# AN OBJECTIVIST ACCOUNT OF PROBABILITIES IN STATISTICAL MECHANICS

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## 1 Introduction

The foundations of classical (meaning nonquantum) statistical mechanics can be characterized by the triplet

(i) classical mechanics  $\rightarrow$  (ii) probability  $\rightarrow$  (iii) thermodynamics, and the primary-level classification of theories of probability is between

- (a) *epistemic interpretations,* in which probability is a measure of the degree of belief (rational, or otherwise) of an individual or group, and
- (b) *objective interpretations*, in which probability is a feature of the material world independent of our knowledge or beliefs about that world.

Hoefer (2007, p. 550) offers the opinion that 'the vast majority of scientists using non-subjective probabilities overtly or covertly in their research feel little need to spell out what they take their objective probabilities to be.' My experience (as a member of that group) accords with that view; indeed it goes further, in finding that most scientists are not even particularly interested in thinking about whether their view of probability is objective or subjective. The irritation expressed by Margenau (1950, p. 247) with 'the missionary fervor with which everybody tries to tell the scientist what he *ought* [his italics] to mean by probability' would not be uncommon. The relevant question here is, of course, the meaning of probability in statistical mechanics, and the approach most often used in textbooks on statistical mechanics (written for a scientific, as distinct from philosophically inclined, audience) is to either sidestep discussion of interpretations<sup>1</sup> or offer remarks of a somewhat ambiguous nature. Compare, for example, the assertion by Tolman (1938, pp. 59–60) that in 'the case of statistical mechanics the typical situation, in which statistical predictions are desired, arises when our knowledge of the condition of some system of interest [his italics] is not sufficient for a specification of its precise state' with the remark two pages later that by 'the

<sup>&</sup>lt;sup>1</sup>See, for example, Lavis & Bell 1999, Ch. 2.

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*probability* [his italics] of finding the system in any given condition, we mean the fractional number of times it would actually be found in that condition on repeated trials of the same experiment.'

The intention of this essay is to propose the use of a particular hard-objective, real-world chance, interpretation for probability in statistical mechanics. This approach falls into two parts and is applicable to any system for which the dynamics supports an ergodic decomposition. Following von Plato 1989b we propose the use of the time-average definition of probability within the members of the ergodic decomposition. That part of the program has already been presented in Lavis 2005 and 2008. It is now augmented by the second part, in which a version of Cartwright's (1999) nomological machine is used to assign probabilities over the members of the decomposition. It is shown that this probability scheme is particularly well adapted to a version of the Boltzmann approach to statistical mechanics, in which the preoccupation with the temporally local increase in entropy is replaced by an interest in the temporally global entropy profile, and in which the binary property of being or not being in equilibrium is replaced by a continuous equilibrium-like property which is called 'commonness.' The place of the Gibbs approach within this program is also discussed.

#### 2 The dynamic system

In this section we introduce the dynamic structure of the system and the idea of ergodic decomposition.<sup>2</sup>

## 2.1 Dynamic flow and invariant subsets

The *states* of the dynamic system are represented by points  $x \in \Gamma$ , the *phase space* of the system, and the dynamics is given by a *flow* which is a semigroup  $\{\phi_t \mid t \ge 0\}$  of automorphisms on  $\Gamma$ , parameterized by time  $t \in \mathbb{Z}^*$  or  $\mathbb{R}^*$ . The points of  $\Gamma$  can also form a continuum or be discrete. The Hamiltonian motion of the particles of a gas in a box is a case where both  $\Gamma$  and t are continuous, the baker's gas (see, for example, Lavis 2005) is a case where  $\Gamma$  is continuous and t is discrete, and the ring model of Kac (1959) (see also Lavis 2008) is a case where both  $\Gamma$  and t are discrete.

In the following we shall, for simplicity, restrict most of the discussion to systems, like that of Ex. 2 below, where  $\Gamma$  is a suitably compactified Euclidean space; implying, of course, a metric measuring the distance between points and a Lebesgue measure, which we denote by  $m_L$ . Ergodic decomposition applies to *compact* metric spaces (see Thm A.2), and also to systems, like Ex. 1 below, which have discrete time and a phase space consisting of a finite number of points;

<sup>&</sup>lt;sup>2</sup>For the interested reader the mathematical underpinning of this section is provided in App. A.

there the ergodic decomposition is just the partition into cycles. For all systems the dynamics is assumed to be<sup>3</sup>

- (i) *forward-deterministic*: if the phase point at some time  $t_0 > 0$  is  $x_0$ , then the *trajectory* of phase points  $x_0 \rightarrow \phi_t x_0$ , for all  $t \ge 0$ , is uniquely determined by the flow;
- (ii) *reversible* (or *invertible*): there exists a self-inverse operator  $\mathfrak{I}$  on the points of  $\Gamma$ , such that  $\phi_t x_0 = x_1 \implies \phi_t \mathfrak{I} x_1 = \mathfrak{I} x_0$ ; then  $\phi_{-t} := (\phi_t)^{-1} = \mathfrak{I} \phi_t \mathfrak{I}$ , and  $\{\phi_t\}$  becomes a group, with  $t \in \mathbb{R}$  or  $\mathbb{Z}$ . A forward-deterministic system defined by an invertible flow is also backward-deterministic and thus simply *deterministic*;
- (iii) *autonomous* (or *stationary*): if  $x_0$  and  $x_1$  are related by the condition that, if  $x_0$  is the phase point at  $t_0$  then  $x_1$  is the phase point at  $t_0+t_1$ , then this relationship between  $x_0$  and  $x_1$  would also hold if  $t_0$  were replaced by any other time  $t'_0$ .

Determinism, as defined by (i) and (ii), means that, if two trajectories  $\{x(t)\}$  and  $\{\tilde{x}(t)\}$  occupy the same state  $x(t_0) = \tilde{x}(t_0)$  at some specified time  $t_0$ , then they coincide for all times. If the system is also autonomous, then the determinism condition is generalized to one in which, if two trajectories  $\{x(t)\}$  and  $\{\tilde{x}(t)\}$  have  $x(t_0) = \tilde{x}(t_0+t')$ , then they coincide with  $x(t) = \tilde{x}(t+t')$ , for all times t. The time parameter now measures relative time differences rather than absolute times, and for the trajectory  $\{x(t)\}$  containing  $x_0$ , which we denote by  $\mathcal{L}_{x_0}$ , we can, without loss of generality, let  $x(0) = x_0$ . Hamiltonian systems, for which the Hamiltonian is nontrivially a function of t, are examples of nonautonomous systems.

For our discussion we need to define on  $\Gamma$  a sigma-algebra  $\Sigma$  of subsets, which is preserved by the flow, meaning that

- (a)  $\sigma \in \Sigma \implies \phi_t \sigma \in \Sigma$ ;
- (b)  $\sigma_1, \sigma_2 \in \Sigma \implies \phi_t(\sigma_1 \cup \sigma_2) = (\phi_t \sigma_1) \cup (\phi_t \sigma_2) \text{ and } \phi_t(\sigma_1 \cap \sigma_2) = (\phi_t \sigma_1) \cap (\phi_t \sigma_2).$

A set  $\sigma \in \Sigma$  is  $\phi$ -invariant iff every trajectory with a phase point in  $\sigma$  is completely contained in  $\sigma$ , that is,  $\phi_t \sigma = \sigma$ . A  $\phi$ -invariant  $\sigma \in \Sigma$  is *Lebesgue-indecomposable* iff there do not exist any  $\phi$ -invariant proper subsets of  $\sigma$ .<sup>4</sup> We denote by  $\Sigma_{\phi}$  the set of  $\phi$ -invariant members of  $\Sigma$  and by  $\widetilde{\Sigma}_{\phi}$  the subset of  $\Sigma_{\phi}$  consisting of Lebesgueindecomposable members. It is not difficult to show that  $\widetilde{\Sigma}_{\phi}$  is a *decomposition* (or

<sup>&</sup>lt;sup>3</sup>Although we state the following assumptions cumulatively, and (ii) and (iii) are predicated on (i), they could be applied separately. Indeed, most of the discussion in this essay could be adapted to a system which is only forward-deterministic.

 $<sup>{}^{4}\</sup>sigma'$  is a proper subset of  $\sigma$  iff  $\mathfrak{m}_{L}(\sigma') > 0$  and  $\mathfrak{m}_{L}(\sigma \backslash \sigma') > 0$ .

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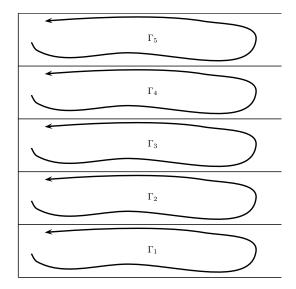


FIG. 1. The ergodic decomposition of  $\Gamma_{\!\!\!,}$  where  $\Gamma_1,\ \ldots,\ \Gamma_5$  are Lebesgue-indecomposable.

*partition*) of  $\Gamma$ , meaning that almost every<sup>5</sup>  $x \in \Gamma$  belongs to exactly one member of  $\widetilde{\Sigma}_{\phi}$ . We denote the members of  $\widetilde{\Sigma}_{\phi}$  by  $\Gamma_{\lambda}$ , where  $\lambda$  could take integer values or a range of real values. This situation is represented schematically in Fig. 1, where  $\widetilde{\Sigma}_{\phi} := {\Gamma_1, \ldots, \Gamma_5}$  and  $\Sigma_{\phi}$  is  $\widetilde{\Sigma}_{\phi}$  together with any unions of its members; thus  $\Gamma_1 \cup \Gamma_2$  belongs to  $\Sigma_{\phi}$  but not to  $\widetilde{\Sigma}_{\phi}$ .

## 2.2 Invariant measures and ergodicity

A measure m is said to be  $\phi$ -invariant if it is preserved by the dynamics; that is,  $\mathfrak{m}(\phi_t \sigma) = \mathfrak{m}(\sigma)$ , for all  $\sigma \in \Sigma$  and t. We denote by  $\mathcal{M}_{\phi}$  the set of  $\phi$ -invariant measures on  $\Sigma$  such that<sup>6</sup>

- (1)  $\mathfrak{m}(\Gamma) = 1$  (the measure is normalized over phase space);
- (2) m is *absolutely continuous* with respect to  $m_L$ , meaning that for all  $\sigma \in \Sigma$ ,  $m_L(\sigma) = 0 \implies m(\sigma) = 0$ .

A set  $\sigma$  is *total* (or *of total measure*) if  $m(\Gamma \setminus \sigma) = 0$  for all  $m \in \mathcal{M}_{\phi}$ , and an important consequence of assuming absolute continuity is that we can interpret 'almost everywhere' as 'in a set of total measure,' which is the condition for the validity of the conclusions reached in this section and App. A. The motivation for

 $<sup>^{5}\</sup>text{'Almost every'}$  means, for all but a set of points of  $m_L\text{-measure zero. 'Almost everywhere' is used in the same sense.$ 

<sup>&</sup>lt;sup>6</sup>We shall assume that  $\mathcal{M}_{\phi} \neq \emptyset$ , which is true (Mañé 1987, Thm 1.8.1) if  $\phi$  is continuous.

restricting attention to normalized absolutely continuous  $\phi$ -invariant measures is discussed in Sec. 3.1 when we define the Boltzmann entropy.

