Quantum Foundations of Statistical Mechanics

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1. Introduction

Statistical mechanics is often taken to be the paradigm of a successful inter-theoretic reduction, explaining high level phenomena (primarily those described by thermodynamics) by the fundamental theories of physics, together with some auxiliary hypotheses.[2] What are the fundamental theories that are taken to explain the thermodynamic phenomena? The lively research into the foundations of *classical* statistical mechanics suggests that using classical mechanics to explain the thermodynamic phenomena is fruitful (see overviews in Sklar 1993; Uffink 2007; Frigg 2008; Hemmo and Shenker 2012; Shenker 2017a,b; and references in all of them). But since in contemporary physics classical mechanics is considered strictly speaking false, the explanation for this success can only be that, where successfully applied, classical mechanics preserves certain explanatory and predictive aspects of the true fundamental theories (see Wallace 2001; Ladyman and Ross 2007). In other circumstances classical mechanics has to be replaced by quantum mechanics (Emch 2007 provides a comprehensive overview of quantum statistical mechanics). In this article we ask the following two questions:

I. How does *quantum* statistical mechanics differ from *classical* statistical mechanics? How are the well known differences between the two fundamental theories reflected in the statistical mechanical account of high level phenomena?

II. How does quantum *statistical* mechanics differ from quantum mechanics *simpliciter*?

To make our main points we need only consider non-relativistic quantum mechanics (see Wallace 2001, Sec. 1 on this point). Most of the ideas described and addressed in this article hold irrespective of the choice of a (so-called) interpretation of quantum mechanics, and so I will mention interpretations only when the differences between them are important to the matter discussed.

2. Quantum mechanical microstates

[1] Forthcoming in Wilson, A. (ed.) *Routledge Companion to the Philosophy of Physics*, Routledge

[2] In my view the scope of statistical mechanics is wider, since it is the type-identity physicalist account of all the special sciences. But in this article I focus on the more traditional and less controversial domain of this theory, namely, that of explaining the thermodynamic phenomena. See Shenker 2017c,d.

The main idea of classical statistical mechanics, for which a quantum mechanical counterpart is sought, is this.[3] According to the *ontology* of classical mechanics every system is, at every moment, in a well defined mechanical state (called *microstate* in statistical mechanics), and this state evolves according to the laws of mechanics.[4] However when we prepare or observe a system we only have *epistemic* access to a *partial description* (or a *coarse grained* description) of its microstate. This partial description pertains to some *aspect* of the system's microstate (*macrovariable* in a term often used to refer to such an aspect). Examples for such aspects are average kinetic energy of the particles, or the energy distribution among the particles, or the time average of these quantities: all give only partial information concerning the system's actual microstates. The great achievement of statistical mechanics is the discovery that such partial knowledge, about an aspect of the prepared microstate of a system, is sufficient to make predictions concerning further aspects of future microstates, and that the thermodynamic properties correspond to those aspects and the thermodynamic regularities correspond to regularities governing those aspects. Of course, the evolution from one microstate to the next (and therefore from one aspect to the next) is governed by the dynamical laws pertaining to the particles, but the discovery is that we don't have to follow all the details of this microevolution to make useful predictions concerning macroscopic phenomena. Instead, the following ideas is used. In general any given aspect of the *actual* microstate (in which a system is prepared, according to the ontology) is shared by many *counterfactual* microstates, that belong to the same equivalence set relative to that aspect (this set is usually called *macrostate*). Since the only thing we know about the actual microstate is that it belongs to some such macrostate, we remain ignorant about which of the microstates in that set is the actual one. Since the microstates in a given macrostate (that *share* a given aspect) *differ* in *other* aspects, their future evolutions may vary from each other quite significantly. And since we do not know which microstate in this set is the actual one, we cannot be sure how the actual microstate will evolve. To express this ignorance notions such as probability or typicality come into play.

(This main idea of statistical mechanics has sometimes been *mistakenly* understood as suggesting that we should be able to observe any aspect of interest and predict its evolution (e.g., the evolution of the aspect of the world's microstate that corresponds to the behavior of the stock market). Sadly, we can only observe *certain specific* aspects of the microstates in our environment, namely those to which our sense organs and measuring devices are physically sensitive, that is, with which they

[3] This idea should be understood in the most general terms, and is shared by the Boltzmannian and the Gibbsian frameworks, discussed in Sec. 3 below.

[4] As used here, the term *microstate* has nothing to do with being small or being part of a whole; as an instructive example think of the microstate of the universe. Others sometimes use the term differently; for example, Goldstein et al. 2016 use "microscopic observable" as pertaining to a small subsystem.

become quantum mechanically entangled due to the interaction Hamiltonian. The thermodynamic magnitudes are some of those aspects.)

Since the terminology in the literature is not uniform we shall use the term *macrovariable* to denote an *aspect* of a microstate, given by its *partial description*, and the term *macrostate* to denote a *set* of microstates that share the same macrovariable. (See discussions of the nature of macrovariables in, e.g., Lebowitz 1993; Callender 1999; Albert 2000; Goldstein and Lebowitz 2004; Earman 2006; Frigg 2008; Wallace 2011[5]).

