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Statistical Mechanics: A Tale of Two Theories

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Abstract

There are two theoretical approaches in statistical mechanics, one associated with Boltzmann and the other with Gibbs. The theoretical apparatus of the two approaches offer distinct descriptions of the same physical system with no obvious way to translate the concepts of one formalism into those of the other. This raises the question of the status of one approach vis-à-vis the other. We answer this question by arguing that the Boltzmannian approach is a fundamental theory while GSM is an effective theory, and we describe some circumstances under which Gibbsian calculations coincide with the the Boltzmannian results. We then point out that regarding GSM as an effective theory has important repercussions for a number of projects, in particular attempts to turn GSM into a non-equilibrium theory.

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1 Introduction

Statistical mechanics (SM) is one of the pillars of modern physics. It predicts equilibrium properties of a wide range of materials; it explains phase transitions; and it successfully reproduces thermodynamic results. Yet things get involved as soon as we ask what SM is. The issue is that there are two different theoretical approaches in SM, one associated with Boltzmann and the other with Gibbs. We refer to them as Boltzmannian SM (BSM) and Gibbsian SM (GSM) respectively. The copresence of two different approaches would itself not be a cause for concern if it were the case that the two formalisms were equivalent, or at least somehow inter-translatable (as, for instance, the Schrödinger and the Heisenberg picture in quantum mechanics). Unfortunately they are not. The theoretical apparatus of the two approaches are fundamentally different. They offer distinct descriptions of the same physical system and there is no obvious way to translate the concepts of one formalism into those of the other.

GSM is the workhorse of the practitioner. It provides the tools and methods to carry out a wide range of equilibrium calculations, which is why physicists often regard it as 'the' formalism of statistical mechanics.[1] However, as Lavis (2005, 246) notes, when confronted with the question of 'what is actually going on' in a physical system, physicists are often quick to desert GSM and offer an account of 'why SM works' in terms of BSM because GSM has number of features that jar with foundational accounts. And discrepancies are not restricted to foundational issues. In non-equilibrium situations BSM is usually the theory of choice because despite many attempts to extend GSM to non-equilibrium, no workable Gibbsian non-equilibrium theory has emerged (see Sklar (1993), Uffink (2007) and Frigg (2008) for reviews). But how can one use one formalism to explain the non-equilibrium behaviour of physical systems and to give a foundational account of SM, while keep using the other formalism for everyday equilibrium calculations?

There have been attempts to downplay the tension between BSM and GSM by arguing that the two formalisms end up producing the same predictions, at least as far as equilibrium calculations are concerned, and that discrepancies concerning foundational issues is something that we can live with.[2] While is is true that Boltzmannian and Gibbsian calculations agree in some cases, this agreement is not universal. There

[1] Two examples illustrate this attitude. Isihara (1971) introduces the Gibbs formalism in a chapter called 'principles of statistical mechanics' and the first chapter of Landau and Lifshitz's (1980) canonical introduction, entitled 'the fundamental principles of statistical physics', is dedicated entirely to a discussion of the Gibbs formalism.

[2] See, for instance, Davey (2009, 566-567) and Wallace (2015, 289). Arguments for special cases are given in Lavis (2005).

are cases in which GSM and BSM either make conflicting *predictions* about a system's equilibrium properties or GSM remains silent (which is the case depends on how GSM is interpreted, as we will see). The two formalisms not only differ in their theoretical characterisation of physical situations; they are also not empirically equivalent. This forecloses the escape route of non-committal pluralism, and any attempt to understand how SM works has to offer an account of the relation between BSM and GSM.

Somewhat surprisingly the problem of the status of one theory vis-à-vis the other has attracted rather little attention. Where it is discussed, either it is argued that GSM and BSM have to be reconciled (Lavis 2005) or it is suggested that GSM is the preferred formulation of SM (Wallace 2015). We are taking a different route and claim that BSM is a fundamental theory while GSM is an effective theory. This means that BSM provides a true description of the systems within the scope of SM; GSM offers an algorithm to calculate values defined by the fundamental theory. The algorithm is often easier to handle than the fundamental theory and provides result where the fundamental theory is intractable. As every effective theory, GSM works only within a certain domain of application. We provide a characterisation of the limits of GSM and show that BSM provides the correct results in cases in which the two theories disagree. This answers the question of how BSM and GSM relate to one another.

The paper is structured as follows. In Section 2 we introduce BSM and GSM and note that they are not empirically equivalent. In Section 3 we draw a contrast between fundamental and effective theories and argue that GSM is an effective theory while BSM is a fundamental theory. Effective theories are not universally applicable, and the most useful effective theories are ones for which we know the domain of applicability. In Section 4 we offer sufficient conditions for GSM to provide correct results. In Section 5 we point out that regarding GSM as an effective theory has important repercussions for a number of projects, in particular attempts to turn GSM into a non-equilibrium theory. In Section 6 we conclude our discussion.