The measure  $\mathfrak{m} \in \mathcal{M}_{\phi}$  is said to be *ergodic with respect to*  $\phi$  if, for all  $\sigma \in \widetilde{\Sigma}_{\phi}$ ,  $\mathfrak{m}(\sigma) = 1$  or  $\mathfrak{m}(\sigma) = 0$ , and we denote the set of such ergodic measures by  $\widetilde{\mathcal{M}}_{\phi}$ . In the case of the simple system illustrated in Fig. 1 there must be exactly five ergodic measures  $\mathfrak{m}(\cdot | \lambda)$ , with  $\mathfrak{m}(\Gamma_{\lambda} | \lambda) = 1$ ,  $\mathfrak{m}(\Gamma_{\lambda'} | \lambda) = 0$ , for  $\lambda, \lambda' = 1, 2, \ldots, 5$  and  $\lambda' \neq \lambda$ , and, in general, it is clear that there is a one-to-one relationship between the ergodic measures  $\widetilde{\mathcal{M}}_{\phi}$  and the Lebesgue-indecomposable sets  $\widetilde{\Sigma}_{\phi}$ . These are thus referred to as *ergodic sets*. A system is *ergodic* if  $\Gamma$  is indecomposable (consists of one ergodic set) and  $\mathcal{M}_{\phi}$  has one member which is ergodic.

Based on a system with this dynamic structure, the objective probability scheme proposed in this essay is founded on two properties of ergodic measures, both of which are derived in App. A:<sup>7</sup>

(i) The ergodic measure associated with  $\Gamma_{\lambda}$  is uniquely given by

$$\mathfrak{m}(\cdot \mid \lambda) := \mathsf{T}(\cdot \mid \Gamma_{\lambda}),$$

almost everywhere in  $\Gamma_{\lambda}$ , where  $T(\sigma | \Gamma_{\lambda})$  is the average time that a phase point moving along a trajectory in  $\Gamma_{\lambda}$  spends in  $\sigma$ .

(ii) Any  $m \in \mathcal{M}_{\phi}$  can be *ergodically decomposed* almost everywhere in  $\Gamma$ , in the form

$$\mathfrak{m}(\,\cdot\,) \,=\, \sum_{\{\lambda\}} \mathfrak{m}(\,\cdot\,|\,\lambda)\,\pi(\lambda), \qquad \sum_{\{\lambda\}} \pi(\lambda) = 1, \tag{1}$$

if the values of  $\lambda$  are discrete, or

$$\mathfrak{m}(\cdot) = \int_{\alpha}^{\beta} \mathfrak{m}(\cdot \mid \lambda) \, \pi(\lambda) \, \mathrm{d}\lambda, \qquad \int_{\alpha}^{\beta} \pi(\lambda) \, \mathrm{d}\lambda = 1, \qquad (2)$$

if  $\lambda \in [\alpha, \beta]$ .

The implication of the caveat with respect to a possible set of points of Lebesguemeasure zero is considered in detail in Sec. 4. Two examples are used to illustrate the discussion:

**Example 1**  $\Gamma$  has a finite number N of points and a discrete time flow, which must necessarily be cyclic, with  $\Gamma$  consisting either of the points of one cycle, making the system ergodic, or of a decomposition  $\{\Gamma_{\lambda}\}$  into a finite number of cycles. Let  $N_{\lambda}$  be the number of points in  $\Gamma_{\lambda}$  and  $N_{\lambda}(\sigma)$  be the number of points of  $\Gamma_{\lambda}$  in  $\sigma \in \Sigma$ . Then m( $\sigma \mid \lambda$ ) =  $N_{\lambda}(\sigma)/N_{\lambda}$ . The Kac ring is an example of such a system. But an even simpler example would be that where  $\Gamma$  consists of N points equally spaced around a circle with the dynamic step consisting of a jump of two phase points in the clockwise direction. It is obvious that, if

<sup>&</sup>lt;sup>7</sup>And subject to the analytic conditions specified there.

*N* is odd, the system is ergodic with each phase point being visited during two passages around the circle and, if *N* is even, there is an ergodic decomposition into two cycles consisting of alternate phase points.

**Example 2**  $\Gamma$  is the 2*N*-dimensional phase space of a system with Hamiltonian H(p, q), where p and q are the *N*-dimensional momentum and configuration vectors. *H* is an isolating integral of motion; meaning that an energy surface  $\Gamma_E := \{ (p,q) \mid H(p,q) = E \}$  divides  $\Gamma$  into invariant regions. If *H* is the only isolating integral of motion then the set of energy surfaces forms an ergodic decomposition of  $\Gamma$  parameterized by the energy *E* (which here replaces  $\lambda$ ). The existence of other isolating integrals of motion would lead to a multiparameter ergodic decomposition. However, for the sake of this example, this is assumed not to be the case.<sup>8</sup> With the change of variables

$$\mathrm{d}\Gamma \rightarrow \left. \frac{\mathrm{d}\Gamma_E \,\mathrm{d}E}{\left| \nabla H(\boldsymbol{p}, \boldsymbol{q}) \right|_{H=E}} \right.$$

where  $d\Gamma_E$  is in terms of local curvilinear variables ( $p_E, q_E$ ) on  $\Gamma_E$ , the induced Lebesgue measure on  $\Gamma_E$  is

$$\mathfrak{m}(\sigma \mid E) = \frac{1}{\Omega(E)} \int_{\sigma \cap \Gamma_E} \frac{\mathrm{d}\Gamma_E}{\left|\nabla H(\boldsymbol{p}, \boldsymbol{q})\right|_{H=E}},$$
(3)

where

$$\Omega(E) := \int_{\Gamma_E} \frac{\mathrm{d}\Gamma_E}{\left|\nabla H(\boldsymbol{p}, \boldsymbol{q})\right|_{H=E}}$$
(4)

is the structure function (Khinchin 1949, Ch. 4).

## 3 Approaches to statistical mechanics

The aim of all programs for classical statistical mechanics is to provide a realization of the triplet: dynamics  $\rightarrow$  probability  $\rightarrow$  thermodynamics, given at the beginning of Sec. 1, where 'thermodynamics' should include both equilibrium and the transition to equilibrium. Broadly classified, there are three approaches to this: that of Boltzmann, that of Gibbs, and an information-theory approach most closely associated with the work of Jaynes.<sup>9</sup> For reasons explained in more detail in Sec. 6, Jaynes' approach is beyond the remit of this essay.<sup>10</sup> This section, however, will give a brief account of the Boltzmann approach and an even briefer

<sup>8</sup>While admitting that the number of systems for which this can be proved, although growing, is still severely restricted. (For an account of recent work, see de Oliveira & Werlang 2007.)

<sup>&</sup>lt;sup>9</sup>The most comprehensive reference for this work is his 1983 collected papers.

<sup>&</sup>lt;sup>10</sup>For discussions of Jaynes' approach, see the contributions in this book by Jos Uffink (pp. 25–49) and by Roman Frigg and Charlotte Werndl (pp. 115–42) and the essay review of Jaynes 1983 by Lavis & Milligan (1985).

account of the Gibbs approach. The imbalance is because, as we shall argue, and have already argued elsewhere (Lavis 2005, 2008), the canonical formulation of statistical mechanics is that of Boltzmann, with the wide and successful use of the Gibbs approach being sanctioned by the fact that its variables approximate to the time averages, along typical trajectories, of those derived from the Boltzmann approach.

## 3.1 The Boltzmann approach

To refer to 'Boltzmann's *approach* [in the singular] to statistical mechanics' is in danger of being misleading, since his 'ideas on the precise relationship between the thermodynamical properties of macroscopic bodies and their microscopic constitution, and the role of probability in this relationship are involved and differed quite remarkably in different periods of his life' (Uffink 2004, p. 1). However, one may (although Boltzmann did not) impose a broad division between his work on kinetic theory (before 1877) and his work on statistical mechanics proper (after that date). The first is important because it includes the evolution of Boltzmann's ideas from distribution functions to probability density functions, but it is not pertinent to this discussion. Although Boltzmann's work from 1877 does not present a coherent development of one approach, the core concept, usually taken (Bricmont 1995, 2001; Goldstein 2001; Lebowitz 1993, 1994, 1999a, 1999b)<sup>11</sup> to be at its heart, is his entropy (Boltzmann 1877).<sup>12</sup>

To describe the Boltzmann approach it is necessary first to introduce some *macroscopic variables*. In general, these will be at the observational level for the system, but will encapsulate more detail than the thermodynamic variables.<sup>13</sup> Examples of these would be local variables which quantify spatial inhomogeneities of density or magnetization. Given such a set of variables let { $\mu$ } be a set of macrostates, with each  $\mu \in \Sigma$  and such that

- (i) every  $x \in \Gamma$  is in exactly one macrostate, denoted by  $\mu_x$ ;
- (ii) each macrostate gives a unique set of values for the macrovariables;
- (iii) the phase points x and  $\Im x$  are in macrostates of the same size;
- (iv) if there exists a symmetry operation  $\mathfrak{S}$  (like a permutation of identical particles) on the points of  $\Gamma$ , such that  $\phi_t x = \tilde{x} \iff \phi_t \mathfrak{S} x = \mathfrak{S} \tilde{x}$ , then x and  $\mathfrak{S} x$  are in macrostates of the same size.

The Boltzmann entropy

$$S_{\rm B}(x) := S_{\rm B}(\mu_x) := k_{\rm B} \ln[c \, {\rm m}(\mu_x)],$$
 (5)

<sup>&</sup>lt;sup>11</sup>These authors will, henceforth, be referred to as 'the Neo-Boltzmannians.'

<sup>&</sup>lt;sup>12</sup>Although the famous formula  $S = k \log W$ , which was engraved on his tombstone, does not appear explicitly in the 1877 paper.

<sup>&</sup>lt;sup>13</sup>Ridderbos (2002) refers to them as 'supra-thermodynamic variables.'

at  $x \in \Gamma$  is a measure of the size of  $\mu_x$ . It is, of course, the case that this definition could use any measure on phase space. However, we choose to impose the condition that  $\mathfrak{m} \in \mathcal{M}_{\phi}$ , and this needs some justification. In the case of condition (1) of Sec. 2.2 the restriction is quite benign; one would wish to have an upper bound on S<sub>B</sub>, and this is provided by *defining* the Boltzmann entropy of the whole of phase space  $S_B(\Gamma) := k_B \ln[c \mathfrak{m}(\Gamma)] = k_B \ln[c]$ .<sup>14</sup> The plausible need for condition (2) relates to a second well-known arbitrary feature of the definition of  $S_{\rm B}$ , that of the choice of macrostates. It is obvious that radically different choices of the set  $\{\mu\}$  are likely to lead to very different temporal evolutions of the entropy, and this can be dealt with only by incorporating, on a case-by-case basis, the choice of macrostates as part of the definition of the model system. However, it is reasonable to demand that  $S_{\rm B}$  be stable with respect to *small* changes in the macrostates. This will be achieved if m has *translational continuity*,<sup>15</sup> and it can be shown (Malament & Zabell 1980) that m is translationally continuous if and only if it is absolutely continuous. Then, as is shown in App. A, the measure is unique if the system is ergodic and otherwise can be expressed as an ergodic decomposition. The remaining condition for  $\mathfrak{m} \in \mathcal{M}_{\phi}$  is  $\phi$ -invariance. It is important to note that we do not impose the condition that the macrostates are  $\phi$ -invariant;  $\phi_t \mu$  is not necessarily a macrostate.<sup>16</sup> However, when  $\phi_t \mu_x$  is the macrostate  $\mu_{\phi_t x}$ , we would expect the Boltzmann entropy to have the same values at *x* and  $\phi_t x$ , and this is achieved by specifying that m is  $\phi$ -invariant.

Since  $S_B(x)$  is a *dynamic* property of the system, once  $\Gamma$  has been partitioned into macrostates, dynamic evolution and the values of  $S_B(x)$  can *in principle* be calculated. But, in practice, this remark needs heavy qualification. It is necessary to obtain, with specified initial conditions, either an analytic, or a numerically stable, solution of the equations of motion. This procedure, leading to entropy profiles, has been implemented for the baker's gas in Lavis 2005 and for the Kac ring model in Lavis 2008; but, of course, these two models are very simple, not least because each has a discrete time parameter.

