We introduce the framework of classical Observational entropy, which is a mathematically rigorous and precise framework for non-equilibrium thermodynamics, explicitly defined in terms of a set of observables. Observational entropy can be seen as a generalization of Boltzmann entropy to systems with initial indeterminate conditions, and describes the knowledge achievable about the system by a macroscopic observer with limited measurement capabilities; it become Gibbs entropy in the limit of perfectly fine-grained measurements. This quantity, while previously mentioned in the literature, has been investigated in detail only in the quantum case [1, 2]. We describe this framework reasonably pedagogically, then show that in this framework, certain choices of coarse-graining lead to an entropy that is well-defined out of equilibrium, and which grows towards thermodynamic entropy as the system reaches equilibrium, even for systems that are genuinely isolated. Choosing certain macroscopic regions, this dynamical thermodynamic entropy measures how close these regions are to thermal equilibrium. We also show that in the given formalism, the correspondence between classical entropy (defined on classical phase space) and quantum entropy (defined on Hilbert space) becomes surprisingly direct and transparent.

I. MOTIVATION

From the introductory pedagogical level to contemporary fundamental research, and in both classical and quantum contexts, the concept of entropy has caused a great deal of confusion. Not only are there many definitions of different type of entropies appropriate to different contexts [3–6], but, we would contend, there are two distinct fundamental notions of to what entropy is meant to refer.

On one hand, entropy per the definitions of Shannon, Gibbs, or von Neumann, is an information-theoretic quantity associated with the probabilities attributed to states of a system. This entropy is preserved in a closed system undergoing evolution via the classical Liouville equation or a unitary quantum operator, reflecting the preservation of information in such systems, but the entropy may change (and will generally rise) if interactions with an external system are allowed.

On the other hand, entropy can measure how “generic” some state-of-affairs is, as described at a coarse-grained or macroscopic level. Thermodynamic entropy, and that defined by Boltzmann as the number of microstates associated with a given macrostate, share this character. This sort of entropy can (and tends to) increase in a closed system, satisfying some version of the Second Law of thermodynamics.

These notions are often conflated because they tend to coincide in equilibrium systems, all converging to the logarithm of the number of states compatible with some set of fixed constraints – whether those states are cells in classical state space, energy levels in quantum theory, or defined otherwise. Yet if we wish to describe systems out of equilibrium, in which entropy can evolve, or to evaluate entropy for small numbers of particles, more conceptual and mathematical precision is necessary.

In this paper we argue that there is a natural and rigorous definition of entropy at the classical level that:

1. Is well-defined in any classical system with a fixed phase-space and probability measure over that phase-space; in particular it is well-defined out of equilibrium and for small numbers of particles.

2. Constitutes a generalization of, and an interpolation between, classical Gibbs and Boltzmann entropies.

3. Is defined in terms of a coarse-graining that corresponds to a partitioning of phase-space.

4. Evolves continuously in time, and generically toward larger values, corresponding to a Second Law.

5. Can be cleanly transcribed into the quantum context – and in fact is the classical version of the quantum “Observational entropy” introduced by [1, 2].

and in addition,

6. It can be used to describe the dynamics of classical systems. Specifically, it can be used to define “dynamical thermodynamic entropy” that changes with the evolution of a system.

The idea coarse-graining has a very long history, going back to Boltzmann [7], and coarse-grained entropies or coarse-grained free energies have emerged in numerous applications, such as fluid dynamics and Navier-Stokes...
equations [8, 9] (clearly present in the continuum hypothesis [10]), statistical mechanics of fields and renormalization group [11–14], in chemical engineering in computing the entropy of mixing [15–17], and in field theory in the guise of renormalization (leading to the 1982 Nobel Prize in Physics for work on critical phenomena using the renormalization group [18]). And there are some definitions of entropy using some type of rigorously-defined coarse-graining, which mostly apply to dynamical systems, such as entropy of partition [19], Kolmogorov-Sinai entropy [19–22], or topological entropy [19, 20].

Nonetheless, in many works coarse-graining is often treated in a rather ad-hoc and non-rigorous manner, with many subtleties swept under the rug. The coarse-grained entropy that we are going to argue for here has also appeared previously in literature[4, 21, 23–26]. However, we have found no clear or comprehensive discussion of it even at the classical level, nor any compelling treatment of applications to thermodynamics.

Thus the aim of this paper is to motivate and define a rigorous mathematical framework of the coarse-grained entropy, which we believe gives an elegant unification of many coarse-graining techniques, then derive its various properties, interpret both from an information-theoretic perspective and from a physical perspective (by connecting it to thermodynamic entropy), and finally spell out its correspondence with the quantum version. In other words, we want to argue that with our definition of coarse-grained entropy, the desiderata in points 1–6 above are indeed satisfied.

II. BOLTZMANN ENTROPY

Although there are variations, the type of “state counting” entropy defined by Boltzmann [7, 27, 28] generally attributes a number $V$ of fundamental microstates to a given macrostate – defined in some terms – attributing an entropy proportional to $\ln V$ to the macrostate. To be more precise, we make use of the following definitions.

The state space of a system can be partitioned into non-overlapping subspaces that sum up to the full state space. This partition is called a “coarse-graining” and denoted by $\mathcal{C}$. An element of this partition is a called a macrostate.

For a microstate $m$ in a macrostate, we attach Boltzmann entropy of $S_B(m) = \ln(V)$ to this microstate (as well as to the macrostate of which it is an element) where $V$ is the number of microstates contained in the macrostate.

This entropy typically rises, at least on average, in any classical dynamical system. Consider for example the prototypical system of a small box of gas that is opened within a larger box, as depicted in Fig. 1, panel (a). In the Boltzmann view, we consider the phase-space of gas particles in the full box, so that immediately post-opening, the gas is in a low-entropy macrostate that might be described as “all particles in the small box.” Under natural evolution the microstate tends to wander out of this macrostate and into the much larger macrostate “particles spread throughout large box.” This is depicted in Fig. 2 (top panel.)

This scheme has the advantage of being defined...
throughout the process, not just in the equilibrium states. But it is problematic in that it changes discontinuously as the macrostate transitions from one macrostate to another, and in that it requires perfect knowledge of the microstate, which is never in practice available. What if one would like to describe a more realistic situation, in which the observer has only a partial knowledge about the state of the system? We will show that in such situations, classical Observational entropy extends the definition of Boltzmann, and leads to the continuously evolving quantity.