We discuss SM in the setting of classical mechanics. We assume that the world is governed by Newton's equation of motion and that force functions are such that the equation has unique solutions, which ensures that the resulting dynamics is deterministic. This is a choice of convenience that we make to keep the technical aspect of the paper manageable. All definitions and results that we appeal to in what follows generalise to stochastic classical systems, and so the conclusions we reach carry over to such systems *mutatis mutandis*.[3] We believe that our conclusions will eventually also bear out in the quantum context, although we note that given the current state

[3]Statements of these relevant definitions and results can be found in our (2017) and (2019a).

of play in quantum SM this claim is largely speculative because no generally accepted quantum formulation of BSM is available.[4]

2 Two Theories

SM describes physical systems like a gas in a container, a magnet on a laboratory table, and a liquid in jar. From a mathematical point of view these system have the structure of a *measure-preserving dynamical system*, i.e. a quadruple $(X, \Sigma_X, \phi_t, \mu)$.[5] X is the system's *state space*, which contains all states that the system's *micro-constituents* could in principle assume. For this reason the states in X are referred to as *micro-states*. In the case of a gas with n molecules, X has $6n$ dimensions: three dimensions for the position of each particle and three dimensions for the corresponding momenta. Σ_X is a σ-algebra of subsets of X, and μ is a measure on Σ_X. The *evolution function* ϕ_t determines how the system's micro-state changes over time. If at a certain time t_0 the system is in micro-state x_0, then it will be in state $\phi_t(x_0)$ at a later time t. If the system is such that the movement of its constituents is governed by an equation of motion such as Newton's equation, then ϕ_t is the solution of this equation. The path that $\phi_t(x_0)$ traces through X as time evolves is the *trajectory through* x_0, and x_0 is the *initial condition*. The system is measure-preserving because it is assumed that ϕ_t and μ are such that the measures of a subsets of X remain invariant under ϕ_t.

At the macro-level the system is characterised by a set of *macro-variables*. Volume, internal energy, and magnetisation are examples of macro-variables. From a mathematical point of view macro-variables are functions hat associate a real number with each point in X; i.e. $f : X \to \mathbb{R}$. If, for instance, f is the magnetisation of the system and the system is in micro-state x, then $f(x)$ is the magnetisation of the system when it is in micro-state x.

BSM and GSM share this characterisation of a system; they disagree on how statistical assumptions are introduced into SM and on what the observables of the theory are. We now introduce each theory and make explicit where and how they differ.

In BSM a system is in a particular *macro-state* at any given time. The macro-state is given by values of the relevant macro-variables. If, for instance, a system is characterised by three macro-variables f_1, f_2, and f_3, then the system's macro-state is

[4] See Dizadji-Bahmani (2011) for a discussion.

[5] Throughout this introduction we aim to keep the technical apparatus to a necessary minimum. Rigorous statements of the relevant definitions and results, as well as further references, can be found in Werndl and Frigg (2015) and (2019b).

defined by a particular set of values for these variables.[6] Macro-states thus defined *supervene* on micro-states, meaning that one cannot change the system's macro-state without also changing its micro-state. This determination relation is usually many-to-one, meaning that many different micro-states are realisers of the same macro-state. For this reason every macro-state M is associated with a *macro-region* X_M consisting of all micro-states for which the system is in M. For a complete set of macro-states the corresponding macro-regions form a partition of X (meaning that the different X_M do not overlap and jointly cover X).

One of these macro-states is the system's equilibrium macro-state. Intuitively a system is in equilibrium when its properties do not change. As an example take a gas in a container that is equipped with measurement devices that record its pressure, volume and temperature. We say that the gas has reached equilibrium if the values of these macro-variables do not change. This intuition is enshrined in thermodynamics, where a system is said to be in equilibrium when all change has come to a halt and the system's thermodynamic properties remain constant over time (Fermi 2000, 4). Unfortunately this definition of equilibrium cannot be implemented unmitigated in SM. The reason is that measure-preserving dynamical systems exhibit Poincaré recurrence and time reversal invariance. This has the consequence that a system, when its time evolution unfolds without any outside influence, will eventually return arbitrarily close to the micro-state where it started. This means that a system that started out of equilibrium (for instance, when the gas was confined to one half of the container) will eventually return to that state. This may take a very long time, but it is a given that it will happen eventually. So in the context of SM no system will remain in any state ad infinitum.

This precludes a definition of equilibrium as the state which the system never leaves once it has reached it. Different formulations of BSM offer different prescriptions of how this state is singled out. We adopt the *long-run residence time definition of equilibrium* which aims to come as close to the thermodynamic definition of equilibrium as the mathematical constraints imposed by measure-preserving dynamical systems permit (Werndl and Frigg 2015).[7] The intuitive idea underlying this approach is to define the *equilibrium mocro-state* of a system as the macro-state in which the system spends most of the time for most of the initial conditions. One way to make this intuition precise is to say that an equilibrium state is such that the system spends

[6]Defining macro-states thought *exact* values is an idealisation and in reality macro-states will be defined through certain ranges of values. Nothing in what follows depends on this.