However, the fact remains that *prima facie* the Boltzmann approach provides a 'probability-free' version of statistical mechanics. And this is further reinforced by the preference on the part of the Neo-Boltzmannians for using the notion of 'typical.' Having first specified that the system is in equilibrium when the phase point is in a particular 'equilibrium' region of phase space and that

<sup>&</sup>lt;sup>14</sup>This does not, of course, mean that Γ is taken as a macrostate, otherwise it would necessarily be the largest macrostate. Note also that all the measures in  $\mathcal{M}_{\phi}$  have the property  $0 < \mathfrak{m}(\sigma) \le 1$ , for all  $\sigma \in \Sigma$ , and this would mean that, in the absence of a constant *c* in (5),  $S_{B}(\mathbf{x}) \le 0$ .

<sup>&</sup>lt;sup>15</sup>The measure m has translational continuity if it is continuous with respect to any small translation in  $\sigma$ , for all  $\sigma \in \Sigma$ .

<sup>&</sup>lt;sup>16</sup>If it were, then  $S_B(\phi_t x) = S_B(x)$ , meaning that the Boltzmann entropy is a constant along a trajectory.

by far the largest volumes [of phase space] correspond to the *equilibrium values* of the macroscopic variables (and this is how 'equilibrium' should be defined) (Bricmont 1995, p. 179),<sup>17</sup>

the expectation is expressed that

 $S_{\rm B}$  will *typically* increase in a way which *explains* and describes qualitatively the evolution towards equilibrium of macroscopic systems. (Lebowitz 1999b, p. S 338)

The idea is that the system, having begun in a small macrostate, with a correspondingly low value of entropy, will typically evolve through increasingly larger macrostates, and higher values of entropy, to the equilibrium state, where the entropy is at its maximum value. Our aim now is to examine this picture and to propose a modified and more general version, which moves from a concentration on the temporally local increase in the Boltzmann entropy to a consideration of its temporally global profile.

3.1.1 Equilibrium in the Boltzmann approach According to the 'standard' Boltzmann approach, summarized above, a certain part of phase space corresponds to the equilibrium state. But is it possible to make such a designation? Because of the system's reversibility and recurrence the possibility that such a region is one which, once entered by x(t), will not be exited, must be discounted. As was well understood by both Maxwell and Boltzmann, equilibrium must be a state which admits the possibility of fluctuations out of itself. Lebowitz (1993, p. 34) and Goldstein (2001, p. 8) refer to a particular macrostate as the equilibrium macrostate, and the remark by Bricmont, cited at the top of this page, is in a similar vein. So is there a single equilibrium macrostate? If so, it must be that in which the phase point spends more time than in any other macrostate and, if the system were ergodic,<sup>18</sup> it would be the largest macrostate  $\mu_{Max}$ ,<sup>19</sup> with the largest Boltzmann entropy. There is one immediate problem associated with this. Suppose the system has entropy levels {  $S_B(\mu)$ :  $\mu$  a macrostate }. Then, as has been shown in Lavis 2005 for the baker's gas and in Lavis 2008 for the Kac ring, these levels may have degeneracies  $\omega(\mu)$  such that, for some  $\mu$  with  $\mathfrak{m}(\mu) < \mathfrak{m}(\mu_{\text{Max}}), \mathfrak{m}(\mu) \,\omega(\mu) > \mathfrak{m}(\mu_{\text{Max}}).^{20}$  The effect of this is that the entropy will be likely, in the course of evolution, to spend more time in a level less than the maximum.<sup>21</sup> An obvious way round this problem would seem to be to take

<sup>17</sup>A similar statement appears in Albert 2000, p. 57.

<sup>&</sup>lt;sup>18</sup>Although the Neo-Boltzmannians deny the need for such a property (see e.g. Goldstein 2001, p. 45), they still seem to make the implicit assumption that a system will spend more time in a larger region of phase space than in a smaller.

<sup>&</sup>lt;sup>19</sup>Assuming, for simplicity, that there is only one largest macrostate.

<sup>&</sup>lt;sup>20</sup>The degeneracy  $\omega(\mu)$  of the entropy level  $S_{\rm B}(\mu)$  is simply the number of macrostates  $\mu'$  such that  $S_{\rm B}(\mu') = S_{\rm B}(\mu)$ . As already indicated, we have assumed that  $\omega(\mu_{\rm Max}) = 1$ .

<sup>&</sup>lt;sup>21</sup>See Lavis 2005, Figs 4 and 5, and Lavis 2008, Fig. 1.

a band of the larger macrostates as the equilibrium state. However, this will lead to an arbitrary division between fluctuations *within* and *out of* equilibrium, according to how the band edge is set. It may be supposed that these problems decrease as the size parameter *N* increases. However, computer studies in Lavis 2008 for a Kac ring of *N* sites indicate that

- (i) just choosing the largest macrostate as the equilibrium region does not guarantee that this region becomes an increasing proportion of phase space as *N* increases; in fact the opposite is the case.
- (ii) If an equilibrium band of the (2k+1) largest macrostates is chosen,<sup>22</sup> then, for it to contain 99.999 % of  $\Gamma$ , we must choose k = 22 for N = 100, k = 70 for N = 1000, and k = 221 for N = 10,000, and, with this proportion of  $\Gamma$  in the equilibrium state, still only about 47 % of a 'typical' trajectory will be in equilibrium.

But why define equilibrium in this binary way? We have already suggested (Lavis 2005, 2008), and propose again here, that the quality which we are trying to capture is a matter of degree, rather than the two-valued property of either being *in equilibrium* or *not in equilibrium*. The proposal is:

All references to a system's being, or not being, in equilibrium should be replaced by references to the **commonness** of the state of the system, with this property being measured by (some, possibly scaled, form of) the Boltzmann entropy.

So commonness could be regarded as just a measure of the degree of 'equilibriumness.' This, the first of our suggested modifications to the Neo-Boltzmannian approach, would leave it largely unaltered, with 'being in equilibrium' now replaced by 'having large commonness,' and 'approaching equilibrium' being replaced by 'exhibiting increasing commonness.'

3.1.2 *Typicality, measure, and probability* For the Neo-Boltzmannians, typical behavior is characterized by evolution from a smaller into a larger macrostate. However, they avoid making an explicit link between probability and typicality and also argue that there is no need for the system to have special properties like ergodicity or mixing. Frigg (2010b) has examined in detail what he discerns to be a number of distinct treatments of typicality and he concludes that they almost all fail either for technical reasons or because they leave unanswered essential questions. In two cases he reserves his judgment. The first of these involves the undeveloped concession (and departure from Neo-Boltzmannian orthodoxy) by Bricmont (2001, p. 16) 'that some form of mixing is important for the approach to equilibrium to take place.'<sup>23</sup> The second is the program proposed by the present

<sup>&</sup>lt;sup>22</sup>There is one largest macrostate and all other macrostates have degeneracy 2.

<sup>&</sup>lt;sup>23</sup>Contrasting with the view of Goldstein (2001) that attempts to explain the approach to equilibrium by appeal to specific dynamical properties such as ergodicity or mixing are 'thoroughly

author (Lavis 2005, 2008) and further developed here. This can be understood in terms of modifications to the 'standard' Neo-Boltzmannian approach, and to see what these are it is useful to consider three questions:

- (a) What type of behavior is being posited as typical?
- (b) What is meant by the behavior being typical?
- (c) Why is the behavior typical?

As we have seen, the Neo-Boltzmannian answer to (a) is clear: entropy temporally increases, or equivalently, the system evolves from smaller to larger macrostates.<sup>24</sup> To answer (b) the Neo-Boltzmannians tend to rely on an ordinarylanguage use of the word 'typical,' meaning that it is behavior which is not 'ridiculously special' (Goldstein 2001, p. 43). With this 'common-sense' view of 'typically' two plausible answers are given to (c). In the first it is argued<sup>25</sup> that, if (at least for large systems) equilibrium corresponds to the overwhelmingly largest macrostate, then the system will quickly evolve into that state. The problems associated with this description of equilibrium have been discussed in Sec. 3.1.1. They are, however, circumvented in a second and even more temporally local answer to (c). In this it is argued (Lebowitz 1999a, p. 521) that the region around a small macrostate will be mainly contained within larger macrostates and thus that typical behavior will be from a smaller to a larger macrostate, with a consequent increase in entropy. The problems with this approach are discussed in Lavis 2008.

We now begin our proposed modifications to this program. The initial step appears quite benign and is prompted by a comparison between 'Boltzmann's Law,' which states that

[if we take] an arbitrary instant of time t' and assume that at that time the Boltzmann entropy  $S_B(t')$  of the system is low, [it is] highly probable that at time t'' > t' we have  $S_B(t'') \ge S_B(t')$ [,] (Frigg 2010a)

and the quote, given on page 59 above, from Lebowitz 1999b, p. S338. This suggests that typical behavior in (b) is translated into having a high *conditional* probability that, given the system has a low entropy  $S_B(t')$  at t', it will have higher entropy  $S_B(t'')$  at t'' > t' (where |t''-t'| is small). It is often supposed that a combination of Boltzmann's Law with the 'Past Hypothesis' (Albert 2000, Ch. 4) provides a way to answer (c). However, it is difficult to envisage the kind of proof that could be given for Boltzmann's Law. As Frigg (2010a) has pointed out, Boltzmann took it to be in the nature of systems that they tend to move from states of lower probability to states of higher probability, and

misguided.'

<sup>&</sup>lt;sup>24</sup>Although little emphasis is placed on this point it is clear that this behavior has to be understood as over a short time-period, since the dynamics is reversible and recurrent.

<sup>&</sup>lt;sup>25</sup>See the quotes from Bricmont 1995 and Lebowitz 1999b, given on p. 59.

the attempt to substantiate this claim by Ehrenfest & Ehrenfest-Afanassjewa (1911, pp. 31–6) is based on a model without deterministic dynamics, making it of limited relevance. However, both Boltzmann's perception and the work of the Ehrenfests make it clear that the problem becomes more tractable if it can be moved from one concerning conditional probabilities (transitions) to one of nonconditional probabilities (being in).

This suggests a more substantial modification to the Neo-Boltzmannian approach. It concerns (a) and involves a change of viewpoint, from the temporally local one espoused by the Neo-Boltzmannians (and others, including Albert (2000)), for which the main preoccupation is the study of the *local* increase of entropy from some initial low-entropy state, to a temporally *global* interest in the overall behavior of entropy. This change is effected by the restatement of the definition of thermodynamic-like behavior in Lavis 2005, p. 255. *Thermodynamic-like behavior* is now characterized as the situation where

the Boltzmann entropy  $S_B$ , for the evolving system, is most of the time close to its maximum value  $(S_B)_{Max} := S_B(\mu_{Max})$ , from which it exhibits frequent small fluctuations and rare large (downward) fluctuations.

This definition makes no reference to probability and, as we shall see below, for an ergodic system a 'Boltzmann account' of statistical mechanics can be given without resort to probabilities, using only an assertion that *thermodynamic-like behavior is 'typical*,' where the explication of that type of typicality (type I) is not susceptible to a probabilistic interpretation. However, part of the aim of this essay is to provide a link between the Boltzmann and Gibbs approaches. For this we need to use the time-average definition of probability to relate thermodynamiclike behavior to the probabilities of the system being in macrostates of different sizes. Probabilities of a different kind (see Sec. 5) also play an essential role in the case of nonergodic systems.