Another goal of this paper, as previously mentioned, is to use this generalized and smoothly-varying definition of Boltzmann entropy to describe thermodynamic entropy as a dynamical quantity, as opposed to the standard definition, which yields a fixed value that is completely determined by the external parameters of a system. To elaborate, in equilibrium systems, thermodynamic entropy (or more precisely, microcanonical entropy) is defined in terms of the density of states near a given overall conserved energy. Illustrated on our example, thermodynamic entropy defined this way changes only during the sudden quench of the Hamiltonian, which changes discontinuously due to the removal of the barrier during stage 1 \( \rightarrow \) 2 in Fig. 1 (a). In other words, this prescription ascribes exactly the same entropy to states 2 and 4, as illustrated in Fig. 1 (b) (top). This conflicts with the fact that the state 2 is a highly non-equilibrium state from which it should be in principle possible to extract a larger amount of work than from the equilibrium state 4. We will show that with a suitable choice of coarse-graining it is indeed possible to define a thermodynamic entropy that does not depend on the barrier removal, but rather on the underlying state of a system, as shown of Fig. 1 (b) (bottom). Moreover, this quantity will correspond to the standard thermodynamic entropy in its respective equilibrium states, increasing continuously from one equilibrium configuration (closed box) to the next (open box after a long time), making it a reasonable definition of a dynamical thermodynamic entropy.

### III. CLASSICAL OBSERVATIONAL ENTROPY

We desire a generalization Boltzmann entropy that can be applied to probability distributions given by phase-space density

\[
\rho(x, p; t)
\]

over initial microstates. This dynamical entropy should act as smoothing-out of the Boltzmann entropy, reducing to the actual Boltzmann entropy for a fully determined system. We also choose the phase-space density to be normalized as

\[
\int \rho(x, p; t) \, dx \, dp = 1.
\]

By phase-space density \( \rho(t) : (x, p) \rightarrow \rho(x, p; t) \) we mean a function parametrized by time \( t \) which attaches a real-valued probability density to each point in phase-space. Thus the probability that the state of the system is in the infinitesimal phase-space volume \( dx \, dp \) at time \( t \) is given by \( \rho(x, p; t) \, dx \, dp \).

Depending on a physical motivation, we assume that observer chooses a certain partition of this space, \( \Gamma = \bigcup_i P_i \). We collect these disjoint subsets – regions of phase-space - into what we call a coarse-graining, and denote \( C = \{P_i\}_i \).

Each region \( P_i \), called a macrostate, is usually defined by some inequality conditions on points of phase-space \((x, p)\). It usually represents a collection of points of phase-space consistent with some macroscopically observed value or property.

The number of states in each macrostate, which we simply call its volume, is linearly proportional to its phase-space volume. The volume of each macrostate is computed as an integral over this macrostate with a constant\(^2\) measure \( \mu \),

\[
V_i = \int_{P_i} \mu \, dx \, dp.
\]

This constant measure determines the inverse of the size of each microstate, and we will typically choose a conventional

\[
\mu = \frac{1}{\hbar^d N},
\]

where \( d \) is number of degrees of freedom of each particle \( (d = 1 \text{ for a particle moving on a line, and } d = 3 \text{ for particle in a 3-dimensional space}) \), \( N \) is number of particles, and \( \hbar \) is the Planck’s constant. The advantage of this specific choice is that its dimensions render \( V_i \) unitless (as required to take a logarithm), and because \( V_i \) then measures the actual number of quantum microstates within each macrostate, since each quantum microstate is considered to take a phase-space volume of \( \hbar^d N \), see e.g. [29].

To calculate the probability of the state being in macrostate \( P_i \), we integrate the phase-space density over this region,

\[
p_i(t) = \int_{P_i} \rho(x, p; t) \, dx \, dp.
\]

\(^2\) We demand the constant measure for the following reason: Due to the Liouville’s evolution, phase-space volume of any state described by a phase-space density \( \rho \) is a constant. If measure \( \mu \) varied depending on \((x, p)\), then the volume \( V_i = \int_{\{(x, p)\} \in (x, p; t) = 0} \mu \, dx \, dp \) associated with phase-space density would change in time. Since this volume is supposed to represent the number of microstates within it, and since it is reasonable to demand that this number stay the same during the evolution, we must demand a constant measure \( \mu \). More generally, Liouville’s equation and the property of time-independent phase-space volume is one of the primary reasons for using phase-space to describe thermodynamics, as opposed to for example configuration space, where the volume of states does not stay constant during the time evolution.
we can write phase-space is equal to one by Eq. (2).

span over several macrostates at the same time. are not known. In such situation the state of the system can signifying that the exact positions and momenta of particles the same evolution, but with indeterminate initial conditions and spends most of its time there. The second picture shows evolves from a small macrostate \( P \) through phase-space. The point in phase-space naturally 

\[
\begin{align*}
\text{FIG. 2. Schematic picture of an evolution of a system} & \text{ through phase-space. The point in phase-space naturally evolves from a small macrostate } P_1 \text{ to a large macrostate } P_4 \text{ and spends most of its time there. The second picture shows the same evolution, but with indeterminate initial conditions signifying that the exact positions and momenta of particles are not known. In such situation the state of the system can span over several macrostates at the same time.}
\end{align*}
\]

This gives a positive value, and all probabilities some up to one, since by definition, integral over the entire phase-space is equal to one by Eq. (2).

Defining projectors as window functions

\[
P_i(x, p) = \begin{cases} 
1, & (x, p) \in P_i \\
0, & (x, p) \notin P_i
\end{cases}
\]

we can write

\[
V_i = \mu \int_T \hat{P}_i(x, p) dx dp,
\]

\[
p_i(t) = \int_T \rho(x, p; t) \hat{P}_i(x, p) dx dp,
\]

where the integral now goes over the entire phase-space. This can be further compacted using the \( L^2 \)-inner product on real-valued functions,

\[
(f, g) \equiv \int_T f(x, p) g(x, p) dx dp,
\]

so that

\[
V_i = (\hat{P}_i, \mu),
\]

\[
p_i(t) = (\hat{P}_i, \rho(t)).
\]

With all this in place, we define classical Observational entropy with coarse-graining \( C \) as

\[
S_{O(C)}(t) = -\sum_i p_i(t) \ln \frac{p_i(t)}{V_i}.
\]

Since the coarse-graining \( C \) can be uniquely defined either by a set of macrostates \( P_i \), or by a set of corresponding projectors \( \hat{P}_i \), we can identify these two otherwise mathematically distinct objects, and write

\[
C = \{ P_i \} \equiv \{ \hat{P}_i \}.
\]

So far, our definition of coarse-grained entropy is mathematically identical to those used by Refs. [4, 23–26]; the next section introduces an important generalization to multiple coarse-grainings.