[7]For a discussion of alternative definitions see Werndl and Frigg's (2015). Those who are familiar with a definition of equilibrium in terms of Boltzmann's combinatorial argument – as introduced, for instance, in Albert's (2000) – can rest assured that the two definitions single out the same equilibrium state in cases where combinatorial considerations apply.

more than half of its time in it. If mathematics was kind on us this would be the case for all initial conditions. However, it is well known that in general there will be initial conditions that fall out of line. So the best one can achieve is to require that *most* initial conditions lie on trajectories that the spend more then half of the time in the relevant macro-state. Formalising this idea yields the following definition of equilibrium. Let α be a real number in the interval $(\frac{1}{2}, 1]$, and let $LF_M(x)$ be the long run fraction of time that a system that starts in initial condition x spends in X_M. Then consider the following condition: for a given macro-state M there exists a subset Y of X so that $\mu(Y) \geq 1 - \varepsilon$ for a very small positive real number ε and so that $LF_M(x) \geq \alpha$ for *all* initial states x in Y. If there exists a macro-state that satisfies this condition, then it is the system's equilibrium macro-state. The corresponding macro-region X_M is its *equilibrium macro-region*. The Boltzmannian *equilibrium value* F of the macro-variable f is the value that f assumes in the equilibrium macro-state: $F = f(x)$, where x lies in the system's equilibrium macro region X_M. If such an equilibrium exists, then one can prove that $\mu(X_M) \geq \alpha(1-\varepsilon)$, which means that the equilibrium macro-region is the largest macro-region.[8]

It is a consequence of this definition of equilibrium that a system is not always in equilibrium and that it can – and in fact does – fluctuate away from equilibrium. This marks a radical departure from thermodynamics, and so it is worth pointing out that this is not merely a concession to the demands of measure-preserving dynamical systems. Having no fluctuations at all is not only mathematically unattainable; it is also physically undesirable. Experimental results show that equilibrium is not the immutable state that classical TD presents us with because systems exhibit fluctuations away from equilibrium (MacDonald 1962; Wang et al. 2002). Thus strict equilibrium is actually *unphysical* and adopting a notion of equilibrium that allows for fluctuations increases the empirical adequacy of the theory.

One may wonder what is 'statistical' about BSM. It turns out the probabilities can be introduced in different ways into BSM. Boltzmann (1877) original idea was to attach probabilities to macro-states themselves and postulate that the probability of finding a system in macro-state M at time t is proportional to the measure of the macro-region of that state: $p_t(M) = c\,\mu(X_M)$, where c is a constant. Contemporary authors, most notably Albert (2000), attach probabilities to micro-states within a macro-region and then use these to calculate transition probabilities from one macro-

[8] An alternative reading takes 'most of the time' to refer to the fact that the model spends more time in the equilibrium state than in any other state, which leads to a different definition of equilibrium. Boltzmannian equilibrium macro-states need not be unique in that a system can have two (or even more) equilibrium macro-states if it spends equal amounts of time in each of them and if these residence times are longer than the residence time for all other macrostates. For details see Werndl and Frigg's (2015)

state to another. Either of these positions has its pros and its cons (see Frigg (2010) for a discussion). In what follows it does not matter which of these approaches is adopted.

The core object of study in GSM is a probability density (or distribution) $\rho(x,t)$ over X.[9] The density $\rho(x,t)$ reflects the probability of finding the state of a system in a region $R \subseteq Z$ at time t:

$$p_t(R) = \int_R \rho(x,t)dx. \tag{1}$$

On physical grounds the probability density must be conserved, meaning that for every region $R(t)$ of X that is moving forward under the time evolution ϕ_t the probability must be constant. If the time evolution is generated by Hamiltonian equations of motion this is the case if, and only if, the Liouville's equation holds (Tolman 1938).

Gibbs introduces what he calls the *condition of statistical equilibrium* (1902, 8). A probability density is in statistical equilibrium iff it is stationary, meaning that it does not change under the dynamics of the system: $\rho(x,t) = \rho(x)$ for all t. Usually there are a large number of stationary density functions for a given ϕ_t and so the question arises which of these should be chosen to characterise a given physical situation. Gibbs showed that the so-called *microcanonical distribution* describes a physical system in equilibrium when the system is completely isolated from its environment and that the so-called *canonical distribution* should be used when the system is in contact with a heat bath.[10]

At this point the question arises how Gibbsian ensembles connect to observations on physical system. According to GSM, what does an experimentalist observes when measuring, say, the magnetisation of a sample of iron? To answer this question we first introduce the *phase average* $\langle f \rangle$ of a macro-variable f:

$$\langle f \rangle = \int_X f(x)\rho(x,t)dx. \tag{2}$$

[9] In Gibbs' (1902) original presentation $\rho(x)$ is glossed as representing an ensemble, an infinite collection of independent systems that are all governed by the same laws of motion but are in different states. Alternative presentations endeavour to avoid reference to ensembles and regard GSM simply as probabilistic algorithm. What follows does not depend on how interpretational issues are settled and so we set this question aside. Different interpretations of GSM are discussed in Frigg and Werndl (2019).