## 3.2 The Gibbs approach to statistical mechanics

The Gibbs approach begins with a slightly extended version of the notion of the  $\phi$ -invariance of measures given in Sec. 2. Now we allow the possibility of measures which are explicit functions of time. Thus  $\mathfrak{m}(\sigma;t)$  will be the measure of  $\sigma \in \Sigma$  at time t, and  $\phi$ -invariance is the condition  $\mathfrak{m}(\sigma;t') = \mathfrak{m}(\phi_t \sigma;t'+t)$ , for all t', t and  $\sigma \in \Sigma$ . The measures  $\mathfrak{m}(\cdot;t)$  parameterized by t are assumed to be members of  $\mathcal{M}_{\phi}$ , and from the Radon–Nikodym Theorem (Mañé 1987, p. 6) they will be associated with density functions  $\rho(\cdot;t)$ , given by<sup>26</sup>

$$\mathfrak{m}(\sigma; t) = \int_{\sigma} \rho(\mathbf{x}; t) \,\mathrm{d}\Gamma, \quad \text{for all } t,$$

<sup>26</sup>We assume, for ease of presentation, that  $\Gamma$  has a continuum of points.

for which the  $\phi$ -invariance condition is Liouville's Equation. This density, for fixed *t*, is normalized over  $\Gamma$  and is taken, without further interpretation, as the probability density function for the distribution of  $x \in \Gamma$  at time *t*. Equilibrium is defined as the situation where the probability density function is stationary, that is to say, not an explicit function of time, when it becomes a function of the global integrals of motion.<sup>27</sup> The statistical-mechanical 'analogues' of thermodynamic quantities are either fixed external parameters, related to phase functions, or functionals of  $\rho$ . In particular, the analogue of thermodynamic entropy is the *Gibbs entropy* 

$$S_{\rm G}[\rho] := -k_{\rm B} \int_{\Gamma} \rho(\mathbf{x}) \ln[\rho(\mathbf{x})] \,\mathrm{d}\Gamma. \tag{6}$$

From a practical point of view this scheme is very satisfactory. However, problems arise when an attempt is made to extend it to nonequilibrium situations, which are given by nonstationary solutions of Liouville's Equation. Specifically:

- (i) When ρ(x) is replaced in (6) by any time-dependent solution ρ(x; t) of Liouville's Equation, S<sub>G</sub>[ρ(t)] remains invariant with respect to time.
- (ii) Given an arbitrary initial condition  $\rho(x; 0)$ , the evolving solution  $\rho(x; t)$  of Liouville's Equation will not, in general, converge to a stationary solution as  $t \to \infty$ .

## 4 The time-average interpretation of probability and typicality

As indicated in Sec. 2, our scheme for assigning probability is predicated upon the system having an ergodic decomposition, and in this section we introduce the time-average definition used for probabilities conditional upon the system being in a particular member of the decomposition. There is a number of well-known objections to this interpretation, which are listed and discussed in Sec. 4.1.

In App. A it is shown that the time-sum in (A.1), or time-integral in (A.3), exists, according to Birkhoff's Theorem (Thm A.1), for all trajectories  $\mathcal{L}_{x_0}$ , except possibly for those for which  $x_0$  lies in a set of Lebesgue-measure zero, which will henceforth be denoted by  $\mathring{\Gamma}$ . It is clear that if  $x_0 \in \mathring{\Gamma}$  then  $x \in \mathring{\Gamma}$ , for all  $x \in \mathcal{L}_{x_0}$ ;  $\mathring{\Gamma}$  consists of the union of a set of 'special' trajectories for which time-integrals (or sums) do not exist.<sup>28</sup> With this in mind, we define the conditional probability that  $x \in \sigma$ , given that  $x \in \mathcal{L}_{x_0}$  and  $\mathcal{L}_{x_0} \nsubseteq \mathring{\Gamma}$ , by

$$\mathsf{P}\left[\left|\mathbf{x}\in\sigma\right|\left|\mathbf{x}\in\mathcal{L}_{\mathbf{x}_{0}}\wedge\mathcal{L}_{\mathbf{x}_{0}}\nsubseteq\mathring{\Gamma}\right]\right] := \mathsf{T}(\sigma\mid\mathcal{L}_{\mathbf{x}_{0}}),\tag{7}$$

where, as defined in App. A,  $T(\sigma | \mathcal{L}_{x_0})$  is the average time that x, moving along the trajectory  $\mathcal{L}_{x_0}$  through  $x_0$ , spends in  $\sigma$ .

<sup>&</sup>lt;sup>27</sup>This is the 'conventional' definition of equilibrium in the Gibbs approach. Van Lith (2001a) has proposed a weakened definition involving a new concept of ' $\varepsilon$ -equilibrium.'

<sup>&</sup>lt;sup>28</sup>With the proviso, of course, that in some cases, like that where Γ consists of a finite number of points and *t* takes discrete values, there will be no set  $\mathring{\Gamma}$ .

With  $\mathring{\Gamma}_{\lambda} := \mathring{\Gamma} \cap \Gamma_{\lambda}$ , when  $x \in \Gamma_{\lambda} \setminus \mathring{\Gamma}_{\lambda}$ , it follows from (A.5) that

$$\left[ \mathbf{x} \in \sigma \mid \mathbf{x} \in \Gamma_{\lambda} \backslash \mathring{\Gamma}_{\lambda} \right] = \mathsf{T}(\sigma \mid \Gamma_{\lambda}) = \mathfrak{m}(\sigma \mid \lambda), \tag{8}$$

and in the special case where the system is ergodic,

$$\mathsf{P}[\mathbf{x} \in \sigma \mid \mathbf{x} \in \Gamma \backslash \mathring{\Gamma}] = \mathsf{T}(\sigma) = \mathfrak{m}(\sigma), \tag{9}$$

m, in this case, being the sole member of  $\mathcal{M}_{\phi}$ .

This leaves the question of how we define  $P[x \in \sigma | x \in \Gamma \setminus \hat{\Gamma}]$  when the system is not ergodic, which cannot, of course, be completely resolved within the context of the time-average definition. However, we do know that any viable definition must correspond to a measure belonging to  $\mathcal{M}_{\phi}$  and hence, from the ergodic decomposition (1) or (2),

$$\mathsf{P}[\mathbf{x} \in \sigma \mid \mathbf{x} \in \Gamma \backslash \mathring{\Gamma}] = \langle \mathsf{T}(\sigma \mid \Gamma_{\lambda}) \rangle_{\pi} := \begin{cases} \sum_{\{\lambda\}} \mathsf{T}(\sigma \mid \Gamma_{\lambda}) \, \pi(\lambda), \\ \int_{\alpha}^{\beta} \mathsf{T}(\sigma \mid \Gamma_{\lambda}) \, \pi(\lambda) \, \mathrm{d}\lambda, \end{cases} \text{ for all } \sigma \in \Sigma \end{cases}$$
(10)

according to whether the ergodic decomposition has a discrete or continuous parametrization. The probability for  $x \in \sigma$  is the *decomposition-mean*  $\langle \cdot \rangle_{\pi}$ , with respect to the probability distribution  $\{\pi(\lambda)\}$  over the members of the decomposition, of the time-average probabilities within each  $\Gamma_{\lambda}$ .

The time-average probabilities are clearly objective. Indeed it can be argued that they 'are some kind of continuous counterparts to limits of relative frequencies' (von Plato 1989b, p. 434).<sup>29</sup> However, it is clear that, in order to construct a wholly objective interpretation for statistical mechanics, an objective interpretation must be given for  $\pi(\lambda)$ . Since this is grounded very specifically in particular models, we reserve discussion of this to Sec. 5. First we show how, in the Boltzmann approach, typicality and thermodynamic-like behavior can be interpreted using (10), and then, in Sec. 4.2, how this is reconciled with the different concepts of equilibrium and entropy in the Gibbs approach and in thermodynamics.

For an ergodic system and all  $x \in \Gamma \setminus \mathring{\Gamma}$ , from (5) and (9), the Boltzmann entropy  $S_{\rm B}(\mu)$  is a monotonically increasing function of  $\mathfrak{m}(\mu) = \mathsf{T}(\mu)$ . Along a trajectory the phase point will thus spend an amount of time in a macrostate proportional to the exponential of the value of the entropy, meaning that it behaves in a thermodynamic-like way.

However, we must consider the set  $\mathring{\Gamma}$ , for which the average time  $T(\mu)$  that the phase point x(t) spends in  $\mu$  is not defined.<sup>30</sup> The event  $x(t) \in \mathring{\Gamma}$  is equivalent

<sup>&</sup>lt;sup>29</sup>This is a contention which is discussed in App. B.

 $<sup>^{30}</sup>$ Or, perhaps more precisely, not quantifiable in terms of the time integral of the indicator function of  $\mu$ .

to  $\mathbf{x}(0) \in \mathring{\Gamma}$  and, as has been pointed out many times in the literature, the fact that  $\mathfrak{m}(\mathring{\Gamma}) = 0$  does not mean that it is impossible for the system to start its evolution in  $\mathring{\Gamma}$ . Nor may it be inferred that  $\mathsf{P}[\mathbf{x} \in \mathring{\Gamma}] = 0$ ; the definition of probability (9) expressly excludes the set  $\mathring{\Gamma}$ , for the points of which probability is *undefined*. We have here (at least in my opinion) a place where typicality must be brought into play and cannot be translated into probability. The choice of an initial point for the evolution in a prespecified set of measure zero would, to use Goldstein's words, be 'ridiculously special,' meaning that the experimenter would need to take ridiculously special steps to ensure the event  $\mathbf{x}(0) \in \mathring{\Gamma}$ . Thus we say that  $\mathbf{x}(0)$  will typically be in  $\Gamma \setminus \mathring{\Gamma}$  and we call this *typicality type I*. An ergodic system will typically (type I) behave in a thermodynamic-like way. Thus we have, for an ergodic system, an answer to question (b) of Sec. 3.1.2 (the meaning of typicality), and the answer to question (c) is the ergodicity of the dynamics.

For a nonergodic system we first consider motion in a particular member  $\Gamma_{\lambda}$  of the ergodic decomposition, for which x(0) will typically (type I) be in  $\Gamma_{\lambda} \backslash \mathring{\Gamma}_{\lambda}$ . Assuming this to be the case, the Boltzmann entropy is still given by (5), but the only part of the macrostate  $\mu$  which is accessible is  $\mu \cap \Gamma_{\lambda}$ . The time spent in  $\mu$  is the time spent in  $\mu \cap \Gamma_{\lambda}$ , which, from (8), is  $\mathsf{T}(\mu \mid \Gamma_{\lambda}) = \mathfrak{m}(\mu \mid \lambda)$ . Now we see what the problem might be. The entropy states are determined by the members of  $\{ \mathfrak{m}(\mu) : \mu \text{ a macrostate } \}$ , whereas the entropy *profile* is determined by  $\{ \mathfrak{m}(\mu \mid \lambda) \colon \forall \mu \}$ . It is tempting to suppose that thermodynamic-like behavior will occur because of an approximate proportionality between these two sets. However, computer experiments with the Kac ring model (Lavis 2008) indicate that this is not always the case. It is quite possible for there to be some macrostates with  $S_{B}(\mu)$  near to  $(S_{B})_{Max}$  and  $\mu \cap \Gamma_{\lambda} = \emptyset$ . For an ergodic system thermodynamic-like behavior was typical (type I); for motion in a member of an ergodic decomposition,  $x(0) \in \Gamma_{\lambda} \setminus \check{\Gamma}_{\lambda}$  is not sufficient to ensure thermodynamic-like behavior. We must establish criteria for thermodynamic-like behavior to be high probability, that is to say, to be typical in a new sense, which we call typicality type II. To do this we need conditions first for the degree to which behavior within the set  $\Gamma_{\lambda}$  is thermodynamic-like and second for the probability of the phase point being within a  $\Gamma_{\lambda}$  for which these conditions are satisfied.