**IV. MULTIPLE COARSE-GRAININGS**

The above definition applies for any coarse-graining, but some coarse-grainings are more relevant than others. To define a thermodynamically relevant specification of Observational entropy, and for other purposes, it is necessary to generalize this entropy to include multiple coarse-grainings. This is done as follows.

Suppose we have several coarse-grainings of the phase-space, \( (C_1, \ldots, C_n) \). We define a joint coarse-graining

\[
C_{1, \ldots, n} = \{ P_{i_1, \ldots, i_n} \}_{i_1, \ldots, i_n}
\]

where the corresponding multi-macrostates are given by overlap of the previous macrostates, and the projectors as a multiple of projectors,

\[
P_i = P_{i_1, \ldots, i_n} = P_{i_1} \cap \cdots \cap P_{i_n},
\]

\[
\hat{P}_i = \hat{P}_{i_1, \ldots, i_n} = \hat{P}_{i_1} \cdot \cdots \cdot \hat{P}_{i_n}.
\]

In the above, we have also employed multi-index \( i = (i_1, \ldots, i_n) \).

Inserting the joint coarse-graining into the definition, Eq. (10), motivates the definition of the Observational entropy with multiple coarse-grainings as

\[
S_{O(C_1, \ldots, C_n)}(t) = -\sum_i p_i(t) \ln \frac{p_i(t)}{V_i},
\]
where
\[ V_i = (\hat{P}_i, \mu), \quad (16) \]
\[ p_i(t) = (\hat{P}_i, \rho(t)) . \quad (17) \]

Indeed, from the definition it follows \( S_{O(c_1, \ldots, c_n)} = S_{O(c_1, \ldots, c_n)} \). (Note the subtle notational difference.) That is, a set of coarse-grainings can also be considered as a single composite coarse-graining. \(^3\)

V. PROPERTIES

We briefly mention some properties of classical Observational entropy. Proofs can be found in Appendix A.

Theorem 1. (Observational entropy is a generalization of the Boltzmann entropy) For a single point in phase-space \((x, p) \in P_i\), equivalent to a delta function \( \rho(\hat{x}, \hat{p}) = \delta(\hat{x} - x, \hat{p} - p) \), we have
\[ S_{O(c)}(\rho) = S_B(\rho) = \ln V_i . \quad (18) \]

Definition 1. (Finer coarse-graining) We say that coarse-graining \( C_2 \) is finer than coarse-graining \( C_1 \) (and denote \( C_1 \rightarrow C_2 \)) when for every \( P_{i_1} \in C_1 \), there exists an index set \( I^{(i_1)} \) such that \( P_{i_2} = \bigcup_{i \in I^{(i_1)}} P_{i_2} \). (That is, each element of \( C_1 \) can be partitioned using elements of \( C_2 \).)

When \( C_1 \rightarrow C_2 \), we can also write \( \hat{P}_{i_1} = \sum_{i \in I^{(i_1)}} \hat{P}_{i_2} \).

Theorem 2. (Observational entropy is a monotonic function of the coarse-graining.) If \( C_1 \rightarrow C_2 \) then
\[ S_{O(c_1)}(\rho) \geq S_{O(c_2)}(\rho) . \quad (19) \]

Definition 2. (Coarse-graining given by an observable) Let \( A : (x, p) \rightarrow a \) be a classical observable, that assigns value \( a \) (property) to each point in phase-space. We define macrostates associated with value \( a \) as \( P_a = \{(x, p)|A(x, p) = a\} \) in case of observable with discrete values, or as \( P_a = \{(x, p)|a \leq A(x, p) < a + da\} \) in case of a continuous observable. \(^4\) We define coarse-graining by the observable \(^5\) \( A \) as \( C_A = \{P_a\}_a \).

\[ \text{Theorem 3. (Observational entropy with multiple coarse-grainings is bounded)} \]
\[ S_{G}(\rho) \leq S_{O(c_1, \ldots, c_n)}(\rho) \leq \ln V \quad (20) \]

where \( S_{G}(\rho) = -\int_\Gamma \frac{\rho(x, p)}{\mu} \ln \frac{\rho(x, p)}{\mu} \; \mu dx dp \), and \( V = \int_\Gamma \mu dx dp \) is the total volume of the phase-space. \( S_{G}(\rho) = S_{G(C_1, \ldots, C_n)}(\rho) \) if and only if \( \rho \rightarrow C_1, \ldots, C_n \), i.e., if the joint coarse-graining is fine enough to distinguish between points in phase-space that have different assigned probabilities.

\( S_{G}(\rho) \) represents Gibbs entropy. \(^6\) Gibbs entropy is invariant under Liouville’s evolution. It is zero for a single point in phase-space, and it is a property of a state, and not of a coarse-graining. This quantity also appears as functional \( H \) in the classical H-theorem, as interpreted by Tolman [31]. Since \( \mu \) is the inverse of the phase-space volume of a single microstate, \( p_i = \rho(x, p) \) is the probability of being in a microstate, so we can as well write \( S_{G}(\rho) = -\sum_{i} p_i \ln p_i \), i.e. the Shannon entropy of these probabilities. The quantum mechanical equivalent of Gibbs entropy is the von Neumann entropy, which is invariant under unitary evolution, is zero for pure states, and which is also property of a state and not of a coarse-graining.

Theorem 4. (Observational entropy is non-increasing with each added coarse-graining.)
\[ S_{O(c_1, \ldots, c_n)}(\rho) \leq S_{O(c_1, \ldots, c_{n-1})}(\rho) \quad (21) \]

for any set of coarse-grainings \((C_1, \ldots, C_n)\) and any phase-space density \( \rho \).

These theorems show that Observational entropy can be elegantly interpreted as the amount of knowledge observer would obtain if he or she were to measure the macroscopic observables that define the coarse-grainings. While Theorem 2 says that an observer with better resolution will get to know more about the system, Theorem 3 says that no matter what coarse-grained measurements they choose to perform, their knowledge will be still limited by an inherent uncertainty in the system given by the Gibbs entropy. On the other hand, no matter the coarse-graining, their knowledge cannot be worse than that measured by the maximal entropy, which signifies complete uncertainty about the system’s state. Theorem 4 then shows an intuitive statement that each additional macroscopic measurement will provide better knowledge of the system, at least on average.

---

\(^3\) As discussed below, this statement does not transfer to quantum mechanics unless the coarse-grainings commute.

\(^4\) The infinitesimal increment \( da \) plays the role of the resolution in measuring the observable \( A \).

\(^5\) Note 1: Although \( \rho \) is not usually considered an observable, it fulfills our definition and we will treat it as such in the theorem that follows. Note 2: we can also define the spectral decomposition of an observable as \( A = \sum \alpha_n P_{\alpha_n} \), or \( A = \int a \rho A da \), where eigenvalues \( a \) are considered to be different from each other. This spectral decomposition is unique, and it plays an identical role in phase-space with inner product (8) as the spectral decomposition of a quantum observable plays in a Hilbert space.