[10] The microcanonical distribution is a constant distribution on the system's energy hypersurface $H(x) = E$, and the canonical distribution is given by $e^{-H(x)/kT}/\zeta_T$, where H is the system's Hamiltonian, T is the temperature, k is the Boltzmann constant, and ζ_T is the so-called *partition function*. For a review of different strategies of justifying the choice of these distributions see Myrvold's (2016), and Frigg and Werndl's (2019).

If the system is in statistical equilibrium, then $\langle f \rangle$ is time-independent. The standard way to establish a connection between Gibbsian ensembles and observable results is to appeal to the *averaging principle* (AP). This principle posits that when observing the physical quantity associated with f on a system in equilibrium, then the observed equilibrium value of f is the phase average $\langle f \rangle$. A recent review of textbooks of statistical mechanics showed that many textbooks on GSM explicitly state and endorse this principle.[11] Examples are Chandler, who calls AP '[t]he primary assumption of statistical mechanics' (1987, p. 58), and Pathria and Beale, who regard AP as the 'the most important result' in SM (2011, p. 31). For this reason we base our discussion in Sections 3 and 4 on a version of GSM that incorporates AP. There is, however, an alternative interpretation of GSM that does not accept AP. We comment on how this alternative version of GSM fits into our tale at the end of Section 3, where we also point out that our main conclusions equally holds in this interpretation.

These brief accounts of BSM and GSM make it clear how different the two theories are. Chief among the differences is their conceptualisation of equilibrium. BSM introduces macro-states and defines the equilibrium macro-state as the macro-state in which the system spends most of its time. It thereby explicitly allows for systems to fluctuate away from the equilibrium state every now and then. GSM does not recognise macro-states and instead introduces a probability density over the system's state space. Equilibrium is a property that pertains to the probability distribution, and is defined as the distribution being stationary. Observable equilibrium properties are equated with the phase averages of macro-variables, which are constant over time if the distribution is in equilibrium.

So we seem to be in a somewhat schizophrenic situation. When we talk about 'statistical mechanics' it is unclear whether we mean BSM or GSM or both, and the two are clearly not just notational variants of the same physical principles. This is disconcerting. A first reaction might be to try to mitigate the severity of the problem by arguing that despite their theoretical differences, the formalisms are empirically equivalent, at least as far as equilibrium properties are concerned.

This raises the question of what it would mean for the to theories to be empirically equivalent. The Boltzmannian notion of equilibrium is designed to mirror the thermodynamic notion of equilibrium, and the Gibbsian notion of statistical equilibrium is connected to thermodynamic equilibrium through the averaging principle. This suggests that Gibbsian phase averages, Bolzmannian equilibrium values, and thermodynamic equilibrium should all coincide. This provides a necessary condition for

[11] For an extensive discussion of this principle see Werndl and Frigg's (2019a) and references therein.

the empirical equivalence of BSM and GSM. Consider a macro-variable f and let F be the Botzmannian equilibrium value of the macro-variable f. It is then a necessary for BSM and GSM to be empirically equivalent that

$$F \approx \langle f \rangle \tag{3}$$

holds for *all* macro-variables f in all systems that fall within the scope of both theories (where $\approx$ means that the two values are approximately equal). We call this the *mechanical averaging principle* and we refer to Equation 3 as the *mechanical averaging equation*.[12]

Unfortunately it turns out that BSM and GSM are not empirically equivalent because F and $\langle f \rangle$ are not always equal, not even approximately. This means that the mechanical averaging equation is not true in general and hence the mechanical averaging principle fails. Boltzmannian equilibrium values and Gibbsian phase averages agree for paradigmatic examples such as the dilute gas with macro-variables that assign the same value to all states that are in the Maxwell-Boltzmann distribution (or in a distribution that is very close to the Maxwell-Boltzmann distribution), but Gibbsian and Boltzmannian calculations come apparat in the six vertex model and the Ising model where Gibbsian phase averages fail to agree with Boltzmannian equilibrium values for important maco-variables such as internal energy, polarisation, and magnetisation (Werndl and Frigg 2019a). These are core examples of SM systems and hence discrepancies between Boltzmannian and Gibbsian predictions cannot be dismissed as formal contrivances at the fringes of the practice of the discipline.