Following Lavis 2008 (with some slight changes of notation), the degree to which the evolution of the system is thermodynamic-like in  $\Gamma_{\lambda}$  is measured by the extent to which

$$\Delta_{\lambda}[S_{\rm B}] := \frac{1}{N} \Big[ (S_{\rm B})_{\rm Max} - \langle S_{\rm B} \rangle_{\lambda} \Big]$$
(11)

and

$$\Psi_{\lambda}[S_{\mathrm{B}}] := \frac{1}{N} \sqrt{\left\langle \left[ S_{\mathrm{B}} - \langle S_{\mathrm{B}} \rangle_{\lambda} \right]^{2} \right\rangle_{\lambda}}$$
(12)

are small, where *N* is an extensive parameter (usually the number of microsystems),  $\langle S_{\rm B} \rangle_{\lambda} := \sum_{\nu} \mathsf{T}(\mu \mid \Gamma_{\lambda}) S_{\rm B}(\mu)$ 

$$\langle S_{\mathrm{B}} \rangle_{\lambda} := \sum_{\{\mu\}} \mathsf{T}(\mu \mid \Gamma_{\lambda}) \, S_{\mathrm{B}}(\mu)$$

is the time average of  $S_B$  along a typical type-I trajectory in  $\Gamma_{\lambda}$ , and  $\Psi_{\lambda}[S_B]$  is the standard deviation with respect to the time distribution. All we now need to do is to set a criterion for the system to be regarded as having thermodynamic-like behavior in  $\Gamma_{\lambda}$  in terms of some small values of  $\Delta_{\lambda}[S_B]$  and  $\Psi_{\lambda}[S_B]$ . Let  $T(\alpha, \beta)$  be the criterion that  $\Delta_{\lambda}[S_B] < \alpha$  and  $\Psi_{\lambda}[S_B] < \beta$ .<sup>31</sup>

We now consider the whole decomposition  $\{\Gamma_{\lambda}\}$  and denote by  $\Gamma^{(T)}$  the union of all members which satisfy  $T(\alpha, \beta)$ , for some specified small (positive) values of  $\alpha$  and  $\beta$ , with  $\Gamma^{(A)} = \Gamma \setminus \Gamma^{(T)}$ . The probability of the phase point  $\mathbf{x}(t) \in \Gamma_{\lambda}$  is  $\pi(\lambda)$ , which is, of course, equivalent to the probability of the *initial* point  $\mathbf{x}(0) \in \Gamma_{\lambda}$ . Thermodynamic-like behavior is now said to be typical type II if

$$\mathsf{P}[\boldsymbol{x}(0) \in \Gamma^{(A)}] = \sum_{\Gamma_{\lambda} \subseteq \Gamma^{(A)}} \pi(\lambda) \ll 1.$$
(13)

An ergodic system is behaving typically (meaning in a thermodynamic way) if it is behaving typically type I. A nonergodic system is behaving typically if it is behaving typically type I *and* type II. Of course, typicality type II is predicated both on chosen values for  $\alpha$  and  $\beta$  and on a level for the inequality in (13). For simple discrete-time systems with a finite phase space (where typicality type I is automatic) it is possible to test every point of  $\Gamma$  to determine (given a choice for  $T(\alpha, \beta)$ ) whether it belongs to  $\Gamma^{(T)}$  or  $\Gamma^{(A)}$ . This allows the numerical value of  $P[\mathbf{x}(0) \in \Gamma^{(A)}]$  in (13) to be computed.

#### 4.1 Problems with the time-average definition of probability

The traditional role of ergodic theory is to give support to the proposition that thermodynamic variables are analogues of the expectation values of phase functions calculated using the microcanonical distribution. This is done by arguing that the measurement of the value of a thermodynamic variable is equivalent to the infinite-time average of the corresponding phase function. This is an attractive idea but the problems associated with it are well known. In particular, rather few systems are ergodic, and while the measurement process may correspond to a long-time average, it is certainly not an *infinite*-time average; this distinction is important for any discussion of equilibrium and nonequilibrium, as we will see below. Van Lith (2001a) discusses the problems associated with the ergodic program in general and with the version which leads to the time-average definition of probability, which as we have seen specializes from the time integral of phase functions in general to those for the indicator functions of sets in phase space.

<sup>&</sup>lt;sup>31</sup>Cases of this for the Kac ring model are discussed in Lavis 2008.

She lists (ibid., p. 587) four problems which still remain for this more specialized use of ergodic theory. In this section we shall consider each of these<sup>32</sup> and show how they are resolved within the program described above:

- **Objection 1:** 'Infinite-time averages need not even exist! It may well be that the limit in [(A.1) or (A.3)] does not exist' (van Lith, ibid.). As is seen in App. A, the time average does exist for almost every  $\mathbf{x}(0) \in \Gamma$ . The exceptional points lie in a set which we have denoted by  $\mathring{\Gamma}$ . We have not argued from  $\mathbf{m}(\mathring{\Gamma}) = 0$  that  $\mathsf{P}[\mathbf{x}(0) \in \mathring{\Gamma}] = 0$ , indeed this probability is not even defined. Nor have we argued that the event  $\mathbf{x}(0) \in \mathring{\Gamma}$  is impossible. We simply argue that, since the implementation of this event would be, for the experimenter, a task requiring exceptional effort, the event  $\mathbf{x}(0) \in \Gamma \setminus \mathring{\Gamma}$  would be typical, designating this as typicality type I.
- **Objection 2:** As is clear from (7), 'the probability of a set  $[\sigma]$  depends on the initial state [x(0)]' (van Lith, ibid.). This objection is clearly invalid for typical (type I) behavior of an ergodic system. The same applies to a system with an ergodic decomposition  $\{\Gamma_{\lambda}\}$  with respect to the location of x(0) within  $\Gamma_{\lambda}$ . The probability of the phase point being in a set  $\sigma$  (or a macrostate  $\mu$ ) does, of course, depend on which member of the decomposition x(0) is in. However, this is provided for in our analysis by proposing in Sec. 5 ways of generating the probabilities  $\{\pi(\lambda)\}$  and giving criteria for whether this leads to typical (type II) behavior.
- **Objection 3:** 'There is no obvious way to extend the application of this notion of probability to time-dependent phenomena, and thus to the more general theory of nonequilibrium statistical mechanics' (van Lith, ibid.). This objection is related to the meaning of equilibrium/nonequilibrium in statistical mechanics. As we have indicated, in Sec. 3.1.1, we do not admit this binary division, which is replaced by degrees of commonness. We have adopted a temporally global view-point, in which the probability of the system being in a state of more or less commonness is time-invariant, with no role for time-dependent measures or probabilities. This having been said, what we take to be the substantive element of van Lith's point still remains to be answered. This could be encapsulated in the following question: Given that, at some time *t*, the system is in a state with a certain commonness, what is the probability that it will be in a state with greater commonness at t' > t (with |t'-t| small)? We must, of course, admit that, apart from the kind of direct calculations carried out for simple models like the baker's gas and the Kac ring, the picture of statistical mechanics proposed here does not include the possibility

<sup>32</sup>For the sake of our discussion these are given in a different order from that of van Lith.

of calculating such transition probabilities. This is a problem which requires much more input than simply the time interval (t'-t) and the measures of the macrostates at t and t'. More particularly, it is necessary to know the distribution and sizes of the macrostates contiguous to  $\mu_{x(t)}$ and the location of x(t) in  $\mu_{x(t)}$ ; different parts of  $\mu_{x(t)}$  can, in general, lead to transitions to different neighboring macrostates. It may, of course, be possible to obtain some insight and some approximate solution by treating the problem using a time-dependent probability density function driven by a kinetic equation. However, we would argue that this does not mean that the system is in some part of its evolution which could be labelled as 'nonequilibrium'; merely that this is a convenient approximation for the part of the global entropy profile where the entropy is increasing steeply.

**Objection 4:** This is the problem of the relationship between the time-average and relative-frequency interpretations of probability asserted in the quotation from von Plato 1989b, p. 434, given on page 64 above. This objection, which is different in kind from the preceding three, presents no threat to the time-average definition of probability per se, but only to putative support for it derived from its being some kind of relative-frequency interpretation. Van Lith (ibid.) identifies what she takes to be a weakness in this argument, arising from the supposed limitation of the relativefrequency interpretation to a sequence of independent trials. She comments that 'the fact that repetitions are determined by a deterministic process puts pressure on the condition that repetitions should be independent.' The question of whether the relative-frequency interpretation is indeed restricted to independent trials and whether it is plausible and illuminating to make a link between it and the time-average interpretation is rather peripheral to our discussion and we have relegated it to App. B.

## 4.2 The Gibbs approach and thermodynamic entropy

Since  $P[x \in \sigma | x \in \Gamma_{\lambda} \setminus \mathring{\Gamma}_{\lambda}] = T(\sigma | \Gamma_{\lambda}) = m(\sigma | \lambda) \in \mathcal{M}_{\phi}$ , it follows from the Radon–Nikodym Theorem that it is associated with the probability density function  $\rho(x_{\lambda} | \lambda)$  by<sup>33</sup>

$$\mathsf{P}\left[\mathbf{x}\in\sigma\mid\mathbf{x}\in\Gamma_{\lambda}\backslash\mathring{\Gamma}_{\lambda}\right] := \int_{\sigma\cap\Gamma_{\lambda}}\rho(\mathbf{x}_{\lambda}\mid\lambda)\,J(\mathbf{x}_{\lambda},\lambda)\,\mathsf{d}\Gamma_{\lambda},\tag{14}$$

<sup>33</sup>As in Sec. 3.2, we assume, for ease of presentation, that  $\Gamma$  has a continuum of points. In the case where  $\Gamma$  consists of a denumerable or finite set of points the integrals in (14), (16), and (17) are replaced by sums. In the integrals on the right-hand sides of (14) and (17) the distinction between  $\Gamma_{\lambda}$  and  $\Gamma_{\lambda} \backslash \mathring{\Gamma}_{\lambda}$  can be ignored since they differ only by a set of measure zero, which would make no contribution.

where  $x_{\lambda}$  represents the local variables on  $\Gamma_{\lambda}$  and  $J(x_{\lambda}, \lambda)$  is the Jacobian of the transformation to the variables  $(x_{\lambda}, \lambda)$ . From (6) and (10), the Gibbs entropy takes the form

$$S_{\rm G}[\rho] = S_{\rm G}[\pi] + \left\langle S_{\rm G}[\rho(\lambda)] \right\rangle_{\!\!\pi}, \qquad (15)$$

where

$$S_{\rm G}[\pi] := -k_{\rm B} \int_{\alpha}^{\beta} \pi(\lambda) \ln[\pi(\lambda)] \,\mathrm{d}\lambda, \qquad (16)$$

$$S_{\rm G}[\rho(\lambda)] := -k_{\rm B} \int_{\Gamma_{\lambda}} \rho(\mathbf{x}_{\lambda} | \lambda) \ln[\rho(\mathbf{x}_{\lambda} | \lambda)] J(\mathbf{x}_{\lambda}, \lambda) \,\mathrm{d}\Gamma_{\lambda}. \tag{17}$$

The entropy is the sum of the entropy  $S_G[\pi]$  of the decomposition and the decomposition-mean of the entropies  $S_G[\rho(\lambda)]$  in the members of the decomposition.

In particular, for Ex. 2 of Sec. 2, from (3),

$$\rho(\boldsymbol{p}_{E},\boldsymbol{q}_{E} \mid E) = \frac{1}{\Omega(E)}, \qquad J(\boldsymbol{p}_{E},\boldsymbol{q}_{E},E) = \frac{1}{\left|\nabla H(\boldsymbol{p},\boldsymbol{q})\right|_{H=E}}, \qquad (18)$$

and, from (4), (17), and (18),

$$S_{\rm G}[\rho(E)] = S_{\rm MC}(E) := k_{\rm B} \ln[\Omega(E)], \qquad (19)$$

the microcanonical entropy (Huang 1963, Sec. 7.2).