To find the quantum mechanical counterpart of this idea we first need to learn what can be the *quantum mechanical microstate*. An option that first comes to mind (but which is problematic as we shall see) is that the microstate of a system is its quantum state: a system is prepared in some definite quantum state, but since many quantum states are compatible with this preparation, we remain ignorant as to which of them is the actual one.[6] The ignorance about the quantum microstate should be quantified, as in the classical case, by a probability distribution. In making predictions, to these ignorance probabilities one adds the Born rule concerning the probabilities for measurement outcomes in each of the possible quantum states. The two kinds of probabilities are in play in predicting measurement outcomes, and their combination is described by a *density matrix*. This case is called (following d'Espagnat 1976) a *proper mixture*.

Two problems arise in this picture. The first is that typically thermodynamic systems are entangled with their environments, and therefore do not have separate definite quantum states that we could identify as their microstates. Consequently, although the reduced state of a subsystem, formally obtained by tracing out the environment, is represented by a density matrix, this density matrix *cannot* be understood as expressing ignorance. For this reason this case is called an *improper mixture* (following d'Espagnat 1976). One may argue that, since entanglement is the rule rather than the exception, pure states should not be understood as microstates in statistical mechanics (see Wallace 2001; Linden, Popescu, Short and Winter 2009). But discussing pure states is nevertheless useful, for two reasons. First, the universe is arguably in a (unknown) pure state, from which the states of affairs with respect to sub-systems are derived (see the considerations in Goldstein, Huse, Lebowitz and Tumulka 2016, Sec. 2). Second, in the prevalent case of decoherence interactions with the environment, the observations of a sub-system of interest may resemble, for practical

[5] In Hemmo and Shenker 2015 the terminology is a bit different, and macrostate is used to denote sets of microstates that share a macrovariable that is accessible for a given observer.

[6] In hidden variables theories the microstate may be different.

purposes, those of a system in an unknown pure state.[7] Therefore in this article we discuss both pure states and reduced states.[8]

The second problem in the above picture arises when we ask ourselves what would it mean to prepare a quantum state that has a certain macrovariable. Suppose that we prepare a collection of systems by measuring on each of them the observable M, of which the eigenvalues are M_0, M_1, etc., and collect only those with eigenvalue M_0 (with the corresponding eigenstate or eigensubspace). Unlike the classical case (and except in the special case described below) the result is that all the systems are prepared in exactly the same quantum state[9] (see Peres 1993 on the notion of quantum mechanical preparation). The ensuing evolutions of different systems prepared with same quantum state will, to be sure, be probabilistic in the sense of the Born rule, but this is a result of quantum mechanics *simpliciter*, not of quantum *statistical* mechanics. (Wallace 2013 also argues that there is no justification for the idea that quantum statistical mechanics involves putting probability distributions over quantum states just as classical statistical mechanics involves putting probability distributions over classical states.)

A way to prepare a system with a certain eigenvalue and nevertheless remain ignorant as to its actual quantum state (thus having quantum mechanical counterpart of the classical notion of macrostate) is to measure a degenerate observable in special circumstances, as follows. In the general case, upon measurement of the observable A on some quantum state $|\psi>$, if the outcome is eigenvalue a_n with degree of degeneracy g_n, then according to the projection postulate, the final state is a (normalized) superposition of all the g_n eigenvectors of A associated with a_n. But if the initial quantum state $|\psi>$ is itself one of the eigenvectors associated with a_n then the final state will remain unchanged and will not become a superposition of all the eigenvectors of a_n. This has the following consequence. Suppose that before A is measured, a non-degenerate observable B is measured non-selectively, and then a suitable Hamiltonian is applied on the resulting proper mixture, such that each of the possible eigenstates b_n of B evolve to one of the eigenstates of the degenerate eigenvalue a_n of A. In this case the state of affairs after the measurement of A can be described in terms of a *proper mixture* of the eigenstates associated with a_n, in which each of the eigenstates associated with a_n can be treated as a microstate, the share eigenvalue a_n can be treated

[7] In decoherence models the environment is described in probabilistic terms, and those probabilities arguably describe ignorance. We do not pursue this point here. See Crull (this volume) for more details of decoherence.
[8] In this article we do not address POVMs, since it is hard to understand them realistically. See Wallace 2013, p. 14 and references there.
[9] The states may differ in hidden variables, but I do not discuss those at the moment

as a shared macrovariable, and the set of these eigenstates can therefore form a macrostate – much like in a classical preparation of a macrostate is the core idea of classical statistical mechanics.

Some interpretations of quantum mechanics leave room for ignorance in other ways. In the GRW theory (or I should say family of theories, see Ghirardi 2016) the observer may be ignorant of the actual state of affairs brought about by unknown spontaneous localizations of the wave function. In hidden variables theories the observer is ignorant of the hidden variable, even when the quantum state is known.

