*, i.e. the macro-region of largest size, is the one where there are N/k constituents taking the value κ_1, N/k constituents taking the value $\kappa_2, \ldots, N/k$ constituents taking the value κ_k. That is, the Boltzmannian equilibrium value is $(\kappa_1 + \ldots + \kappa_k)N/k$. The *Gibbsian equilibrium value* obtained by phase averaging is also $(\kappa_1 + \ldots + \kappa_k)N/k$ because one simply takes the average over all sequences of the $\{\kappa_1, \ldots, \kappa_k\}$ and the κ_i are equally probable.

The proof does not make any assumptions about the dynamics of the system; in particular it doesn't assume that the system is ergodic. The crucial assumptions of the theorem are (i) that the macro-variable is a sum of the observable on the constituent space and (ii) that the macro-variable on the constituent space corresponds to a partition with cells of equal probability. This theorem is important because it applies to many examples in SM. Consider, for instance, the baker's gas discussed in Section 3. The gas involves a partition of the unit square (the phase space for one particle) into cells $\{\omega_1^{bg}, \ldots, \omega_k^{bg}\}$, $k \in \mathbb{N}$, of equal size $\delta\omega$. Suppose that a particle in ω_i^{bg} takes value κ_i for all $i = 1, \ldots, k$. Now the macro-variables often

[8] N is assumed to be a multiple of k, i.e. $N = k \times s$ for some $s \in \mathbb{N}$.

considered for the baker's gas are of the form $K(x) = \sum_{i=1}^{N} \kappa(x_i)$ (e.g. Lavis 2005).[9] Then the assumptions of Theorem 1 are satisfied. Thus the Boltzmannian equilibrium value is the same as the value obtained by Gibbsian phase space averaging, namely $(\kappa_1 + \ldots + \kappa_k)N/k$.

The KAC-ring with the standard macro-state structure given by the magnetisation and the ideal gas with the standard macro-states afford further examples of systems satisfying the conditions of the theorem (these examples are discussed in Werndl and Frigg 2015a). In the Boltzmannian framework one often considers macro-variables of the type as assumed in the theorem (Frigg 2008, 110). In these cases the Gibbsian and Boltzmannian equilibrium calculations lead to the same results.

The examples discussed earlier in the paper, showing that equilibrium calculations in Boltzmannian and Gibbsian SM do not lead to the same results, violate the relevant assumptions. In the baker's system with the macro-variables as discussed in Section 3 and in the Ising model with the internal energy as an observable significant chunks of the phase space are taken up by non-equilibrium states, which results in the Khinchin condition not being satisfied. These two examples do not satisfy the assumptions of EET either because the macro-variables of both the baker's gas and the Ising model are not the sum of a one-component macro-variable whose outcomes have equal probability. What does the work in these two examples is that significant parts of the phase space are taken up by non-equilibrium states and that the Boltzmannian equilibrium state has the lowest value of the macro-variable. This results in the phase average being different from the lowest value of the macro-variable (the Boltzmannian equilibrium value).

These examples show that Gibbsian and Boltzmannian calculations can but need not

[9]Note that this macro-variable is very different from the one in Section 3.

provide the same results.[10] An important task of the foundations of SM is to classify under which conditions the two frameworks lead to the same results and under which conditions they do not. The Khinchin condition and EET provide partial answers to this question. The answers are partial because both offer only sufficient but not necessary conditions for Gibbsian and Boltzmannian results being the same.

7 Conclusion

There is widespread belief that Gibbsian and Boltzmannian SM provide the same equilibrium values. We argued that this is false. There are important cases where the Boltzmannian and Gibbsian equilibrium calculations will lead to different results. Furthermore, the conditions under which an equilibrium exists are different for Gibbsian and Boltzmannian SM. It is, however, true that the equilibrium values coincide under special circumstances. We proved a new theorem giving conditions under which this is the case.

This raises the question of what happens in cases where the two do not coincide. Is the Gibbsian or the Boltzmannian equilibrium the correct one? For the Ising model the correct empirical conclusions follow from the Boltzmannian and not the Gibbsian calculations, and we suspect that this will be the same for other cases. Which framework provides the correct values and under which circumstances is a question for future research.

[10]This discrepancy is not an artefact of the use of our own definition of the Boltzmannian equilibrium. The same results would follow if one adopted the standard definition of the equilibrium as the largest macro-region.

8 Appendix: Proof of Theorem 1

First, we determine the value of the largest macro-region. Recall that N is a multiple of k and that the observable on the one-constituent space takes the values $\{\kappa_1, \ldots, \kappa_k\}$ with equal probability. Hence for the macro-region of largest size there are N/k particles taking the value κ_1, N/k particles taking the value $\kappa_2, \ldots,$ N/k particles taking the value κ_k. Therefore, the value of the largest macro-region is $(\kappa_1 + \ldots + \kappa_k)N/k$.