Lavis 2005 proposed a general scheme for relating a phase function f, defined on  $x \in \Gamma$ , to a macro-function  $\mathcal{F}$  defined on the macrostates  $\{\mu\}$  and then to a thermodynamic function F. The first step is to coarse-grain f(x) over the macrostates to produce  $\mathcal{F}(\mu)$ .<sup>34</sup> The second step (assuming typicality type I) is to define the thermodynamic variable F along the trajectory  $\mathcal{L}_x$  as the time average  $\langle \mathcal{F} \rangle_x$  of  $\mathcal{F}$  along the trajectory. The special case of interest here is the relationship between the Boltzmann and thermodynamic entropies. Now the first step is unnecessary since  $S_B$  is already, by definition, coarse-grained over the macrostates. The dimensionless thermodynamic entropy is then identified with  $\langle S_B \rangle_x$ . For a system with an ergodic decomposition this would yield a different thermodynamic entropy  $S_\lambda$  for each member of the decomposition, with, from (11),

$$S_{\lambda} := \langle S_{\rm B} \rangle_{\lambda} = (S_{\rm B})_{\rm Max} - N \Delta_{\lambda} [S_{\rm B}].$$

When the behavior is thermodynamic-like in  $\Gamma_{\lambda}$ , the ratio  $S_{\lambda}/N$  differs from  $(S_{\rm B})_{\rm Max}/N$  by at most some small amount and, if (13) holds, this will be the case for measurements along typical trajectories. In the case of the Kac ring, with N = 10,000 and the trajectory investigated for Figs 1 and 2 of Lavis 2008,  $\Delta_{\lambda}[S_{\rm B}] = 0.58122723 \times 10^{-2}$ , a value which is likely to decrease with increasing *N*.

 $<sup>^{34}</sup>$ It is argued that  $\mathcal{F}$  is a good approximation to f for the phase functions relevant to thermodynamics since their variation is small over the points in a macrostate.

To connect the Boltzmann and Gibbs entropies it is first necessary to make a suitable choice of *c* in (5) so that, as defined in Sec. 3.1, the Boltzmann entropy of the whole of phase space  $S_{\rm B}(\Gamma) = k_{\rm B} \ln[c] = S_{\rm G}$ . It is often said that in 'equilibrium [the Gibbs entropy] agrees with Boltzmann and Clausius entropies (up to terms that are negligible when the number of particles is large) and everything is fine' (Bricmont 1995, p. 188). In the present context this means that the good approximation  $(S_B)_{Max}$  for the entropy of a system for which thermodynamic-like behavior is typical, can be replaced by  $S_{\rm G} = S_{\rm B}(\Gamma)$ . The advantage of this substitution is obvious, since  $(S_B)_{Max}$  is dependent on the division into macrostates and  $S_{\rm B}(\Gamma)$  is not. However, a little care is needed in justifying this substitution. It is valid not because, as asserted in the quote from Bricmont 1995, p. 179, on page 59 above,  $\mu_{Max}$  occupies an increasing proportion of  $\Gamma$  as the system size increases. Indeed, as was shown in Lavis 2008 for the Kac ring, the reverse is the case. That proportion becomes vanishingly small as the number N of sites increases. However, the required substitution can still be made, since, for that model,

$$\frac{(S_{\rm B})_{\rm Max}}{S_{\rm G}} \simeq 1 - \frac{\ln(N)}{2N\ln(2)}, \quad \text{as } N \to \infty.$$
<sup>(20)</sup>

Although it may seem that the incorrect intuition on the part of Neo-Boltzmannians concerning the growth in the relative size of the largest macrostate, leading as it does to the correct conclusion with respect to entropy, is easily modified and of no importance, it has been shown in Sec. 3.1.1 that it has profound consequences for the attempt to define equilibrium in the Boltzmann approach.

In Sec. 3.2 we indicated that, in the Gibbs approach, equilibrium and nonequilibrium states correspond to the probability density function not being or being an explicit function of time. In the picture we are now advocating, the only part of the approach which features is that with a time-independent probability density function. The Gibbs entropy (6) is no longer taken as that of some (we would argue) nonexistent equilibrium state, but as an approximation to the true thermodynamic entropy, which is the time average over macrostates of the Boltzmann entropy. The reason for using a time-independent probability density function for the Gibbs entropy is not that the system is in equilibrium but that the underlying dynamics is autonomous.<sup>35</sup> The thermodynamic entropy approximated by the Gibbs entropy (6) remains constant if  $\Gamma$  remains unchanged, but changes discontinuously if a change in external constraints leads to a change in  $\Gamma$ . An example of this, for a perfect gas in a box when a partition is removed, is considered in Lavis 2005, where it is shown that the Boltzmann entropy follows closely the step-change in the Gibbs entropy.

<sup>35</sup>A nonautonomous dynamic system will not yield a time-independent solution to Liouville's Equation.

## 5 Interpreting $\{\pi(\lambda)\}$ : Stochastic nomological machines

We now consider the problem of building into our model an objective procedure for assigning the probabilities  $\{\pi(\lambda)\}$ . Once this is done, and assuming typicality type I (that  $\mathbf{x}(0) \notin \mathring{\Gamma}_{\lambda}$ ), it can be determined whether thermodynamiclike behavior is typical (type II). If  $\mathbf{x}(0)$  were fixed to lie in a particular  $\Gamma_{\lambda_0}$ (specifically, in terms of Ex. 2 given in Sec. 2, if the system were thermally isolated with energy  $E_0$ ), then  $\pi(\lambda)$  would be a delta-distribution at  $\lambda = \lambda_0$ and the system evolution would be thermodynamic-like or not according to whether the specified  $T(\alpha, \beta)$  criterion were satisfied.<sup>36</sup> Typicality type II implies a non-delta probability distribution which has most probable behavior which is thermodynamic-like according to the criterion (13). For this to have meaning the system must *include as part of its definition* a probability-generating mechanism for assigning  $\mathbf{x}(0)$ . The contention of this section is that this mechanism can be understood as a *stochastic nomological machine*, and to make this case it is necessary to outline the origin of this idea and to show that it validly applies in this case. A *nomological machine* was described by Cartwright (1999, p. 50) as

a fixed (enough) arrangement of components, or factors, with stable (enough) capacities that in the right sort of stable (enough) environment will, with repeated operation, give rise to the kind of regular behavior that we represent in our scientific laws.

A 'fixed arrangement' and a 'stable environment' are needed to give meaning to 'repeated operation,' and they imply what she calls 'shielding conditions' (ibid.) preventing intrusion of extraneous external effects from one operation to the next. The planetary motion of the solar system is, for her, a rare example of a naturally occurring nomological machine. More usually they are either the result of laboratory experiment or a theoretical construct. The power of a nomological machine to generate regular behavior is what Cartwright calls its 'capacity,' and here our interest is in a machine which has the capacity to generate probabilities. Such a nomological machine is called by Cartwright a *chance setup* (ibid., p. 152) and by Hoefer (2007, p. 574) a *stochastic nomological machine* (SNM).<sup>37</sup> So, in practical terms, what are the ingredients of an SNM and is such a one compatible with our assumed deterministic system? The answer to the first part of this question would, of course, answer the second part if it is the case that SNMs

<sup>&</sup>lt;sup>36</sup>Or we could, of course, redefine the Boltzmann entropy (5) in terms of macrostates and a measure on  $\Gamma_{\lambda_0}$ , in which case the system would be effectively ergodic, with thermodynamic-like behavior typical type I.

<sup>&</sup>lt;sup>37</sup>Hoefer develops this idea into a theory of 'Humean objective chance' supported by a version of Lewis's (1980) Best-System Analysis and representing a 'third way' for defining objective probabilities differing from, on the one hand, hypothetical (infinite) or actual (finite) frequencies and, on the other, the various versions of propensities. This will not be our concern, since our interest is simply in defining the part of the system which gives the probability distribution { $\pi(\lambda)$ } of initial points as an SNM.

can be constructed in a deterministic world. However, as Hoefer (2007, p. 568) points out, their 'characterization is obviously vague,' and he approaches the problem by giving some examples. The first two of them: the chance of getting double-zero on an American roulette wheel and the probability of heads (say) from good coin flips,<sup>38</sup> exemplify two important features of one kind of SNM:

- [1.1] The system behaves in a pseudo-random way. This is achieved by a setup which is sensitive to initial conditions (of the ball and the wheel in roulette and the velocity and position of the flip of the coin). While the coin flip is good in the sense that it is shielded against bias, in both cases random external influences (from air currents etc.) will make things more randomlooking.
- **[1.2]** The system has some kind of symmetry in terms of which a probability distribution can be hypothesized.

If we are engaged in theoretic model construction, these conditions will be enough to satisfy us that SNMs can be constructed in a deterministic world.<sup>39</sup> But if our aim is to physically construct something that works then we shall need to test reliability using relative frequencies. It is now quite easy to apply these ideas to Ex. 1 of Sec. 2.

One possibility is to take a well-shuffled pack of *N* cards, with each card identified with a point in  $\Gamma$  and  $N_{\lambda}$  in 'suit'  $\lambda$ . Draw a card and run the system, starting at that initial point in  $\Gamma$ . The chance of obtaining a card in suit  $\lambda$  is  $\pi(\lambda) = N_{\lambda}/N$ . So

$$\mathsf{P}[\mathbf{x} \in \sigma] = \frac{1}{N} \sum_{\{\lambda\}} N_{\lambda}(\sigma) = \frac{N(\sigma)}{N},$$

where  $N(\sigma)$  is the number of points in  $\Gamma$  belonging to  $\sigma$ . A procedure of this kind was applied to the Kac ring model in Lavis 2008, except that the pack of cards was replaced by a random number generator. Runs were tested for thermodynamic-like behavior by comparing them with a benchmark created by supposing that the system were ergodic.

Another example given by Hoefer, that of the decay of radium atoms, is of a different kind. Here the important features which enable the system to be characterized as an SNM are the following:

**[2.1]** The stochastic behavior (the emission of alpha particles by <sup>226</sup>Ra, say) is given by a physical system.

<sup>&</sup>lt;sup>38</sup>'Good' is used by Hoefer (2007, p. 567) to include conditions for shielding from bias, both in the way the coin is flipped and in the physical structure of the coin.

<sup>&</sup>lt;sup>39</sup>And as Hoefer (2007, p. 566) points out it would still be a good scheme even if the suggested machine never had been, and probably never would be, constructed: like a roulette wheel with 43 slots.

**[2.2]** The probability distribution is given by a physical theory (quantum mechanics). Specifically the probable number of particles emitted in a fixed time interval is given by a Poisson distribution.

It is clear that the two elements defining an SNM, namely stochastic behavior and a probability distribution, are present in [1.1], [1.2], and in [2.1], [2.2]. However, their origin is different and, importantly for us, the latter scheme is more closely akin to Ex. 2 of Sec. 2.