3. Quantum mechanical macrostates and synchronic functional relations

The central idea of statistical mechanics (described above) is that in order to account for the thermodynamic regularities only partial information about the microstates is needed, concerning some *macrovariables* of them, that is, concerning the fact that they belong to certain *macrostates* in which all the microstates share the same macrovariables (but differ otherwise). A famous example of a *classical* macrovariable is the *Maxwell-Boltzmann energy distribution* (see Frigg 2008): the very partial information about the microstate of an ideal gas, which says that the energy is distributed among the particles of the gas in the Maxwell-Boltzmann way, yields important explanations and predictions about the gas's behaviour (e.g., that it will obey the *ideal gas law*; see Uffink 2007). In certain conditions however, (of high density or low temperature,) the classical approximation of Maxwell-Boltzmann energy distribution no longer captures the relevant aspects of the gas, and therefore yields wrong predictions. In these circumstances the quantum mechanical distinction between bosons and fermions becomes significant, and the so-called *Bose-Einstein* and *Fermi-Dirac statistics* must be applied to describe the distribution of particles between energy levels (see Emch 2007, Secs. 2.4-2.5).[10] It is natural to *prima facie* treat these statistics as analogous to the classical Maxwell-Boltzmann distribution, and to think of them as quantum mechanical macrovariables, that is, as aspects (given by partial descriptions) of the quantum state. However, as we saw in the previous section, the distinct non-classical features of quantum mechanics entail that the classical notion of macrovariables does not have a straightforward counterpart in quantum mechanics, and that the idea that one can remain partly ignorant concerning the microstate even after a measurement has been carried out is applicable in the quantum domain only in special cases. For this reason we can either focus on these special cases, or opt for a completely different conceptual framework (e.g. that there is no quantum statistical mechanics above and beyond

[10] These cases raise interesting questions concerning individuation, see French and Redhead 1989, and for more recent studies Ladyman 2015 and in this volume.

quantum mechanic simpliciter; see Sec. 6 below and Wallace 2013). We now turn to describe various approaches to quantum statistical mechanics that are offered in the literature.

To describe the different approaches to quantum statistical mechanics it is useful to distinguish between two kinds of regularities that are addressed by thermodynamics: One kind involves *synchronic functional relations*, especially those that hold in equilibrium, like the ideal gas law, and the other involves *diachronic relations*, especially the approach to equilibrium and the second law of thermodynamics (for the distinction between the two latter ones see Brown and Uffink 2001). In this section we focus on synchronic relations, and discuss the diachronic ones in the next section.

In *classical* statistical mechanics there are two main theories concerning synchronic functional relations, usually referred to as stemming from the works of Boltzmann and of Gibbs (see the chapters by Frigg and Werndl in this volume and references therein). In the Boltzmannian theory measured magnitudes are understood as macrovariables, that is, as aspects of the microstates that obtain during a measurement. In the Gibbsian theory measured magnitudes are understood as weighted functions over the entire phase space. (For conceptual problems with the latter theory see Callender 1999, Wallace 2013; for an approaches that combines both theories and thus accounts for both, see Lavis 2005, 2008; Hemmo and Shenker 2012 Ch. 11). In *quantum* statistical mechanics there are two corresponding views. The first view (called "individualist" by Goldstein and Tumulka 2011) states that a system has a given thermodynamic property if it is *either* in a pure state with high amplitudes for eigenvalues corresponding to that thermodynamic property, *or* in a reduced state that entails high probability for the corresponding thermodynamic observations (see Goldstein, Huse, Lebowitz and Tumulka 2016; Linden, Popescu, Short and Winter 2009, and references in both). The second view (called "ensemblist" in Goldstein and Tumulka 2011) states that a system has a given thermodynamic property if it is in an appropriate statistical state, given by a density matrix, which entails a certain expectation value. Perhaps Von Neumann's concept of thermal equilibrium is ensemblist (see Goldstein, Huse, Lebowitz and Tumulka 2016 sec. 9.2; Goldstein and Tumulka 2011; Goldstein, Lebowitz, Mastrodonato, Tumulka and Zanghi 2010), and Emch (2007) seems to follow this line as well. The conceptual problems in the classical Gibbsian approach carry over to the quantum mechanical domain, *mutatis mutandis* (see Wallace 2001, 2013). From now on we focus mainly on individualist approaches.

An important example of a (synchronic) thermodynamic property, that needs to be explained in quantum statistical mechanics, is that of *being in thermal equilibrium*. In thermodynamics, thermal equilibrium has three main characteristics. First, the temperature is spatially uniformly distributed;

we call this condition "*uniformity*" (in other kinds of equilibrium this condition is replaced by similar ones, e.g. spatially uniform pressure or spatially uniform chemical mixture). Second, the uniformity condition is stationary: the system reaches it and remains there indefinitely; we call this condition "*stability*". Third, when the uniformity and stability conditions obtain the *entropy* of the system is maximal (the notion of entropy is addressed below). Statistical mechanics adds a fourth condition: In the *individualist* theory of *classical* statistical mechanics it was argued (by Boltzmann, see Uffink 2004) that the set of microstates of an ideal gas that satisfies the uniformity condition has the largest Lebesgue measure; we call this the "*big set*" condition. The Lebesgue measure of macrostates has since then been associated with entropy, thus connecting the third and fourth conditions; and attempts have been made to show that this set also satisfies the stability condition (we expand on these attempts in the next section).[11] The idea that the four conditions of uniformity, stability, entropy and big set are interconnected has been generalized to the quantum mechanical realm. In the next section we discuss the quantum mechanical counterparts of the stability condition, and in the present section we will say a few words about the quantum mechanical counterparts of the big set and uniformity conditions, and (finally) of the notion of entropy.