Let us now determine the phase average. The proof is by mathematical induction. We will show that the sum over all sequences of length N whose elements are in $\{\kappa_1, \ldots, \kappa_k\}$ is $k^{N-1}N(\kappa_1 + \ldots + \kappa_k)$. Because each sequence has equal probability $1/k^N$, the desired result follows that the phase average is

$$\frac{1}{k^N} k^{N-1} N(\kappa_1 + \ldots + \kappa_k) = \frac{N}{k}(\kappa_1 + \ldots + \kappa_k). \tag{11}$$

$N = 1$: Because $k \leq N$, $k = 1$, and the the sum over all sequences of length N is
$\kappa_1 = 1^{1-1}1\kappa_1 = \kappa_1$.
$N \rightarrow N + 1$: We need to determine the sum over all sequences of length $N + 1$. One obtains sequences of length $N + 1$ by adding to sequences of length N one element at the end of the sequences. One can add k possible elements at the end and so a contribution to the sum over all sequences of length $N + 1$ is k times the sum of the sequences of length N, i.e.

$$k \times k^{N-1} N(\kappa_1 + \ldots + \kappa_k). \tag{12}$$

What is still missing is the contribution from the element at the end. There are k^N sequences of

length N to which a κ_i can be added, and hence this contribution is

$$k^N(\kappa_1 + \ldots + \kappa_k). \tag{13}$$

Adding these two contributions leads to:

$$k \times k^{N-1}N(\kappa_1 + \ldots + \kappa_k) + k^N(\kappa_1 + \ldots + \kappa_k) = k^N(N+1)(\kappa_1 + \ldots + \kappa_k). \tag{14}$$

References

Baxter, Rodney J. 1982. *Exactly Solved Models in Statistical Mechanics*. London: Academic Press.

Berger, Arno. 2001. *Chaos and Chance: An Introduction to Stochastic Aspects of Dynamics*. New York: De Gruyter.

Cipra, Barry. 1987. "An Introduction to the Ising Model." *American Mathematical Monthly* 94:937-54.

Davey, Kevin 2008. "The Justification of Probability Measures in Statistical Mechanics" *Philosophy of Science*: 75 (1), 28-44.

Frigg, Roman. 2008. "A Field Guide to Recent Work on the Foundations of Statistical Mechanics." In *The Ashgate Companion to Contemporary Philosophy of Physics*, ed. Dean Rickles, 99-196. London: Ashgate.

Goldstein, Sheldon. 2001. "Boltzmanns Approach to Statistical Mechanics." In *Chance in Physics: Foundations and Perspectives*, ed. Jean Bricmont, Detlef Dürr, Maria Carla Galavotti, Gian Carlo Ghirardi, Francesco Petruccione, and Nino Zangh, 39-54. Berlin: Springer.

Khinchin, Alexandr I. 1949. *Mathematical Foundations of Statistical Mechanics*. Mineola/NY: Dover Publications.

Lavis, David. 2005. "Boltzmann and Gibbs: An Attempted Reconciliation." *Studies in History and Philosophy of Modern Physics* 36:245-73.

Lebowitz, Joel L. 1993. “Boltzmanns Entropy and Times Arrow.” *Physics Today* 46:32-38.

Malament, David B., and Sandy L. Zabell. 1980. “Why Gibbs Phase Averages WorkThe Role of Ergodic Theory.” *Philosophy of Science* 56:339–49.

Secular, Paul. 2015. “Monte-Carlo simulation of small 2D Ising lattice with Metropolis dynamics.” http://secular.me.uk/physics/ising-model.pdf

Uffink, Jos. 2007. “Compendium of the Foundations of Classical Statistical Physics.” In *Philosophy of Physics*, ed. Jeremy Buttereld and John Earman, 923-1047. Amsterdam: North Holland.

Werndl, Charlotte, and Roman Frigg. 2015a. “Rethinking Boltzmannian Equilibrium.” *Philosophy of Science* 82:1224-35.

———. 2015b. “Reconceptionalising Equilibrium in Boltzmannian Statistical Mechanics.” *Studies in History and Philosophy of Modern Physics* 49:19-31.

———. Forthcoming*a*. “Boltzmannian Equilibrium in Stochastic Systems.” In Proceedings of the EPSA15 Conference, ed. Michela Massimi, and Jan-Willem Romeijn. Berlin and New York: Springer.

———. Forthcoming*b*. “When Does a Boltzmannian Equilibrium Exist?.” In *Quantum Foundations of Statistical Mechanics*, ed. Daniel Bedingham, Owen Maroney, and Christopher Timpson. Oxford: Oxford University Press.

———. Forthcoming*c*. “Transcript of the Talk and Discussion at the Oxford Workshop in Honour of David Wallace.”, In *Proceedings of the Quantum Foundations of Statistical*

Mechanics Workshop in Oxford, ed. Bendingham, Daniel, Owen Marony, and Christopher Timpson. Oxford: Oxford University Press.