\(^6\) Definition of Gibbs entropy is not consistent in literature. Our definition seems to be the most common, and is used for example in [3]. Sometimes, Gibbs entropy is defined as Shannon entropy of probabilities of energy distribution (which has a quantum equivalent called diagonal entropy [30]), and what is called Gibbs entropy in [26] is actually our Observational entropy.
In addition, rewriting Eq. (15) as
\[ S_{O(c_1, \ldots, c_n)}(t) \equiv -\sum_i p_i(t) \ln p_i(t) + \sum_i p_i(t) \ln V_i \] (22)
provides an intuitive information-theoretic interpretation. The first term denotes an uncertainty as measured by the Shannon entropy regarding to which macrostate the microstate of the system belongs. In other words, if one were to make a coarse-grained measurement at time \( t \) given by the coarse-graining (for example a measurement determining the system’s energy) the first term measures the uncertainty in the measurement outcomes in such a coarse-grained measurement. The second term measures the average remaining uncertainty about the microstate after this coarse-grained measurement was done. Put together, Observational entropy measures the average amount of uncertainty about a microstate of a system, from a point of view of an observer that can track only certain macroscopic properties by his/hers ability to perform coarse-grained measurement.

VI. THERMODYNAMICALLY RELEVANT NON-EQUILIBRIUM ENTROPY: \( S_{xE} \)

The treatment thus far has pertained to any possible coarse-graining. However, even if entropy increase is generic, there is no reason to expect that an arbitrary coarse-graining will be closely connected with thermodynamics, e.g. it relates temperature, energy and entropy.

In this section we introduce a (composite) coarse-graining that lead to an entropy relevant for closed classical systems, that is perfectly defined for systems outside of equilibrium, and grows to the equilibrium thermodynamic value when the system thermalizes. This dynamical quantity will describe physical regions coming into equilibrium with each other.

Let us consider a system of \( N \) particles contained in a 1-dimensional box from position of \( L_1 \) to \( L_2 \) of size \( L = L_2 - L_1 \). We coarse-grain this box into \( m \) physical regions (bins) of size \( \Delta x = \frac{L}{m} \). Considering the vector of positions as \( x = (x_1, \ldots, x_N) \), and vector of number of particles in each part of the box as \( n = (n_1, \ldots, n_m) \), we define positional (configuration) macrostates as
\[ P_n \equiv \{(x,p)|n_1 \text{ particles with position } L_1 \leq x < L_1 + \Delta x, \ldots, n_m \text{ particles with position } L_1 + (m-1)\Delta x \leq x < L_2\} \] (23)

Clearly, we can easily generalize this to any number \( d \) of spatial dimensions. This coarse-graining corresponds to measuring number of particles in each one of the \( d \) bins, i.e., to a coarse-grained measurement of local particle numbers, and we denote it \( C_X \equiv \{P_n\}_n \). For example, \( P_{(3,0,1)} \) corresponds to a macrostate where three particles are in the first bin, zero in the second, and one in the third.

We also define energy macrostates with width \( \Delta E \), as
\[ P_{E,\Delta E} \equiv \{(x,p)|E < H(x,p) \leq E + \Delta E\} \] (24)
where \( H \) denotes the Hamiltonian. When \( \Delta E = dE \) is an infinitesimal increment, we simply denote \( P_E \equiv P_{E,dE} \), its corresponding projector as \( \hat{P}_E \equiv \hat{P}_{E,\Delta E} \), and volume as \( V_E \equiv V_{E,\Delta E} \). We call coarse-graining with such an infinitesimal energy increment a “fine-graining” in energy, and denote it \( C_E \equiv \{P_E\}_E \) (considering definition (2), \( C_E \equiv C_H \)). It is important to emphasize here that \( dE \) is fixed to be the same for all energies \( E \).

The position-energy macrostates are then defined as \( P_{nE} \equiv P_n \cap P_E \), and the respective projectors are \( P_{nE} = P_n P_E \). With macrostate volumes \( V_{nE} = (P_{nE},\mu) \), and probabilities \( p_{nE} = (\hat{P}_{nE},\rho) \), we define thermodynamically relevant coarse-grained entropy
\[ S_{xE}(t) \equiv S_{O(c_X,c_H)}(t) \equiv -\sum_{n,E} p_{nE}(t) \ln \frac{p_{nE}(t)}{V_{nE}}. \] (25)

Figure 3 gives an example of these quantities for a single particle in a Harmonic potential.

As we will show in the next section, this quantity\(^8\) has all the desired properties expected of dynamical definition of thermodynamic entropy.

VII. THERMODYNAMIC BEHAVIOR

We now take a closer look at the thermodynamic behavior of \( S_{xE} \). We will show that for systems in equilibrium, the \( S_{xE} \) and thermodynamic entropy coincides.

---

\(^7\)For example, one could also think of an energy coarse-graining \( C^{\text{eigen}}_E \equiv \{P^{\text{eigen}}_E\}_E \), consisting of projectors onto “eigenstates” of the classical Hamiltonian, where we fit the width of each energy shell \( dE \) so that \( V^{\text{eigen}}_E = 1 \), meaning that each macrostate corresponds to a single microstate. In that case \( dE = dE(E) \) will generally depend on the energy. Projectors (window functions) \( P^{\text{eigen}}_E \) are then a classical equivalent of projectors onto quantum energy eigenstates \( |E\rangle \langle E| \). However, this would not give a desirable long-time behavior for \( S_{xE} \); in particular, the entropy assigned to a microstate in a given energy macrostate \( P_E \) would not be the correct microcanonical entropy, which is defined as a logarithm of number of microstates in energy shell \( \{E, E + dE\} \). Projectors \( P_E \in C_E \) with fixed \( dE \) correspond to the sum \( \sum_{E,E+dE} |E\rangle \langle E| \) in quantum mechanics. We also note that correspondence between projectors onto eigenstates of the Hamiltonian \( |E\rangle \langle E| \) (called stationary Liouville eigenstates) and \( P^{\text{eigen}}_E \) have been explored in \[32\] and references therein. It was shown that the Wigner function of \( |E\rangle \langle E| \) converges to a distribution that can be viewed as a highly peaked \( P^{\text{eigen}}_E \) in the \( \hbar \to 0 \) limit (see Eq. (24) in \[32\]).