An example of the big set condition in quantum statistical mechanics is given by Goldstein and Tumulka (2011). Consider a quantum state ψ, expressed as a superposition of energy eigenstates all of which are in a given energy shell. And suppose that there is a subspace H_{eq} whose dimensionality is almost that of the entire space H: $\dim(H_{eq})/\dim(H)\approx 1$. Then ψ satisfies the big set characterization of equilibrium if the projection P_{eq} of ψ onto H_{eq} is $<\psi|P_{eq}|\psi>\approx 1$. Of course, the only reason for focusing on the big set condition to begin with is the thought that that it is connected to the other characteristics of thermodynamic thermal equilibrium. The quantum mechanical counterpart of the uniformity condition, in this context, could be that upon measurement of the appropriate observables on ψ one is extremely likely to end up with eigenvalues that correspond to a uniform temperature distribution (see the characterization of this desideratum in Goldstein, Huse, Lebowitz and Tumulka 2015, 2016. Linden, Popescu, Short and Winter 2009 generalize the quantum mechanical uniformity condition.).

In order to examine the (alleged) connection between the big set condition and that of high entropy we must first identify the quantum mechanical counterpart of the thermodynamic notion of entropy. In thermodynamics entropy difference is usually understood as quantifying the change in the degree

[11] In the ensemblist approach the "big set" condition is replaced by the condition of a dynamically invariant probability distribution.

to which the energy of a system can be exploited to produce work.[12] In mechanics, in general, the more *control* one has over the system's microstate, the more one can exploit its energy; and assuming that more information about a system's state contributes to its controllability, it is reasonable to say that the more *information* we have about a system's state, the more its energy is exploitable, and therefore it is natural to associate entropy with information (see more on control in this context in Wallace 2014).[13] In classical (Boltzmannian) statistical mechanics this idea is realized by associating entropy with the (logarithm of the) Lebesgue measure of a set of microstates. What would be an analogue of the notion of entropy in quantum mechanics that can be understood along these lines? One possibility that immediately comes to mind is the (logarithm of the) dimension of the subspace corresponding to the degenerate eigenvalue of the thermodynamic observable (i.e., the degenerate eigenvalue that corresponds to a macrovariable, as explained in the previous section). The big set characterization of equilibrium in Goldstein and Tumulka (2011) and Goldstein, Huse, Lebowitz, and Tumulka. (2016) and Linden, Popescu, Short, and Winter (2009) (described below) seem to go along these lines.

Another prevalent candidate for the quantum mechanical counterpart of thermodynamic entropy is the so-called *Von Neumann entropy*, $\mathrm{Tr}(\rho\log\rho)$ (see, e.g., Peres 1993, p. 270). Following Von Neumann (1932), all the arguments for this idea are grounded in thought experiments of the kind one finds in thermodynamics: in a cycle of operation, the entropy is balanced by adding the Von Neumann entropy at the right stage. In previous writings (Shenker 1999; Hemmo and Shenker 2006) we have shown that in systems with a finite number of particles the entropy balance is kept without this addition, and concluded that Von Neumann's entropy does not correspond to thermodynamic entropy since it does not satisfy the corresponding functional relations. An alternative line of argument, in support of the claim that Von Neumann's expression refers to thermodynamic entropy, could be that this quantity expresses the essential feature of thermodynamic entropy, namely, the degree of energy exploitability (Peres 1993 seems to have this in mind; see, e.g., pp. 369-70).[14] This may work, as follows. The Von Neumann's entropy corresponds to the degree of uniformity of the probability distribution over the possible outcomes of the next measurement, and if higher uniformity corresponds to lower control over what will be the next quantum state of the system, and if we take degree of control as an essential feature of thermodynamic entropy, then Von Neumann's entropy can be said to correspond to the

[12] This holds only if the Second Law of Thermodynamics is universally true, that is, if Maxwellian Demons are impossible, a topic we discuss in Section 7 below; see Fermi 1936; Hemmo and Shenker 2012, Ch. 1.

[13] The spin echo experiments can be understood as a case where control over the microstate is available despite lack of information concerning it; see Hemmo and Shenker 2012, sec. 6.7.

[14] As we said in a footnote above, entropy is a measure of the exploitability of energy only if the second law of thermodynamics is universally true.

thermodynamic entropy. It should be noted, however, that this quantity is more naturally seen as part of a Gibbsian ("ensemblist") understanding of thermodynamic properties than to a Boltzmannian ("individualist") notion.