3 A Tale

The failure of empirical equivalence brings to a head the problem of the status of BSM and GSM vis-à-vis each other. It also raises the question of which prediction is correct if they disagree. The solution to this conundrum, we suggest, lies in the realisation that BSM and GSM are not alternative theories that are on par with each other: BSM is a fundamental theory while GSM is an *effective theory*, and in situations where Boltzmannian and Gibbsian equilibrium values come apart, the Boltzmannian values are the correct values.

What is an effective theory? Physicist James Wells offers the following following characterisation:

[12]The qualification 'mechanical' indicates that the principle connects two mechanical quantities, namely equilibrium values in BSM and GSM.

> "'Effective Theories" are theories because they are able to organise phenomena under an efficient set of principles, and they are effective because it is not impossibly complex to compute outcomes. The only way a theory can be effective is if it is manifestly incomplete. [...] Any good Effective Theory systematises what is irrelevant for the purposes at hand. In short, an Effective Theory enables a useful prediction with a finite number of input parameters.' (2012, 1)

As examples of effective theories Wells discusses Galileo's law of falling bodies, the harmonic oscillator, classical gravity, and effective theories of particle masses. Hartmann (2001) discusses low-energy approximations to quantum chromodynamics in nuclear physics and the BCS theory of superconductivity as effective theories.

We suggest adding GSM as a further item to this list because GSM meets Wells' criteria. First, by characterising equilibrium in a wide array of different materials and across different phases as an ensemble with a stationary distribution it offers an *organisation* of phenomena under the umbrella of small set of principles. Second, the principles of GSM are an efficient tool for the *computation* of equilibrium values. In fact, as note earlier, in many applications it is GSM that delivers the results because it offers actionable principles and tractable methods to calculate equilibrium values of large array of materials. Third, GSM is *incomplete* in a number of ways. As we have seen in Section 1, GSM is unconcerned with the dynamics of the model. The role of the system's dynamics in GSM is limited to ensuring that a stationary distribution emerges from the dynamics, but no other features of the dynamics is taken into account. GSM considers neither equations of motion nor dynamical laws; it completely disregards trajectories; no time averages along trajectories are studied; and the initial conditions are left unspecified.[13] In fact the Gibbs formalism does not even distinguish between models with deterministic and a stochastic time evolution! The Gibbsian phase averages are the same for all time evolutions that are such that ρ is invariant over time, no matter how different they may otherwise be. The system's dynamics is considered immaterial to understanding equilibrium as long as it – somehow – produces the stationary distribution that enters into the calculations.[14]

[13]Notions of this kind are sometimes considered in attempts to justify the Gibbsian formalism, but they are not part of the formalism itself. For a discussion of justificatory endeavours see, for instance, Sklar (1993).

[14]The system's Hamiltonian is used in formulating the most common Gibbsian distributions. But a Hamiltonian by itself does not pin down the system's dynamics; it specifies a system's time evolution only when combined with an equation of motion. The same Hamiltonian can give rise to deterministic time evolution when plugged into Hamilton's equations of motion, or to a stochastic time evolution when used in the formulation of a stochastic process. If we allow for the substitution of classical variables by self-adjoint operators, we can also plug the same Hamiltonian into the Schrödinger equation and thereby generate a quantum time evolution. The differences between

Finally, GSM is explicit about what it regards as immaterial and about what it omits. In this sense GSM *systematises* what it regards as irrelevant.

BSM is quite unlike GSM in these respects. Dynamical considerations occupy centre stage in BSM. It introduces macro-states with corresponding macro-regions, and then defines equilibrium in explicitly dynamical terms (namely as the macro-state whose macro region is such that, in the long run, the system's state spends most of its time in that macro region). As noted in the introduction, we work under the assumption that the world is governed by Newton's equation of motion. In such a world the dynamics considered in BSM is the true dynamics at the fundamental level: the unabridged and unidealised dynamics with all interactions between all micro-constituents of the system. Equilibrium results from macro-states that are defined in terms of macro-variables that supervene on the true micro-dynamics of the system, and where a system fluctuates away from equilibrium it does so as a result of the true underlying dynamics. In a classical world the theory gives a full account of all this - nothing is left out and nothing is averaged over. BSM tells the complete fundamental theory of SM systems.

True complete fundamental theories cannot be wrong, which implies that the BSM results are the correct ones when BSM and GSM disagree. Experimental results confirm this. Consider the example of magnet with the macro-variable of total magentization m. Such system can be represented by the Ising model. Calculations in BSM show that below the critical temperature the Ising model has two Boltzmannian equilibrium values $m = M$ and $m = -M$, corresponding to the maximum magnatization pointing upward and downward (Baxter 1982). The system flips back and forth between these states spending an equal amount of time in each state, and the frequency of the flips gets lower as the size of the system increases. GSM by contrast yields a phase average of $\langle m \rangle = 0$. Experimental results show that magnets indeed flip back and forth between $m = M$ and $m = -M$ and the magnetisation is hardly ever zero.