\(^8\)We note that another choice of coarse-graining also leading to thermodynamically relevant entropy is one related to measuring local energies. We will not elaborate on this choice here, and instead refer an interested reader to the fully quantum version of this entropy described in Ref. \[1\], \[2\].
where the right position-energy macrostate, left position-energy macrostate is the same as the volume of jump out of its energy shell, but only rotate through it (blue time as shown in Fig. 1. We model this by a Hamiltonian physical scenarios such as the expansion of an ideal gas.

FIG. 3. Phase-space of a single particle in a Harmonic potential, with a positional (configuration) coarse-graining, and energy coarse-graining. The blue positional macrostate \( P_{(1,0)} \) corresponds to statement “the particle is on the left side of the box”, while the red energy macrostate \( P_E \) corresponds to “particle has energy between \( E \) and \( E + dE \)”. Overlap of these two macrostates \( P_{(1,0)E} \) (purple) is a position-energy macrostate which corresponds to “the particle is on the left side of the box and has energy between \( E \) and \( E + dE \)”. Energy macrostates — shells of constant energy of width \( dE \) — form ellipses in this example because they are given by equations \( E = \frac{1}{2}m p^2 + \frac{1}{2}kx^2 = \text{const} \). The volume of the energy macrostate \( V_E \) is proportional to the red area (including purple) in the picture, and it defines the microcanonical entropy \( S_{\text{micro}}(E) \equiv \ln V_E \). In an isolated system, a particle will never jump out of its energy shell, but only rotate through it (blue arrow). In the situation depicted, where the volume of the left position-energy macrostate is the same as the volume of the right position-energy macrostate, \( V_{(1,0)E} = V_{(0,1)E} = \frac{1}{2} V_E \), the dynamical thermodynamic entropy has a constant value \( S_{x,E}(t) = \ln(\frac{1}{2}V_E) = S_{\text{micro}}(E) - \ln 2 \), which is the same as microcanonical entropy of a particle in a half of the box.

and that this entropy effectively measures dynamical physical scenarios such as the expansion of an ideal gas.

Consider the prototypical example of a gas contained in the first half of the box, expanding into its full volume, as shown in Fig. 1. We model this by a Hamiltonian undergoing quench (a sudden discontinuous change) at time \( t = 0 \),

\[
H(x, p, t) = \begin{cases} 
H_1(x, p) = H_0(x, p) + U_1(x), & t < 0 \\
H_2(x, p) = H_0(x, p) + U_2(x), & t \geq 0 
\end{cases}
\]

where \( H_0 \) denotes Hamiltonian of the particles themselves (which may or may not contain interaction between the particles), and

\[
U_1(x) = \begin{cases} 
0, & \forall i, \ 0 < x_i < \frac{L}{2} \\
+\infty, & \text{otherwise} 
\end{cases} 
\]

\[
U_2(x) = \begin{cases} 
0, & \forall i, \ 0 < x_i < L \\
+\infty, & \text{otherwise} 
\end{cases} 
\]

denote two infinite potential wells.

For Hamiltonian \( H \), the microcanonical entropy is defined as the logarithm of number of microstates in each energy shell [33], which we can write two ways as

\[
S^{(H)}_{\text{micro}}(E) = \ln V_{E,\Delta E} = \ln(\rho(E)\Delta E). 
\]

\( V_{E,\Delta E} \) is the volume of an energy macrostate, and \( \rho(E) \) denotes the energy density of states. \( \Delta E \) is the width of the energy macrostate which can be fixed to some small but non-zero value\(^9\) that is considered to be independent of \( E \). More generally, we can define thermodynamic entropy as

\[
S^{(H)}_{\text{th}} \equiv S_{O(C_H)},
\]

which coincides with the definition of microcanonical entropy for a single point in phase-space, and with canonical entropy for a canonical distribution \( \rho(x, p) = \frac{1}{Z} e^{-\beta H(x, p)} \), where \( \beta \) denotes inverse temperature, and \( Z = \int e^{-\beta H(x, p)} dx dp \) is the partition function.

In the following, we consider \( S_{x,E} \equiv S_{O(C_X, C_H)} \) with positional coarse-graining \( C_X \) that halves the box \( (n = (n_1, n_2)) \), \( L_1 = 0 \), \( L_2 = L \), \( \Delta x = \frac{L}{2} \), and with energy coarse-graining \( C_{H_2} \) given by the Hamiltonian after the quench.

From Theorem 4, we can immediately see that thermodynamic entropy of the entire box bounds the \( S_{x,E} \):\(^10\)

\[
S_{x,E} = S_{O(C_X, C_{H_2})} = S_{O(C_{H_2}, C_X)} \leq S_{O(C_{H_2})} = S^{(H_2)}_{\text{th}}.
\]

Now we move onto studying the actual dynamics of \( S_{x,E} \).

A. Dynamics of \( S_{x,E} \) for deterministic initial conditions

First we assume a fully-determined state of \( N \) particles contained in the left part of the box, described by a state

----

\(^9\) Since \( \rho(E) \) rises exponentially with \( E \) and \( \ln(\rho(E)\Delta E) = \ln \rho(E) + \ln \Delta E \), the choice of \( \Delta E \) ultimately does not matter, because \( \ln \Delta E \) acts only as an additive constant which is small compared to the first term. Moreover, since we are usually interested in changes in entropy, rather than in absolute values, in such situations value of this additive term becomes completely irrelevant.

\(^10\) Symmetry \( S_{O(C_X, C_{H_2})} = S_{O(C_{H_2}, C_X)} \) holds for classical Observational entropy, but not for quantum Observational entropy [2].
If initial conditions were indeterminate, we plot the 16-dimensional phase-space as four single particle phase-spaces stacked onto each other. **1** Particles start in the left side of the box, which corresponds to macrostate \( P_{(4,0)E} \) ("four particles on the left, zero on the right"), where \( E \) denotes the total energy of the system. This configuration gives microcanonical entropy of the left half of the box, \( S_{xE}^{(H_1)} = \ln V_{(4,0)E} = S_{\text{micro}}(E) \). **2** As particles evolve, they wander into the largest macrostate \( P_{(2,2)E} \) ("two particles on the left, two on the right") allowed by the given energy, which is 6 times bigger than the initial macrostate, and they spend most of their time there. The entropy of this largest macrostate is equal to the microcanonical entropy of the entire box up to some correction, \( S_{xE} = \ln V_{(2,2)E} = S_{\text{micro}}(E) - \frac{1}{2} \ln(2\pi) \), \( m = 2 \) in Eq. (33). **3** If the initial state was not fully determined, then after some time the particle positions become uncertain, and the phase-space density becomes quite uniformly smeared over the entire energy shell \( P_{E}^{(4,0)E} \), which is the effect known as mixing. This erases corrections to the entropy, which then exactly equals the microcanonical entropy of the entire box: \( S_{xE}^{(H_2)} = \ln V_{E} = S_{\text{micro}}^{(H_2)}(E) \).