It is plausible to suppose that, while we may be able to isolate this system, which for the sake of brevity we denote as  $\mathcal{H}$ , with a fixed energy at t = 0, it may be more difficult to specify the exact value of that energy. So we consider one possible way of 'letting the physics' prepare an initial distribution of chances over different values of  $0 \le E < \infty$ . Suppose that, at some t < 0, the system  $\mathcal{H}$  is weakly coupled to a similar system  $\mathcal{H}'$  with Hamiltonian H'(p', q') and phase space  $\Gamma'$ . The weak coupling means that the single global constant of motion is H(p,q) + H'(p',q') and the system  $\mathcal{H} + \mathcal{H}'$  is ergodic on an energy surface  $H(p,q) + H'(p',q') = E^*$  in  $\Gamma \times \Gamma'$ . Given that the motion on this surface is typical type I, and using the time-average definition of probability, it can be shown (Khinchin 1949, Ch. 4) that

$$\mathsf{P}[H(\boldsymbol{p},\boldsymbol{q})=E] = \frac{\Omega(E)\,\Omega'(E^{\star}-E)}{\Omega^{\star}(E^{\star})},\tag{21}$$

where  $\Omega'(E')$  is the structure function of  $\mathcal{H}'$  and

$$\Omega^{\star}(E^{\star}) := \int_0^{\infty} \Omega(E) \, \Omega'(E^{\star} - E) \, \mathrm{d}E$$

is the structure function of  $\mathcal{H} + \mathcal{H}'$ . Now suppose that, at t = 0, the system  $\mathcal{H}$  is detached from  $\mathcal{H}'$ . The distribution of energies given by (21) is preserved.

$$\pi(E) = \frac{\Omega(E) \,\Omega'(E^* - E)}{\Omega^*(E^*)} \tag{22}$$

and, from (18),

$$\rho(\boldsymbol{p}_E, \boldsymbol{q}_E, E) = \rho(\boldsymbol{p}_E, \boldsymbol{q}_E \mid E) \pi(E) = \frac{\Omega'(E^* - E)}{\Omega^*(E^*)}.$$

giving, from (15), (19), and (22),

$$S_{\rm G}[\rho] = S_{\rm MC}^{\star}(E^{\star}) - \left\langle S_{\rm MC}^{\prime}(E^{\star}-E) \right\rangle_{\pi},$$

where  $S_{MC}^{\star}(E^{\star})$  and  $S_{MC}^{\prime}(E^{\prime})$  are respectively the microcanonical entropies of  $\mathcal{H} + \mathcal{H}^{\prime}$  and  $\mathcal{H}^{\prime}$ . It should perhaps be emphasized that, although (21) is normally

seen as part of the derivation of the canonical distribution in statistical mechanics,<sup>40</sup> it is not a consequence of any additional use of statistical-mechanical theory; it results simply from the *mechanical* properties of the system, together with the use of the time-average definition of probability. Here we have used contact of  $\mathcal{H}$  with  $\mathcal{H}'$  as a mechanical SNM for assigning objective probabilities to the energies of  $\mathcal{H}$ .

## 6 Conclusions

As indicated in Sec. 1 we have chosen to interpret 'objective,' when used to qualify probability, in the 'hard' sense of real-world chance. An alternative to this, where the probability distribution is derived according to some agreed procedure from a certain specified state of knowledge of (or information about) the system, could also be construed as objective but in a 'softer,' interpersonal sense. Such a program for statistical mechanics has, as was indicated above, been developed by Jaynes (1983), who called it 'predictive statistical mechanics' (ibid., p. 2). However, for him, this is 'not a physical theory but a form of statistical inference' (ibid., p. 416) and it has (at least for the present writer) the undesirable consequence that 'entropy is an anthropomorphic concept, not only in the well-known statistical sense that it measures the extent of human ignorance as to the microstate. *Even at the purely phenomenological level, entropy is an anthropomorphic concept* [his italics]' (ibid., p. 86).

The problem with developing a hard-objective theory of probability for statistical mechanics is not that there is a variety of possible interpretations, which, developed for probability theory in general, can be 'taken off the shelf' and applied to statistical mechanics, but rather that there is a paucity of suitable interpretations. That, for most practitioners, this has not seemed to be an urgent problem, is partly because of the way the probability distribution appears in statistical mechanics. Unlike other areas of science and economics, where the power of a theory is given directly in terms of the predicted probability of an event, in statistical mechanics the probability distribution is buried deep in the theory. Predictions are made for heat capacities, susceptibilities, critical temperatures, etc. Although there is, within the theory, something which can be understood as a prediction for the probability that x(t) lies in  $\sigma \subset \Gamma$ , there is no pretence that this can (even approximately) be tested. Bearing this in mind, it is relevant to ask for the possible hard-objective answers to the question: 'What is meant by the probability  $P|x(t) \in \sigma|$ ?' In this essay an answer to this question has been proposed based on the ergodic decomposition of  $\sigma$  into the subsets  $\{\sigma \cap \Gamma_{\lambda}\}$ 

<sup>&</sup>lt;sup>40</sup>The rest of the derivation (see, for example, Khinchin 1949, Ch. 5) establishes that, when  $\mathcal{H}$  is small in comparison with  $\mathcal{H}'$ ,  $\Omega'(E^* - E)/\Omega^*(E^*) \simeq \exp(-\beta E)/Z(\beta)$ , where  $Z(\beta) = \int_0^\infty \exp(-\beta E) dE$  and  $\beta$  is the solution of  $d \ln[Z(\beta)]/d\beta = -E^*$ , which is subsequently identified as  $1/k_BT$ .

and the assignment of probabilities within the subsets using the time-average definition of probability, and between subsets using an SNM. Of course, the future may yield other interpretations and in particular offer plausible alternatives to the use of an SNM. However, with the exception of the 'traditional' ensemble approach such do not seem to be currently on offer. It is therefore worth considering whether the use of ensembles is really an alternative view to that proposed here.

The ensemble picture is usually credited to Gibbs (1902),<sup>41</sup> who invites his readers to 'imagine a great number of independent systems, identical in nature, but differing in phase' (ibid., p. 5). This 'mental picture of such a collection of systems is called an *ensemble* [his italics]' (Huang 1963, p. 144) and  $P|x(t) \in \sigma|$ is the proportion of the number of representative phase points of the ensemble which lie in  $\sigma$  at time t. The use of the term 'ensemble' is widespread in statistical mechanics and, although it sometimes seems little more than a synonym for 'distribution,' it is worthwhile examining whether it gives a hard-objective interpretation of probability in statistical mechanics. We are invited to enter the imaginary world in which we have a large number of systems, identical (in some specified way) apart from the locations of their phase points. These phase points are then 'sprinkled' in a single phase space Γ. Accepting that this gives a conceptually useful picture, does it give a *practically* useful picture? The ensemble is meant to represent *all* systems sharing certain properties. But does it lead to a specification of the probability distribution? The answer is clearly 'no.' The only practical consequence of this point of view is Liouville's Equation, which is just the conservation condition for the flow of phase points. It is then necessary to justify in some other way the appropriate solution to Liouville's Equation for the various ensembles. Thus, for example, Gibbs (1902, p. 33) justifies the canonical distribution on the grounds that it

seems to represent the most simple case conceivable, since it has the property that, when the system consists of parts with separate energies, the laws of the distribution in phase of the separate parts are of the same nature,– a property which enormously simplifies the discussion.

The crucial features to be taken into account in the assignment of a probability distribution are dynamic structure and preparation. The strengths of the present work are that it applies to a wide class of systems (those whose dynamic structure gives an ergodic decomposition)<sup>42</sup> and that it demonstrates that part of the probability assignment (that between members of the decomposition) is essentially the probability associated with the mode of preparation. In this

<sup>&</sup>lt;sup>41</sup>Who, however, cites (ibid., p. viii) an earlier reference to the use of the picture of 'a great number of systems' by Boltzmann. For a discussion of this historical question, in which Maxwell also appears, see Emch & Liu 2002, p. 105.

<sup>&</sup>lt;sup>42</sup>The precise conditions for ergodic decomposition are given in Thm A.2.

context we have recognized that it is possible, although very difficult, to prepare the system in a state for which the subsequent evolution will not support the time-average definition of probability. We have argued that this is a place where the Neo-Boltzmannian idea of typicality is not synonymous with 'highly probable' and we have called system preparation and subsequent evolution which avoids this exceptional (measure-zero) set 'typical type I.' We have then given criteria for the system to be such that thermodynamic-like behavior is typical type II, where this type of typicality is to be understood as meaning 'highly probable.'

The weaknesses of our use of SNMs are evident. These are essentially blackbox probability generators, whether they are justified, as recommended by Hoefer (2007), as the result of best-systems analysis or, as not recommended by Hoefer, as something with a certain propensity. Either way the SNM is the part of the system which for the experimenter or model constructor is most arbitrary. The aim should be to make the choice which is most plausible for a model which aims to reflect the 'overall pattern of actual events in the world [which] ... make these chances exist' (ibid., p. 558). Inevitably this needs to be done on a case-by-case basis, as we have demonstrated in Sec. 5 for the two examples introduced in Sec. 2.

### Appendix A: Ergodicity and ergodic decomposition

It is convenient at this stage to represent time as discrete and, to avoid confusion, it is denoted by an integer superscript, rather than subscript; thus  $\phi := \phi^1$  and  $x_n = \phi^n x_0$  on the trajectory  $\mathcal{L}_{x_0}$ . If the underlying time parameter *t* is continuous then it is discretized with a small interval  $\Delta t$  and  $t := n \Delta t$ ,  $\phi := \phi_{\Delta t}$ . An important part of this discussion is *Birkhoff's Theorem*:<sup>43</sup>

**Theorem A.1** Let  $\mathfrak{m} \in \mathcal{M}_{\phi}$ , let f be a phase function integrable over  $\Gamma$  with respect to  $\mathfrak{m}$ , and let  $\Upsilon \in \Sigma_{\phi}$  with  $\mathfrak{m}(\Upsilon) \neq 0$ . Then, for almost every  $\mathbf{x}_0 \in \Upsilon$ , the infinite-time average of f along  $\mathcal{L}_{\mathbf{x}_0}$ , which is the limit

$$\hat{f}(\mathbf{x}_0) := \lim_{n \to \infty} \frac{1}{n} \sum_{k=0}^{n-1} f(\phi^k \mathbf{x}_0),$$
(A.1)

exists, with

$$\hat{f}(\phi^n \mathbf{x}_0) = \hat{f}(\mathbf{x}_0), \qquad \int_{\mathbf{Y}} \hat{f}(\mathbf{x}) \,\mathrm{d}\mathbf{m} = \int_{\mathbf{Y}} f(\mathbf{x}) \,\mathrm{d}\mathbf{m}. \tag{A.2}$$

For a system with continuous time made discrete by taking a time interval  $\Delta t$ , (A.1) is equivalent, as  $\Delta t \rightarrow 0$ , to

<sup>&</sup>lt;sup>43</sup>In this appendix we draw on the notation and definitions given in Sec. 2.

$$\hat{f}(\boldsymbol{x}_0) := \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau f(\phi_t \boldsymbol{x}_0) \, \mathrm{d}t.$$
 (A.3)

(For a proof, see, for example, Mañé 1987, Sec. 2.1.)

Any function *g* for which  $g(\phi x) = g(x)$ , for all  $x \in \Gamma$ , is said to be  $\phi$ -invariant. It is clear, from (A.1) and (A.2), that  $\hat{f}$  is such a function.<sup>44</sup>

Now, substituting into (A.1) or (A.3)  $f = i_{\sigma}$ , the indicator function of some  $\sigma \in \Sigma$ , gives, for almost all  $x_0 \in Y$ ,  $\hat{f}(x_0) = T(\sigma | \mathcal{L}_{x_0})$ , the average time spent by  $x(t) \in \mathcal{L}_{x_0}$  in  $\sigma$ .

Although  $T(\sigma | \mathcal{L}_{x_0})$  is constant along  $\mathcal{L}_{x_0}$ , that is, independent of the particular point  $x_0$  chosen to specify the trajectory, it will, in general, differ between trajectories. However, if Y is Lebesgue-indecomposable (that is to say, according to the definition in Sec. 2.1, one of the ergodic sets in  $\tilde{\Sigma}_{\phi}$ ), then  $T(\sigma | \mathcal{L}_{x_0})$  is constant almost everywhere in Y (Mañé 1987, Sec. 2.2); meaning that it takes the same value, denoted by  $T(\sigma | Y)$ , along all trajectories in Y for which it is defined. From (A.2),

$$\mathsf{T}(\sigma \mid \mathsf{Y}) = \frac{\mathfrak{m}(\sigma \cap \mathsf{Y})}{\mathfrak{m}(\mathsf{Y})}.$$
 (A.4)

The right-hand side of (A.4) is the average time spent by the phase point x(t) in  $\sigma$ , as it moves along a trajectory, which, as we have seen, for an autonomous system can be uniquely identified by specifying x(0). It follows from the assumed Lebesgue-indecomposability of Y that this time will be the same for almost all specifications of  $x(0) \in Y$ . The exceptional set of points of Lebesgue-measure zero corresponds to cases where the infinite-time sum or time-integral, in (A.1) or (A.3) respectively, does not exist.