There is often a tradeoff between fundamentality and practicality, and our case is no exception. Not only does BSM not offer an effective algorithm of computation; it is often intractable. If one wants to find out whether a Boltzmannian equilibrium exists, and if so, determine the equilibrium state, then one has to explicitly specify the macro-state structure of the model and determine the macro-states' macro-regions; one has to know enough about the underlying dynamics to be able to calculate the long-run fractions of time that a model spends in each macro-region; and one has to be able to estimate the measure of the set of initial conditions that lie on trajectories

these different time evolutions is not reflected in the Gibbs formalism.

that do not have well-behaved long-run fractions of time. In many cases this is asking for too much because it requires more information than we have.[15]

Against this background we come to see GSM's omissions as an advantage rather than as a weakness – they are precisely what makes GSM effective! But relegating a host of things to the realm of irrelevance comes at a cost. Wells point out that whenever we recognise a theory as an effective theory we have to

> 'confront a theory's flaws, its incompletenesses, and its domain of applicability as an integral part of the theory enterprise. The most useful Effective Theories are ones where we know well their domains of applicability, and can parametrically assess the uncertainties induced by ignoring the "irrelevant."' (*ibid.*)

So the flipside of recognising a theory as an effective theory is that we should be able to delimit its range of application: we have to be able to say when a theory yields trustworthy results and when its procedures fail to deliver. In concrete terms we are now faced with the question: under what conditions does GSM yield correct results, i.e. results that coincide with BSM?

4 Domains of Effectiveness

As noted in Section 2, for BSM and GSM to agree on a system's equilibrium properties it must be the case that $F \approx \langle f \rangle$, where F is the Boltzmannian equilibrium value. This can be the case under different conditions. In this section we discuss two conditions that are individually sufficient for this result to hold: the Khinchin condition and the requirement that fluctuations be small. These conditions are, however, not necessary and there will be other conditions, such as the so-called average equivalence theorem and the cancelling out theorem (Werndl and Frigg 2019a). In fact, currently there is no complete list of conditions under which $F \approx \langle f \rangle$, and we have doubts that there will ever be such a list.

Phase averages and Boltzmannian equilibrium values are trivially identical if the macro-variables under considerations take the same value everywhere: $f(x) = c$ for all x in X and a constant c. In this case we have $F = \langle f \rangle = c$. Such macro-variables are uninteresting, but the they raise a useful question: how far does one have to move away from the case $f(x) = c$ to obtain an interesting condition while still retaining the basic idea? An answer to this question is provided by what is now known as

[15] If ϕ_t is ergodic, then BSM readily yields results. But ergodic systems are few and far between, and it is often difficult to determine whether or not a given dynamical law is ergodic.

the Khinchin condition.[16] To formulate the condition we introduce the notion of a *fluctuation*. Take a micro-state x and consider the difference between the value $f(x)$ (the true value if the model is in state x) and the phase average:

$$\Delta f(x) = f(x) - \langle f \rangle. \tag{4}$$

$\Delta f(x)$ is the fluctuation when the system is in micro-state x, and $|\Delta f(x)|$ the *magnitude* of the fluctuation. The *Khinchin condition* then states that there is a subset $\bar{X}$ of X with $\mu(\bar{X}) = 1 - \delta$ for a very small $\delta \geq 0$ such that $|\Delta f(x)| = 0$ for all x in $\bar{X}$.

If the condition is satisfied, then $F = \langle f \rangle$. Assume that a Boltzmannian equilibrium exists and let F be the Boltzmannian equilibrium value of f. The Khinchin condition then guarantees that there are only a few states (of at most measure δ) whose macro-values differ from $\langle f(x) \rangle$. These 'exceptional' states cannot form the Boltzmannian equilibrium macro-state because, as we have seen in Section 2, the macro-region corresponding to the Boltzmannian macro-state is large. For this reason the set of micro-states for which $f(x) = F$ must be the macro-region of the Boltzmannian macro-state, and for the states in that region we have $F = \langle f(x) \rangle$. Hence, if the Khinchin condition is satisfied, then BSM and GSM equilibrium macro-values agree. The paradigmatic examples of such a system is the dilute gas with macro-variables that assign the same value to all states that are in the Maxwell-Boltzmann distribution, or in a distribution that is very close to the Maxwell-Boltzmann distribution (Ehrenfest and Ehrenrest-Afanassjewa 1959).