**FIG. 4.** Evolution of \( N=4 \) particles in the phase-space, with position-energy coarse-graining taken from Fig. 3. We plot the 16-dimensional phase-space as four single particle phase-spaces stacked onto each other. **1** Particles start in the left side of the box, which corresponds to macrostate \( P_{(4,0)E} \) ("four particles on the left, zero on the right"), where \( E \) denotes the total energy of the system. This configuration gives microcanonical entropy of the left half of the box, \( S_{xe} = \ln V_{(4,0)E} = S_{\text{micro}}^{H_1}(E) \). **2** As particles evolve, they wander into the largest macrostate \( P_{(2,2)E} \) ("two particles on the left, two on the right") allowed by the given energy, which is 6 times bigger than the initial macrostate, and they spend most of their time there. The entropy of this largest macrostate is equal to the microcanonical entropy of the entire box up to some correction, \( S_{xe} = \ln V_{(2,2)E} = S_{\text{micro}}^{H_2}(E) - \frac{1}{2} \ln(2\pi) \), \( m = 2 \) in Eq. (33). **3** If the initial state was not fully determined, then after some time the particle positions become uncertain, and the phase-space density becomes quite uniformly smeared over the entire energy shell \( P_{E} \), which is the effect known as mixing. This erases corrections to the entropy, which then exactly equals the microcanonical entropy of the entire box: \( S_{xe} = \ln V_{E} = S_{\text{micro}}^{H_2}(E) \).

**FIG. 5.** Simulation of evolution of \( S_{xe} \) of a system of \( N = 64 \) particles in a 2-dimensional box coarse-grained into \( m = 4 \) physical regions, evolving through a Hamiltonian including weak inter-particle interactions, and taking periodic boundary conditions. The green and red dashed lines represent thermodynamic entropy of the bottom left quarter, and the full system respectively. As the system evolves, the particles spread throughout the regions, and the \( S_{xe} \) grows to the thermodynamic entropy of the full system, up to some finite-size corrections, as expected from Eq. (33). Illustrations of the particle spread are the real snapshots of the system at different times of evolution in our simulation.
\((x_0, p_0) \in P_{(N,0)E}\). We have

\[ S_{xE}(x_0, p_0) = \ln V_{(N,0)E} = \ln V_E^{(H_1)} = S_{\text{micro}}^{(H_1)}(E). \quad (32) \]

The first equality comes from Theorem 1, and the second comes from the fact that macrostate of \(N\) particles in the left side of the box with energy \(E\) is identical to the energy macrostate of the initial Hamiltonian, \(P_{(N,0)E} = P_E^{(H_1)}\). Therefore, for initial particles contained in the left side of the box, \(S_{xE}\) gives the microcanonical entropy of this side of the box.

As the particles evolve, some of them will go to the right side of the box and some remain. After some time, the state of the system becomes what we can describe as "about a half of the particles are on the left, and about a half of the particles are on the right side of the box".

We can say the same by saying that the point in phase-space will wander around, and will most likely end up in one of the largest macrostates. In the current situation, the largest macrostate corresponds to a statement "a half of the particles is on the left side of the box, a half is on the right, and the total energy is \(E^n\). This is schematically depicted as stages 1 → 2 in Fig. 4.

Due to the slow growth of the logarithm, the entropy associated with either of those large macrostates will not differ much: there will be some corrections, but they will become irrelevant in the thermodynamic limit. So in order to find the long-time behavior of \(S_{xE}\), it is therefore enough to calculate the entropy for the largest of the macrostates, which is what we do in Appendix C. We find that for \(m\) bins,

\[ \lim_{t \to +\infty} S_{xE}(\rho(t)) = S_{\text{micro}}^{(H_2)}(E) + \frac{1}{2} \ln(2\pi N) - \frac{m}{2} \ln \frac{2\pi N}{m} - \frac{m}{2} \ln \frac{m}{2}. \quad (33) \]

This means that in the case of perfect knowledge of the system, \(S_{xE}\) matches microcanonical entropy of the full system, up to some small corrections. The second term becomes negligible compared to the first in the thermodynamic limit of particle number \(N \to \infty\). The last term represents a finite-size effect, which for small number of bins \(m\) (or equivalently, large bin sizes) is also small in comparison with the first term. We will see in the next section that these corrections are an artifact of taking the deterministic initial conditions: they disappear in case of indeterminate initial conditions.

**B. Dynamics of \(S_{xE}\) for indeterminate initial conditions**

Let us define the phase-space density of a microcanonical ensemble as

\[ \rho_{E,\Delta E}^{(\text{micro})}(x, p) \equiv \begin{cases} \frac{\mu}{V_E^{(H_1)}}, & (x, p) \in P_{E,\Delta E} \\ 0, & (x, p) \notin P_{E,\Delta E} \end{cases}. \quad (34) \]

Equivalently, we can write

\[ \rho_{E,\Delta E}^{(\text{micro})} = \frac{\mu}{V_E^{(H_1)}} P_{E,\Delta E}. \quad (35) \]

It is easy to see that for this microcanonical ensemble, as long as \(dE \ll \Delta E\) (i.e., the energy coarse-graining is fine enough to determine the width of the ensemble), \(S_{xE}\) gives the microcanonical entropy:

\[ S_{xE}(\rho_{E,\Delta E}^{(\text{micro})}) = \ln V_{E,\Delta E} = S_{\text{micro}}(E), \quad (36) \]

where \(\rho(E)\) denotes the energy density of states.

More generally, in Appendix A we prove a theorem that gives meaning to all stationary states: For phase-space densities that are mixtures of energy macrostates (such as the microcanonical and canonical ensembles), \(S_{xE}\) gives the thermodynamic entropy:

**Theorem 5.** For phase-space density of form \(\rho = \mu \sum_{E} f(E) P_E\), where \(f(E)\) is any function of energy \(E\) normalized as \(\sum_E f(E)V_E = 1\),

\[ S_{xE}(\rho) = S_{\text{O}(\mathcal{H}_2)} = \rho_{\text{th}}(\rho). \quad (37) \]

Now for the dynamics. We consider initial state at some time \(t < 0\) that is a microcanonical state of \(N\) particles contained in the left part of the box, and none in the other half, which we can denote as a microcanonical ensemble of the initial Hamiltonian,

\[ \rho_0 \equiv \rho_{E,\Delta E}^{(\text{micro};H_1)}. \quad (38) \]

Since this is a stationary state of \(H_1\), \(\rho(t) = \rho_0\) for \(t < 0\).