Up to this point we have made no assumption about the measure m, except that it belongs to  $\mathcal{M}_{\phi}$  and is non-zero on Y. However, an important consequence of (A.4) is that, to within normalization over Y, it is unique and given by  $T(\sigma | Y)$ .

In Sec. 2.1 it was shown that the members of  $\widetilde{\Sigma}_{\phi}$  form a decomposition of  $\Gamma$ , denoted by  $\{\Gamma_{\lambda}\}$ . So, by setting  $Y = \Gamma_{\lambda} \in \widetilde{\Sigma}_{\phi}$ , it is clear that, starting with any  $\mathfrak{m} \in \mathcal{M}_{\phi}$  for which  $\mathfrak{m}(\Gamma_{\lambda}) \neq 0$ , (A.4) will yield a unique ergodic measure

$$\mathfrak{m}(\cdot \mid \lambda) := \mathsf{T}(\cdot \mid \Gamma_{\lambda}) = \frac{\mathfrak{m}(\cdot \cap \Gamma_{\lambda})}{\mathfrak{m}(\Gamma_{\lambda})}.$$
 (A.5)

To complete the mathematical results, we now need the *Ergodic Decomposition Theorem*, and given that the range of application of our approach depends on the applicability of this theorem, it is useful to state it in full technical detail:

**Theorem A.2** If  $\Gamma$  is a compact metric space with  $\mathcal{M}_{\phi} \neq \emptyset$  then the set of points  $\mathbf{x} \in \Gamma$  which can be associated with measures, according to the formula  $\mathfrak{m}(\cdot | \mathbf{x}) := \mathsf{T}(\cdot | \mathcal{L}_{\mathbf{x}})$ ,

<sup>&</sup>lt;sup>44</sup>This does not mean, of course, that *f* is constant throughout Y; only along a particular trajectory.

*is total*<sup>45</sup> *and any other*  $\mathfrak{m} \in \mathcal{M}_{\phi}$  *can be expressed as a linear combination of these measures* (Mañé 1987, Sec. 6.2).

In Sec. 4 we denoted the set of points, of measure zero, in  $\Gamma$  for which the time average  $T(\cdot | \mathcal{L}_x)$  was not defined as  $\mathring{\Gamma}$ , with  $\mathring{\Gamma}_{\lambda} = \Gamma_{\lambda} \cap \mathring{\Gamma}$ . Then it follows, from Thm A.2, that, since every  $x \in \Gamma_{\lambda} \setminus \mathring{\Gamma}_{\lambda}$  is associated with the same ergodic measure  $\mathfrak{m}(\cdot | \lambda)$ , given by (A.5), any  $\mathfrak{m} \in \mathcal{M}_{\phi}$  can be decomposed into a linear combination of the ergodic measures  $\widetilde{\mathcal{M}}_{\phi}$ , in the form given by (1) or (2).

# Appendix B: The relative-frequency and time-average interpretations of probability

The starting point of the relative-frequency interpretation is a space  $\Omega := \{\omega\}$  of outcomes of a trial or experiment and a sequence  $\mathcal{E}_n$  of *n* repetitions of the trial. For some particular  $\omega \in \Omega$ , and k = 1, 2, ..., n, let  $\xi_k(\omega) := 1$  if the outcome of the *k*-th trial is  $\omega$ , and zero otherwise. Then

$$\Xi(\omega \mid \mathcal{E}_n) := \frac{\xi_1(\omega) + \xi_2(\omega) + \dots + \xi_n(\omega)}{n}$$

counts the relative frequency of the outcome  $\omega$  in the *n* trials, and von Mises (1928, pp. 28–9) specified two conditions necessary to relate this to probability:

(i) The *convergence criterion*: that, when the sequence of trials is infinitely extended to  $\mathcal{E}$ ,

$$\lim_{\omega \to \infty} \Xi(\omega \mid \mathcal{E}_n) =: \Xi(\omega \mid \mathcal{E}) \quad \text{exists for all } \omega \in \Omega.$$
 (B.1)

(ii) The *randomness criterion*, which is defined as the nonexistence of an implementable gambling strategy<sup>46</sup> which could determine an infinite subsequence *E'* of *E* for which the relative frequency of any ω ∈ Ω had a limiting value Ξ(ω | *E'*) ≠ Ξ(ω | *E*).

The probability of the occurrence of  $\omega$  is then *defined* to be  $\Xi(\omega \mid \mathcal{E})$ .

Aside from the question<sup>47</sup> that the only realizable sequences of trials are of finite length, the von Mises approach is operational. A procedure is carried out to determine (to within some level of accuracy) a relative frequency, which is then taken to be a probability. In this straightforward sense it is clear that the relative-frequency approach has little or no relevance to statistical mechanics; no one takes literally the idea that the probability density function can be obtained by

<sup>&</sup>lt;sup>45</sup>The definition of a total set is given in Sec. 2.2.

<sup>&</sup>lt;sup>46</sup>The way that this can be done is by means of a *recursive gambling system*, for which the rigorous mathematical development is due to Wald and Church. For references to their work and for a summary of their conclusions see Gillies 2000a, pp. 105–9.

<sup>&</sup>lt;sup>47</sup>Discussed in detail by Gillies (2000a, pp. 96–105).

a sequence of experiments on a single system or simultaneous experiments on an ensemble of systems. The connection to relative frequencies is not through gathering data, but through the dynamics. We consider motion with discrete (or discretized) time along the trajectory  $\mathcal{L}_{x_0}$ . With a particular  $\sigma \in \Sigma$  and  $\Omega := \{\sigma, \Gamma \setminus \sigma\}$ , let

$$\xi_k(\sigma) := \mathfrak{i}_{\sigma}(\phi^k \mathbf{x}_0) \quad \text{for all } k.$$

It then follows from Birkhoff's Theorem (Thm A.1) that the convergence criterion is satisfied with  $\Xi(\sigma | \mathcal{E}) = T(\sigma | \mathcal{L}_{x_0})$ , for all  $\mathcal{L}_{x_0}$  for which  $x_0 \notin \mathring{\Gamma}$ ; that is to say, for all trajectories which are typical type I, these being the only ones for which we have used the time-average definition of probability. Thus we have at least a partial relationship between the relative-frequency and timeaverage definitions. The problem is the randomness criterion (ii). The sequence  $\xi_1(\sigma), \xi_2(\sigma), \xi_3(\sigma), \ldots$  is determined by specifying  $x_0$  and the dynamics, and the time-average probability is part of the theory. As in von Mises' treatment of a gas, 'the possibility of a direct determination of the probability does not exist' (1928, p. 21)<sup>48</sup> and consequently the possibility of choosing a subsequence cannot arise. So in order to understand the relationship to the relative-frequency interpretation, it is necessary to investigate the role of condition (ii). What is von Mises aiming to avoid by imposing this condition and what, if anything, is needed to replace it in our case of dynamic determination of the sequence?

It would seem that the underlying aim is to avoid the possibility of a *bias* leading to different values for the limiting frequency. Von Mises (1928) explicitly excludes biases arising from subsequence selection. But given, as we have seen, that such a selection cannot be made for our dynamic system, it is still necessary to consider other possible ways in which it could, in principle, be possible to obtain different values for the time average. In fact there is only one way, which is to choose different initial points x(0); once this is done the dynamics takes over and determines whether the time average exists and if so its value. For systems without any ergodic properties this will happen; different x(0) not lying on the same trajectory will yield different time averages. In the case of an ergodic system this possibility is eliminated for all cases for which we use the time-average definition, that is to say, for all  $x(0) \notin \tilde{\Gamma}$ . Then, from (9), the probability of  $x(t) \in \sigma$  is  $\mathfrak{m}(\sigma)$ , where  $\mathfrak{m}$  is the unique member of  $\mathcal{M}_{\phi}$ . For a system with an ergodic decomposition, and  $x(0) \notin \tilde{\Gamma}$ , it is, of course, the case that the probability of  $x(t) \in \sigma$  will have a different value depending on the member  $\Gamma_{\lambda}$  of the decomposition containing x(0). However, we have used the time-average definition of probability *only within the ergodic sets*  $\{\Gamma_{\lambda}\}$ , and in each of these the probability  $\mathbf{x}(t) \in \sigma$  is  $\mathfrak{m}(\sigma \mid \lambda)$  for all  $\mathbf{x}(0) \in \Gamma_{\lambda} \setminus \mathring{\Gamma}_{\lambda}$ . Although

<sup>&</sup>lt;sup>48</sup>He, however, goes on to say that 'there is nevertheless no fundamental difference between it' and other examples, which he cited, where such measurements are possible.

motion along a trajectory is not random, the role played by the randomness criterion (ii) is here played by ergodicity and ergodic decomposition.

We now return to van Lith's fourth objection and ask why she sees independence as a necessary ingredient of the relative-frequency interpretation. Von Mises (1928) introduces his relative-frequency definition of probability in Lecture 1 without stating that the trials are independent. But this is hardly surprising, since independence is a *probabilistic concept*<sup>49</sup> whereas the relative-frequency limit (B.1) is a means of *defining* probability. The question of independence arises only if the order of the argument is reversed. That is: Given that the random variables  $\xi_1(\omega), \xi_2(\omega), \dots, \xi_n(\omega)$  are jointly distributed with a given probability, under what conditions does the limit on the left-hand side of (B.1) exist? One answer to this question is that it converges to  $\lim_{n\to\infty} \langle \Xi(\omega \mid \mathcal{E}_n) \rangle$  with probability 1 if the Strong Law of Large Numbers is satisfied. The argument is then completed by the proof (Loève 1963, p. 14) that the Strong Law of Large Numbers is satisfied if the random variables are independently and identically distributed.<sup>50</sup> In that sense independence justifies the relative-frequency interpretation of probability, and it is clear, in particular from his discussion of Bernoulli and non-Bernoulli sequences (von Mises 1928, pp. 112-13), that von Mises equated randomness, at least in an informal way, with a physical concept of the independence of the trials in the sequence. In this sense van Lith's objection has weight, since, as she says, the only systems for which the steps along the flow are independent are Bernoulli systems, like the baker's gas, at the top of the ergodic hierarchy, and we have not restricted our discussion to such systems. A partial reply to this point is contained in von Mises' lectures. In his discussion of the Law of Entropy Increase (ibid., pp. 192-3) he considers 'linkages of events' in the form of Markov chains, the example being the distribution of molecules of a gas over the macrostates. He expects

with very great probability that the different distributions occurring in the natural time succession will appear with relative frequencies which are approximately equal to the corresponding probabilities [calculated from the combinatorial formula]. And [that] this holds even though this succession does not exhibit complete randomness.

If randomness means (in some sense) independence then he does not regard it as a sacrosanct element of the relative-frequency interpretation, always provided (presumably) that it is replaced by something which fulfils the same role. Given, as we have argued, that this role is to avoid bias, this is achieved by ergodicity.

<sup>&</sup>lt;sup>49</sup>The events A and B are independent if, according to an already defined probability,  $P[A \land B] = P[A] P[B]$ .

<sup>&</sup>lt;sup>50</sup>In fact the Strong Law of Large Numbers is satisfied for sequences which satisfy the weaker condition of exchangeability (ibid., p. 400).

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