An alternative approach focusses on the statistics of fluctuations and shows that GSM reproduces, under certain circumstances, the fluctuation pattern of BSM. To see how this happens, let us first have look at fluctuations in GSM. The core idea of the fluctuation approach in GSM is to use the probabilities given in Equation 1 to calculate the probability that a fluctuation of a certain magnitude occurs. Consider an interval $\delta := [\delta_1, \delta_2]$, where δ_1 and δ_2 are real numbers such that $0 \leq \delta_1 \leq \delta_2$. Equation (1) can then be used to calculate the probability for a fluctuation of a magnitude between δ_1 and δ_2 to occur:

$$p(\delta) = \int_D \rho(x) dx, \tag{5}$$

where $D = \{x \in X \mid \delta_1 \leq |\Delta(t)| \leq \delta_2\}$.

[16] The name of the condition is owed to the fact that Khinchin (1949) instigated a systematic study of functions that satisfy strong symmetry requirements and therefore have small fluctuations for systems with a large number of constituents. The condition comes in two version. We here discuss only the first version, which is appealed to in Wallace (2015, 289), Lavis (2005, 267-268); Malament and Zabell (1980, 344-345), and Vranas (1998, 693). The second version originates in Ehrenfest and Ehrenfest-Afanassjewa's (1959, 46-52); for a discussion see Werndl and Frigg's (2019c).

It is important to be clear about the scope of this equation. The probabilities in Equation 1 are sometimes interpreted as being universal in the sense that ρ is seen as providing the correct probabilities for a system's state to be in region R at time t and for *all* R in X and for *any* time t. Under this assumption the fluctuation probabilities in Equation 5 are then seen as beeing universal the sense that for any magnitude and for any time t, $p(\delta)$ would be the correct probability for a fluctuation of a certain magnitude to occur at t. Unfortunately universality of this kind fails. A careful look at GSM reveals that at least one of two conditions have to be met for this to be the case (Frigg and Werndl 2019). The *masking condition* requires either that the system can access all parts of the phase space, or, if that is not the case, that f must be such that the proportion of states for which f assumes a particular value is the same in each invariant subset of X. The condition of *f-independence* (roughy) states that the the system's dynamics must be such that the probability of finding a specific value of f in two consecutive yet sufficiently temporally distant measurements must be independent of one another. The Gibbsian ρ can be used to calculate correct fluctuation probabilities only if ϕ_t and the macro-variable f work in tandem to guarantee that at least one of these conditions is satisfied. These conditions limit the scope of GSM in determining fluctuations because both conditions are strong and their satisfaction cannot be taken for granted.

Let us now look at BSM and first focus on the masking condition to explain, from the perspective of BSM, why the fluctuation probabilities of equation (5) turn out to be right. The starting point here is to consider the fluctuations that arise in the same system when we observe its behaviour over time. This amounts to tracking a system over an infinite period of time when the system starts in a particular initial condition and its state evolves under the dynamics of the system. If the masking condition holds, either the system can access all parts of X or the proportion of states for which f assumes a particular value is the same in each invariant subset of X. This immediately implies from a Boltzmannian perspective that the fluctuations that arise in the same system over an infinite period of time are equal to the probabilities assigned to the fluctuations by the measure ρ, i.e. equation (5) holds. In particular, assume that a system spends, say, β of its time in a certain macro-state for which the function f assumes the value F'. For this macro-state the magnitude of the fluctuation away from the phase average is $|F' - \langle f \rangle|$. Assume δ_0 is the interval that consists only of $|F' - \langle f \rangle|$. The probability $p(\delta_0)$ must then be β.

Let us now focus on the second case of f-independence and explain from the perspective of BSM why the fluctuation probabilities of equation (5) turn out to be right. Consider again a system and an observable f with a finite number of macro-states. Then suppose that the dynamics of the system is such that for two points of time t_1

and t_2 that are sufficiently far apart f-independence is satisfied, i.e. the probability of finding a specific value of f in the two measurements are approximately independent of each other. Then it immediately follows from the Boltzmannian perspective that, given a specific macro-value at t_1, the probability of finding the system in a macro-value at t_2 is given by the probability measure ρ, i.e. equation (5) holds. In particular, assume that the measure assigns β to a certain macro-state for which the function f assumes the value F'. For this macro-state the magnitude of the fluctuations away from the phase average is $|F' - \langle f \rangle|$. Assume δ_0 is the interval that consists only of $|F' - \langle f \rangle|$. Then, given that the system was in a certain macro-state at t_1 the probability of obtaining the fluctuation δ_0 at t_2 is given by the probability $p(\delta_0)$ and is β.

In sum, we have seen that GSM can be used as an effective theory if the macro-variable satisfies the Khinchin condition, or if the system satisfies either the masking condition and the f-independence condition. As noted previously, these are sufficient but not necessary, and so there can be other conditions under which GSM can be used as an effective theory.