4. Diachronic functional relations in quantum statistical mechanics: "finite time" arguments concerning the approach to equilibrium

The thermodynamic law of approach to equilibrium (which is part of, or assumed by, the second law of thermodynamics) says that systems, prepared in non-equilibrium states, will invariably evolve to equilibrium states fixed by the constraints on these system, and remain in them indefinitely (see Brown and Uffink 2001). In mechanics, however, due to the *velocity reversal invariance* of the fundamental microscopic dynamics, given any Hamiltonian, if there are entropy-increasing trajectory segments in the system's state space, then there are also entropy-decreasing ones, and so the thermodynamic law cannot be strictly true. The standard explanation for why we do not encounter anti-thermodynamic evolutions is that those are extremely a-typical or unlikely. The meaning of probability in this context is a subject of ongoing debates in classical statistical mechanics, which carry over to quantum statistical mechanics, as we shall see. (For the debate on the meaning of *typicality* in this context and the difference between typicality and probability see Frigg 2011, Pitowsky 2012, Goldstein 2012, Frigg and Werndl 2012, Hemmo and Shenker 2014).

In the classical domain, two kinds of accounts have been proposed for the law of approach to equilibrium, and both have quantum mechanical counterparts: I call them the *finite time* and *infinite time* accounts. The *finite time* account aims to prove that a system prepared in a microstate that belongs to some non-equilibrium macrostate is highly likely to evolve to equilibrium within a characteristic time interval. The *infinite time* account aims to prove that as time goes to infinity, *typical* systems spend *most* of their time in equilibrium, and therefore if a system is observed at some randomly sampled moment (as it were) then it will most likely be found in equilibrium, and if found out of equilibrium then it is most likely to be in a minimum entropy state from which its entropy will increase. I now expand on the finite time account, and address the infinite time account in the next section.

Consider Figure 1. Suppose that a system is prepared in a microstate which is a member of the macrostate M_0, in which all microstates share the macrovariable M_0. And suppose further that the dynamics is such that the evolution of each microstate in M_0 takes the system to a microstate within region $B(t_1)$ (with the same Lebesgue measure, according to Liouville's theorem) so that if we measure the system at t_1, we shall find it in either macrostate M_0 or M_1 depending on its actual trajectory, with the probability for each such possibility given by the measure of the region of overlap of $B(t_1)$ with M_0 and M_1, respectively. Let us assume, as is usual, that increasingly larger macrostates (by Lebesgue measure) correspond to increasingly uniform temperature distributions, so that the largest macrostate (M_2 in the figure) is the one in which the uniformity condition of equilibrium is satisfied (such assumptions are usually based on combinatorial arguments, following Boltzmann; see Uffink 2007). In these mechanical terms the law of approach to equilibrium would say that the dynamics is such that, with time, the regions $B(t)$ have increasingly larger overlaps with increasingly large macrostates, where "large" is understood relative to some appropriate measure.[15] (For a description of what in statistical mechanics can be proven from mechanics by itself and what requires auxiliary hypotheses see Shenker 2017a,b.) An example for a detailed finite time proof is Lanford's theorem (see Uffink and Valente 2010, 2015).

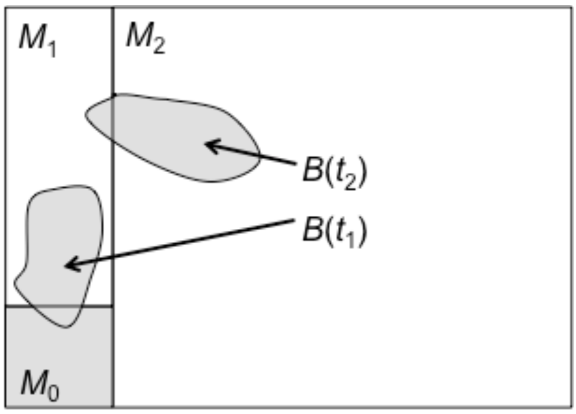

Figure 1: The interplay between dynamics and macrovariables.

A major difficulty in the finite times account (which has a counterpart in quantum statistical mechanics, discussed below) is that due to the *retrodiction invariance* of the underlying dynamics, proving that entropy is highly likely to increases towards the future entails that entropy is equally likely to increase towards the past: this is the so-called parity of reasoning (or minimum entropy) problem. (This holds if pairs of velocity-reversed microstates belong to the same macrostate. This condition is normally assumed implicitly.) Since this result makes the theory internally inconsistent (since entropy is at a minimum at every moment, but is not constant), it had to be solved by adding symmetry-breaking postulates to the theory, that allow only histories in which past entropy was low; in contemporary literature this idea is often called the *past hypothesis* (see Feynman 1965; Albert 2000; Winsberg 2004; Earman 2006; Shahvisi, this volume).

[15] Conceptually, the measure of overlap (that gives rise to probability) and the measure of the macrostates (associated with entropy) need not be the same; see Hemmo and Shenker 2012.