Similar to Eq. (32), we find that for \(t < 0\),

\[ S_{xE}(\rho_t) = \ln V_{E,\Delta E}^{(H_1)} = S_{\text{micro}}^{(H_1)}(E). \quad (39) \]

(See Appendix B for details.) In other words, \(S_{xE}\) of the initial state is equal to the microcanonical entropy of the first half of the box.

At time \(t = 0\), the available phase-space suddenly expands, and phase-space density \(\rho(t)\) starts to explore the full extent of it. That first leads to a quick increase of entropy due to the same reasons as for the case of deterministic conditions, i.e., because the phase-space density will wander into the largest macrostate. However, due to mixing [34], after with time the positions of the particles will become increasingly uncertain, and the phase-space density will become uniformly smeared over all points in each energy shell. This is depicted as stages 2 → 3 in Fig. 4.

Mathematically, this means that the phase-space density converges to microcanonical state of the second Hamiltonian,

\[ \lim_{t \to +\infty} \rho(t) = \rho_{E,\Delta E}^{(\text{micro};H_2)}. \quad (40) \]
According to Theorem 5, $S_{x,E}$ of this state must be equal to the microcanonical entropy of the entire box,

$$\lim_{t \to +\infty} S_{x,E}(\rho(t)) = \ln V_{E,\Delta E}^{(H_2)} \equiv S_{\text{micro}}^{(H_2)}(E). \quad (41)$$

Clearly, one can generalize this to any initial ensembles, since due to mixing, any initial phase-space density will become a stationary state of Hamiltonian $H_2$, in a sense of Theorem 5.

Having indeterminate initial conditions therefore results in $S_{x,E}$ converging to thermodynamic entropy exactly, without the corrections of Eq. (33).

C. Simulations

To support our analytical arguments, we have performed a simulation of a thermodynamic system of gas in $d = 2$ spatial dimension, and for 4 and 16 partitions. The case of 4 partitions is depicted in Fig. 5.

We take $N = 64$ particles of identical mass $m = 1$, initialize them in the lower left corner of size $8 \times 8$, within the full box of size $16 \times 16$ with periodic boundary conditions. The velocity of each particle has been randomly drawn from the Normal distribution. Particles interact via a Lennard-Jones potential

$$u(r) = \frac{K_0}{r^{12}} - \frac{K_1}{r^6}, \quad (42)$$

where $K_0 = 0.008333$ and $K_1 = 0.016667$ and $r$ denotes distance between each two particles. Particles are then evolved via a velocity Verlet algorithm with time step $10^{-4}$.

As particles and heat spread from one region to the others, entropy $S_{x,E}$ grows from thermodynamic entropy of the first bin to the thermodynamic entropy of the full system, up to some finite-size corrections as expected from Eq. (33), effectively modelling thermalization of an expanding gas.

D. Interpretation

We have shown that $S_{x,E}$, which is well-defined out of equilibrium, corresponds to the thermodynamical entropy of the initial subsystem, and it grows to thermodynamic entropy of the full system, for both cases of determinstic and non-determinstic initial conditions. Thus, $S_{x,E}$ behaves as expected of a dynamical thermodynamic entropy.

Physically, we can interpret $S_{x,E}$ as a measure of thermal equilibrium between the different physical regions given by coarse-graining in position. The regions are in thermal equilibrium with each other when $S_{x,E}$ is equal to thermodynamic entropy. When $S_{x,E}$ is low, it means that many particles and energy is contained in one or a few small regions, and the system is therefore in a highly non-equilibrium state.

Mathematically, for a single point in phase-space $(x, p)(t) \in P_{(n_1, \cdots, n_m)}E$, the $S_{x,E}$ gives value

$$S_{x,E}(t) = \ln V_{(n_1, \cdots, n_m)}E, \quad (43)$$

which is exactly the thermodynamic entropy that one would assign to a system of $N$ particles distributed into $m$ bins, in the situation if the energy were allowed to be exchanged between the bins, but particle number in each bin were fixed. $S_{x,E}(t)$ therefore measures an immediate thermodynamic entropy of a system, as if one were to infinitely quickly insert elastic membranes in between the bins at time $t$, that allow for energy transfer but not for particle transfer, and then wait until the system relaxes.

In other words, $S_{x,E}(t)$ gives an immediate thermodynamic entropy of the full system subject to constraints on the number of particles in each bin.

VIII. COMPARISON OF CLASSICAL AND QUANTUM OBSERVATIONAL ENTROPY

In the same way that a point in phase-space describes a classical system, a vector in a Hilbert space describes a quantum system. This state-vector (or wave-function) encodes every property of a quantum system and is evolved using the Schrödinger equation. More generally, a quantum system with indeterministic initial condition is described by a density matrix $\hat{\rho}$, which is a positive semi-definite operator acting on the Hilbert space. The density matrix is a quantum equivalent of phase-space density, and is evolved through the von Neumann equation, as compared to Liouville’s equation in classical system.

In classical systems, the coarse-graining is defined as a partitioning of phase-space. These partitions/regions — subsets of phase-space — are called the macrostates. To define coarse-graining in quantum physics, we have to partition a Hilbert space. However, partitions of Hilbert space are not composed of subsets but of subspaces combined in a direct sum: $H = H_1 \oplus H_2 \oplus \cdots$. We can form these subspaces for example by choosing a basis of the Hilbert space, and putting every basis vector into a group. A subspace is then created by taking all the linear combinations of vectors in the group. For example, real three-dimensional space could be partitioned as
TABLE I. Classical and quantum descriptions of an isolated physical system.