As noted in Section 2, there is an alternative interpretation of GSM that does not include AP. On such an interpretation the theoretical core of GSM contains only ρ, while Equation 3, the mechanical averaging equation, has the status of a pragmatic rule that is adopted *only when it provides correct results*. When this equation fails, GSM is simply silent about the correct equilibrium values. This move immunises GSM against arriving at calculations that disagree with the calculations of BSM, but it does so at the cost of further restricting the scope of GSM. This is not *per se* objectionable, but it changes nothing fundamentally in our argument. On this alternative interpretation GSM is an still an effective theory with a limited range of applicability (and the limits are identical to the limits of the standard interpretation). The only difference is that in cases where GSM would disagree with BSM, it is now seen not as giving wrong results but as it providing no results at all.[17]

[17]Furthermore, as argued in Frigg and Werndl (2019), there is no single reasonable interpretation of Gibbs that can make sense of all the successful applications of Gibbs. Reasonable interpretations of Gibbs such as the fluctuation account can always only explain some of the applications of GSM. That there is no single reasonable interpretation of Gibbs that can account for all successful applications of GSM further strenghtens the view that GSM is an effective theory.

5 Reverberations

Classifying GSM as an effective theory is not merely physical botany for the consolation of those interested in labels. It has far-reaching consequences for foundational debates. If we understand GSM as an effective theory, this implies that GSM does not address foundational questions and that such questions should not be discussed in that theory. The relevant question to ask about GSM is: under what conditions does it provide accurate results? Asking whether GSM provides a correct fundamental description of the world, or, if the answer to this question is negative, trying to revise GSM so that it does provide such a description, is a mistaken endeavour. Effective theories do not offer fundamental descriptions; they are calculatory devices of instrumental value; no more and no less.

This has profound implications for non-equilibrium SM. Consider the approach to equilibrium. It is a well-known problem that Gibbs entropy is a constant of motion, which undercuts attempts to describe the approach to equilibrium as a process of increasing entropy.[18] This sparked an entire research programme aiming to revise GSM in such a way that the Gibbs entropy increases over time. Coarse-graining combined with a mixing dynamics, interventionism, and attempts to redefine Gibbsian equilibrium in a way that avoids reference to stationary distributions are but the most prominent proposals in that programme.[19] For those who regard GSM as effective theory such attempts get started on the wrong foot. If the Gibbs entropy does not change over time, we should conclude that GSM does not offer an effective description of non-equilibrium processes and limit its range of applicability to equilibrium situtions rather than trying to turn GSM into a correct description of non-equilibrium processes. Such a programme would be justified only if it turned GSM into an effective theory of non-equilibrium processes. But at least so far this has not happened. Non-equilibrium versions of GSM are not effective non-equilibrium theories. Not only do they not offer manageable algorithms to compute outcomes (thereby violating Wells' first criterion); they often also are not empirically adequate (spin echo experiments are a case in point). Unless there is clear instrumental upshot, the effort to turn the Gibbs entropy into a non-conserved quantity is an ill-motivated project.

Foundational questions concerning GSM remain valid when they concern the empirical adequacy of the theory or its connection to the fundamental theory, BSM. An example of such a question is the one we addressed in the previous section, namely under what circumstances Gibbsian and Boltzmannian values coincide. Another is

[18] The Gibbs entropy is defined as $\int_X \rho \ln(\rho) dx$.

[19] For a review and discussion of these proposals see Frigg (2008), Sklar (1993) and Uffink (2007).

the problem of the justification of maximum entropy methods. In many applications one does not first write down the fundamental dynamics and then derive the invariant outcome measure from that dynamics. What happens is rather the opposite: one first postulates the outcome measure and then narrows down a class of dynamical laws to the ones that are such that the postulated measure turns out to be invariant (for instance, to ergodic motions in the deterministic case or irreducible Markov chains in the stochastic case). The choice of the outcome distribution is often guided by maximum entropy considerations, and there is a legitimate question why these considerations work. For want of space we cannot pursue this question here and refer the reader to Uffink (1995, 1996) for a discussion.

6 Conclusion

We argued that the schism between the Boltzmannian and the Gibbsian approaches in SM is resolved by recognising that they are not theories on equal footing. While BSM is a fundamental theory, GSM is an effective theory. We presented an account of effective theories and showed that GSM matches the relevant criteria. Effective theories have a limited range of application, which raises the question under what condition GSM yields correct results. We point out that this can happen under different conditions and discuss two of them explicitly, namely the Khinchin condition and the fluctuations account together with the condition that fluctuations satisfy certain additional conditions. These conditions are individually sufficient but not necessary, and other sufficient conditions exist. There currently is no complete list of such conditions and so there are open questions, first, about what other conditions there are to ensure the correctness of Gibbsian results and, second, whether there is complete list of such conditions. Finally, we argued that recognising GSM as an effective theory has clear implications for foundational debates. For instance, if GSM is recognised as an effective theory, programmes that aim to extend GSM to cover non-equilibrium cases seem unmotivated.

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