What would be the quantum mechanical counterpart of the classical finite time account of the approach to equilibrium? Suppose that the quantum state ψ has high amplitude for some *non equilibrium* eigenvalue, and the quantum state φ has high amplitude for the *equilibrium* eigenvalue (that satisfies the quantum mechanical counterparts of the four conditions above). A Schrödinger evolution from ψ at t_0 to φ at t_1 is deemed a quantum mechanical counterpart of an approach to equilibrium. However, due to the quantum mechanical counterpart of the classical velocity reversal symmetry, to each such quantum mechanical thermodynamic evolution there exists a corresponding anti-thermodynamic evolution, from the complex conjugate φ^* at t_0 to the complex conjugate ψ^* at t_1. Why then don't we observe anti thermodynamic evolutions? One intuition here employs an analogy to the classical way of thinking: Every standard preparation gives rise to two kinds of quantum states: some states evolve thermodynamically and some evolve anti thermodynamically; and for typical Schrödinger evolutions of thermodynamic systems, the former set is larger (by an appropriate measure). But this line of thinking requires that standard preparations give rise to two kinds of quantum states – whereas, as we said in Section 2, in general quantum mechanical preparations (by measuring some quantum observable M and selecting the systems that end up in some eigenvalue M_0) result in all the prepared systems being in exactly the same quantum state. One solution to this problem, described in Section 2 above, is to suppose that the thermodynamic magnitudes correspond to degenerate eigenvalues of quantum observables, and that the preparations of thermodynamic systems are as outlined in Section 2.[16] Given this assumption the task, of proving a quantum mechanical counterpart of the law of approach to equilibrium, is to follow the dynamical evolution of this set of states and to find the probability (calculated with the suitable density matrix) of finding the system in eigenvalues the correspond to equilibrium.

The parity of reasoning problem has its quantum mechanical counterpart: if – given an appropriately constructed initial quantum macrostate – evolution to quantum states with high amplitudes for equilibrium is highly likely, then it is equally likely that such were the quantum states in the past. A quantum mechanical symmetry breaking *past hypothesis* is, then, needed. In this context the temporal asymmetry of the projection postulate may become significant. Von Neumann (1932) thought that the time asymmetric nature of the projection postulate should be explained on the basis of the thermodynamic regularities (and so the former cannot explain the

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[16] Peres considers a different case, in which there is ignorance concerning the *dynamics* (not the quantum state). He writes: "[A] quantum system prepared in a pure state remains pure when it evolves in a perfectly controlled environment. More generally, the entropy S =-Tr($\rho\log\rho$) remains invariant under the unitary evolution $\rho \to \rho' = U\rho U^\dagger$. On the other hand, if the environment is not perfectly controlled and is only statistically known, we must replace the evolution operator U by an ensemble of unitary matrices Uα , with respective probabilities pα . The dynamical evolution then is [such] that the entropy never decreases" (Peres 1993, p. 369). (We discuss the Von Neumann entropy -Tr($\rho\log\rho$) in Section 6 below.)

latter; *contra* the view described in Sec. 6 below). He wrote (ibid., p. 358): "It is desirable to utilize the thermodynamical method of analysis, because it alone makes it possible for us to understand correctly the difference between [Schrodinger's unitary transformation] and [the measurement transformation], into which reversibility questions obviously enter." (For more details on this argument by Von Neumann see Shenker 1999, Hemmo and Shenker 2006.)

5. Diachronic functional relations in quantum statistical mechanics: "infinite time" arguments

We now turn to the *infinite time* account of the thermodynamic law of approach to equilibrium. According to this approach, "for physical initial states ψ_0 of suitable macroscopic quantum systems, the system will spend most of its time in thermal equilibrium." (Goldstein and Tumulka 2011). Given a quantum mechanical macrostate (in the above sense of the term), and assuming a Schrodinger evolution that is typical of thermodynamic systems,[17] most of the quantum states in this macrostate evolve in such a way that, as time goes to infinity, they spend most of their time in equilibrium (that is, in quantum states in which there is high amplitude for equilibrium eigenvalues). Presumably this approach is made empirically significant by taking it to entail that if a system is observed at some random moment then it is highly likely to be found in equilibrium (in that sense).

A well-known problem in this account is that it entails that if one prepares a system in a non-equilibrium state, the approach to equilibrium could take *eons* and the account would still hold, since it pertains to the *infinite time* limit (see Earman and Redei 1996). Another problem is that (on this view) the probability of equilibrium is already high *immediately after* the system is found far from equilibrium, regardless of the system's dynamics and even if this requires superluminal speeds (see the debate in Allori 2013; Hemmo and Shenker 2015; Allori 2015). These problems, known in the classical context, carry over to the quantum mechanical case. The infinite time approach is nevertheless prevalent, perhaps due to its advantages, especially the fact that it is not subject to the reversibility and parity of reasoning problems (since a system that spends most of the future in equilibrium also spent most of the past in equilibrium.)

Several recent papers in quantum statistical mechanics offer arguments in this spirit. Here we describe very briefly the general gist of two of these arguments, and refer the reader to the literature for the details. One is by Goldstein, Huse, Lebowitz and Tumulka (2016). First these writers show

[17] In its classical version this account is inspired and illustrated by Boltzmann's own arguments in which the dynamics is assumed to be ergodic, where ergodicity should be understood *á la* Birkhoff and Von Neumann, see Frigg 2008, sec. 3.2.4.

that *most* of the pure states in a given energy shell in Hilbert space satisfy a counterpart of the *uniformity condition* of equilibrium, that is: upon measurement of the appropriate observables there is high probability of outcomes that correspond to thermodynamic equilibrium, in the sense of our uniformity condition above. Then they show that those quantum states that satisfy this uniformity condition also satisfy a counterpart of the *big set condition*: they are all close to a certain subspace H_{eq} which (for many systems) has the overwhelming majority of dimensions in the energy shell. Next they need to prove the *stability condition*, which they understand as an *infinite time* theorem. To do so they decompose the Hilbert space into a sum of orthogonal subspaces (called "macrospaces", corresponding to classical sets of microstates that share macrovariables) using approximate commutativity, and identify one of them as H_{eq} ,which has most of the dimensions. Since only a set of states with measure zero lies in subspaces of less than full dimension, most of the states in the energy shell will have their dominant part in H_{eq} and so most of those will also satisfy the (quantum counterpart of the) uniformity condition. They also prove a stronger theorem, namely, that small subsystems of pure state equilibrium systems, entangled with the rest of the system, are also in equilibrium in the sense that if we were to take a quantum measurement of a relevant observable in that subsystem, then the probability distribution over the measurement outcomes would agree with the thermal distribution.

The second infinite time argument we describe here is by Linden, Popescu, Short and Winter (2009). These writers focus on the reduced state of a small system that is entangled with a heat bath, and prove that the subsystem equilibrates for every one of its possible states and for almost every possible state of the bath, and for (what they argue are) prevalent Hamiltonians. While the authors describe thermal equilibrium in terms that are close to our thermodynamic uniformity condition, this is not part of their main theorem; they consider equilibrium to be any state at which the system stays most of the time, which is the stability condition. Their proof connects the big set condition (concerning the relatively very small dimensionality of subspaces of small subsystems) with the stability condition: "Whenever the state of the whole system – and in particular of the bath – goes through many distinct states, any small subsystem reaches equilibrium," and the uniformity condition is supposed to be a special case of this general proof.

Both of the above described results pertain to *most* states, namely, to a large majority of the states considered. Goldstein, Huse, Lebowitz and Tumulka (2016) write that "throughout this paper, 'most' means 'the overwhelming majority of' (or 'all except a small set') relative to the relevant uniform distribution" (Sec. 1 and 4.1), and Linden, Popescu, Short and Winter (2009) write: "In this situation, we have proved that for every state of the subsystem and *almost* every state of the bath, the subsystem equilibrates" (p. 8, our italics). In both cases the idea is that if a condition is true of most cases, this suggests that the condition is also true of a concrete given system, unless we have reason to expect otherwise. Indeed, as in the classical case, all the proofs of the approach to equilibrium in quantum statistical mechanics, both the finite time and infinite time ones, are valid only for *most* of the initial conditions. This also holds for our own proposals in Hemmo and Shenker 2001; 2003; 2005: These results hold only for systems in which the initial conditions lead to environmental decoherence, and according to prevalent decoherence models these results hold at best for most quantum states of the universe, given the right measure.

To establish such *most* proofs one needs to rely on a measure, and the idea is that the theoretical context suggests certain *natural* measures (see also Goldstein, Lebowitz, Mastrodonato, Tumulka, and Zanghi 2010). What makes a measure natural for determining which set of states contains the *most*? The prevalent arguments in *classical* statistical mechanics for taking the Lebesgue measure to be natural for counting initial conditions rely on the fact that this measure has a special status in the diachronic regularities: for example, it is invariant under the dynamics according to Liouville's theorem. However this dynamical fact is irrelevant for counting initial conditions (see Hemmo and Shenker 2014, who criticize on similar grounds also the preference of the quantum mechanical measure in Bohmian mechanics). But in quantum mechanics there seems to be another resource for choosing a measure: can the probabilities in quantum statistical mechanics be the result of the Born rule at the microscopic level? In the next section we describe an attempt to achieve such a result.

6. Can statistical mechanical probabilities be reduced to quantum mechanical probabilities?

Albert (2000, Ch. 7) proposes an approach to quantum statistical mechanics in which the only kind of probabilistic statements are those derived from the micro-dynamics, namely, those of the Born rule. In this proposal standard quantum mechanics is replaced with the GRW dynamics (Ghirardi, Rimini and Weber 1986; Bell 1987). There are several versions of this dynamics (see Ghirardi 2016; Lewis, this volume), but for our purpose it is useful to describe it briefly as follows: Every quantum state φ_1 evolves for some time according to the Schrödinger equation to another quantum state φ_2, and then collapses spontaneously into a third state φ_3, which is a Gaussian superposition of positions centered around some point x. The probability that the spontaneous collapse will take place at any given moment is fixed by the temporal constant in the stochastic equation of motion, and the probability of the position x is fixed by the amplitude of x in φ_2.

Although the GRW spontaneous localizations are in position, when applied to macroscopic systems the result can also appear in the form of thermodynamic magnitudes, which can then be characterized in terms of their proximity to thermodynamic equilibrium (according to the four conditions of equilibrium mentioned above). In order to talk about the approach to equilibrium we shall use the following terminology. Suppose that the eigenvalue a_{eq} of the observable A corresponds to an equilibrium state (e.g., it corresponds to the uniformity condition of thermal equilibrium), and suppose that given a certain Hamiltonian H the quantum state $\psi(t_1)$ evolves to $\psi(t_2)$. If, according to the Born rule, the probability for a GRW spontaneous collapse to a_{eq} is higher in $\psi(t_2)$ than in $\psi(t_1)$ then we shall say that $\psi(t_1)$ is a *thermodynamic* quantum state *relative to H* (Albert 2000 uses the term "thermodynamically normal"). If, given the same dynamic evolution, the probability for a GRW spontaneous collapse to a_{eq} is lower in $\psi(t_2)$ than in $\psi(t_1)$, we shall say that $\psi(t_1)$ is an *anti-thermodynamic* quantum state *relative to H*. The proviso "relative to *H*" is necessary since we ascribe the property of being thermodynamic (or anti-thermodynamic) to the initial state $\psi(t_1)$, although this property is about the relation between $\psi(t_1)$ and the time evolved state $\psi(t_2)$.

Given these definitions, Albert makes the dynamical hypothesis, that the Hamiltonian H that governs thermodynamic systems has the following characterization: *Every* (not only most!) initial state $\psi(t_0)$ has high Born probability to collapse under the GRW dynamics to another quantum state $\psi(t_1)$ which is thermodynamic relative to H, regardless of whether or not $\psi(t_0)$ itself was thermodynamic relative to H. That is, with high probability the state $\psi(t_0)$ will collapse to a state $\psi(t_1)$ that will evolve deterministically, under the Hamiltonian H, to another quantum state $\psi(t_2)$, in which the amplitude for a GRW spontaneous collapse to a_{eq} will be higher than it is in $\psi(t_1)$.

Albert provides no proof for this hypothesis, and his only plausibility argument for it is based on the fact that observed systems are actually thermodynamic. (In comparison, Linden, Popescu, Short and Winter 2009, for example, provide arguments for the plausibility of the particular sort of Hamiltonian they rely on.) Thus Albert's theorem is not a *proof* from first principles that the world is thermodynamic, but only a *conjecture* or an *empirical generalization* that it is so. (See more on Albert's approach in Sklar 2015; Uffink 2002; Callender 2016.)

7. Quantum mechanical Maxwellian Demon

In 1867 J.C. Maxwell proposed a thought experiment, in which a tiny automaton (that came to be known as *Maxwell's Demon*) manipulates the individual molecules of a gas that is initially in uniform temperature, directing the relatively hotter (that is, faster) molecules to one side and the colder (i.e. slower) one to the other side, thus creating a temperature difference, which amounts to an entropy decrease. The result is a total decrease in the entropy of the universe, in violation of the second law of thermodynamics. Since, as things stand now, there is no general proof from first principles that the second law of thermodynamics is (probabilistically) universally true (in neither classical nor quantum statistical mechanics, neither finite nor infinite arguments, neither individualist nor ensemblist approaches), the question of whether a Maxwellian Demon is compatible with fundamental physics became an indirect route to asking about the universal validity of the second law. For this reason numerous attempts have been made to "exorcise" the Demon, that is, show that it is *incompatible* with fundamental physics and hence the second law is true (see Leff and Rex 2003 and Earman and Norton 1998, 1999). But all have failed, and in recent years the *compatibility* of Maxwell's Demon with classical mechanics has been proven (Albert 2000; Hemmo and Shenker 2010, 2011, 2012, 2013, 2016). Interestingly, some central attempts to exorcise the Demon that appear to rely on quantum mechanics (such as Zurek 1984) have turned out to be grounded in classical statistical mechanical ideas (on Zurek's argument see Earman and Norton 1999[18]). It has recently been shown that Maxwellian Demons are also compatible with quantum mechanics, either with or without collapse (Hemmo and Shenker 2012, 2017). These results are significant in that they entail that attempts at a universal proof of the law of approach to equilibrium and the second law of thermodynamics are futile; there is hope only for proofs pertaining to special circumstances – namely, special Hamiltonians and specially prepared quantum states. This realization goes against deeply entrenched convictions, according to which the second law of thermodynamics expresses a universal truth. But if quantum mechanics is the fundamental theory, then this conviction will have to be relinquished.[19]

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[18] Zurek's argument relies on the Landauer-Bennett thesis that was disproved in Hemmo and Shenker 2013.
[19] Scully, Zubairy, Agarwal and Walther (2003) show that a quantum heat engine allows us to extract work from a single thermal reservoir, in violation of Carnot's principle.

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