| Classical | Quantum |
|-----------|---------|
| **phase-space \( \Gamma \)** | **Hilbert space \( \mathcal{H} \)** |
| defines a classical system, is a space of all possible classical states, all states are orthogonal, employs \( L^2 \)-inner product for observables | defines a quantum system, is a space of all possible quantum states, employs Hilbert space inner product, employs Hilbert-Schmidt inner product for observables |
| **Point in phase-space \((x, p)\)** | **Vector in Hilbert space \( |\psi\rangle \)** |
| describes a state of a classical system, is evolved through Hamilton’s equations of motion, is also called a microstate. | describes a state of a quantum system, is evolved through Schrödinger equation, is also called a macrostate. |
| **phase-space density \( \rho \)** | **Density matrix \( \hat{\rho} \)** |
| describes a state of a classical system with indeterminate initial conditions, is evolved through Liouville’s equation. Point in phase-space is described by a delta function, \( \rho(x, p) = \delta(x - x, p - p) \), | describes a state of a quantum system with indeterminate initial conditions, is evolved through von Neumann equation. Vector in Hilbert space is described by a rank-1 density matrix, \( \rho = \rho \). |
| **Coarse-graining \( \mathcal{C} = \{P_i\}_1 \)** | **Coarse-graining \( \mathcal{C} = \{\mathcal{H}_i\}_1 \)** |
| is a complete set of regions of phase-space, \( \Gamma = \bigcup_i P_i \). Equivalently, \( \mathcal{C} = \{\hat{P}_i\}_1 \) is a complete set of orthogonal window functions, \( \sum_i \hat{P}_i = 1 \). Joint coarse-graining of multiple coarse-grainings always exists. | is a complete set of subspaces, \( \mathcal{H} = \bigoplus_i \mathcal{H}_i \). Equivalently, \( \mathcal{C} = \{\hat{P}_i\}_1 \) is a complete set of orthogonal projectors, \( \sum_i \hat{P}_i = \hat{1} \). Joint coarse-graining exists only if the coarse-grainings commute. |
| **Observable \( \hat{A} \)** | **Observable \( \mathcal{A} \)** |
| is a real-valued function \( A : (x, p) \rightarrow a \) acting on a phase-space, admitting spectral decomposition \( \hat{A} = \sum_i a \hat{P}_i \), with expectation value \( \langle \hat{A} \rangle = \langle A(x) \rangle \), where the probability of observing \( a \) is \( p_a = \left( \hat{P}_a, \rho \right) \), and coarse-graining given by an observable is \( \mathcal{C}_A = \{ \hat{P}_a \}_a \). | is a Hermitian operator acting on a Hilbert space, admitting spectral decomposition \( \mathcal{A} = \sum_i a \hat{P}_i \), with expectation value \( \langle \mathcal{A} \rangle = \text{tr}[\hat{A} \rho] \), where the probability of observing \( a \) is \( p_a = \text{tr}[\hat{P}_a \rho] \), and coarse-graining given by an observable is \( \mathcal{C}_A = \{ \hat{P}_a \}_a \). |

**Dynamical thermodynamic entropy**

| \( S_{xE} \equiv S_{\text{O}(\mathcal{C}_X, \mathcal{C}_E)} = -\sum_{n,E} p_n E \ln \frac{p_n}{\rho_{E}^\mathcal{C}_E} \) | \( S_{xE} \equiv S_{\text{O}(\mathcal{C}_X, \mathcal{C}_E)} = -\sum_{n,E} p_n E \ln \frac{p_n}{\rho_{E}^\mathcal{C}_E} \) |
|\( \mathcal{C}_X = \{P_n\}_n \) is a set of positional macrostates, and \( \mathcal{C}_E \) is a set of energy macrostates, which are defined as energy shells of the Hamiltonian, \( P_E = \{(x, p) | E \leq H(x, p) < E + dE \} \) (\( dE \) independent of \( E \)). | \( \mathcal{C}_X = \{P_n\}_n \) is a set of positional macrostates, and \( \mathcal{C}_E \) is a set of energy macrostates, which are defined as energy shells of the Hamiltonian, \( P_E = \{|E\} \). |

\( \mathbb{R}^3 = \mathbb{R}^2 \oplus \mathbb{R} \), where subspace \( \mathbb{R}^2 = \text{span}\{(1, 0, 0), (0, 1, 0)\} \) describes the x-y plane, and \( \mathbb{R} = \text{span}\{(0, 0, 1)\} \) the z-axis. We call these subspace macrostates, and their collection a coarse-graining, \( \mathcal{C} = \{\mathcal{H}_i\}_1 \). As we did with the classical system in Eq. (6), also here we can switch from describing the coarse-graining as a collection of subspaces, and describe it as a collection of projectors that project onto these subspaces instead. In other words, for each subspace \( \mathcal{H}_i \) there exists a unique projector \( \hat{P}_i \) that projects onto this subspace, and the coarse-graining \( \mathcal{C} = \{ \hat{P}_i \}_1 \) is then defined as a complete set
of orthogonal projectors (∅₂ = ∅₁, ∅₁ = ∅, ∅ᵢ, ∅ᵢ = δᵢⱼ, ∑ᵢ ∅ᵢ = ∅).

With an ordered set of coarse-grainings (C₁, ..., Cₙ), we define volume of a multi-macrostate i = (i₁, ..., iₙ) as

\[ V_i = \text{tr}[\hat{P}_{i₁} ... \hat{P}_{iₙ}], \]

and the probability of being in a macrostate as

\[ p_i(\hat{\rho}) = \text{tr}[\hat{P}_{i₁} ... \hat{P}_{iₙ}\hat{\rho}\hat{P}_{i₁} ... \hat{P}_{iₙ}]. \]

This probability can be also interpreted as a probability of obtaining the sequence of outcomes i when performing a sequence of measurements in measurement bases (C₁, ..., Cₙ) on the system.

The (quantum) Observational entropy is defined identically to the classical case, Eq. (15), but with the use above definitions for Vᵢ and pᵢ(\hat{\rho}):

\[ S_{O(C₁,...,Cₙ)}(\hat{\rho}) = - \sum_i p_i(\hat{\rho}) \ln \frac{p_i(\hat{\rho})}{V_i}. \]

We compare descriptions of classical and quantum systems in Table I. Notably, coarse-grainings in the classical scenario always commute, while in quantum scenario they need not. As a consequence, a joint coarse-graining may not exist in the quantum case, and switching order of non-commuting coarse-grainings leads to different Observational entropies. Surprisingly, this does not affect many other properties, as theorems equivalent to 1-5 still hold.

Due to the non-commutativity of coarse-grainings, there are two quantum versions of SₓE: one that corresponds to first measuring the coarse-grained position, and then energy (denoted SₓE), and one that corresponds to measuring coarse-grained energy with resolution ∆, and then coarse-grained position (denoted SₓE). Their properties were explored in Ref. [2]. Quantum SₓE converges to thermodynamic entropy as the system equilibrates, even when the system is genuinely isolated, as in the examples shown here. The behavior of SₓE depends heavily on the resolution. However, for an appropriate ∆ it behaves very similarly to classical SₓE; but it differs from quantum SₓE for systems at low temperatures, when the positional coarse-grained size ∆ₓ is small.

IX. CONCLUSION AND OUTLOOK

This paper has discussed in detail the framework of classical “Observational entropy,” an idea previously defined in the quantum context [1, 2]. This quantity is

\[ \text{defined precisely in or out of equilibrium, is generically non-decreasing, and corresponds to thermodynamic entropy in equilibrium. Our treatment has aimed to define this quantity clearly and rigorously, while also exhibiting in detail three core sets of relations.} \]

First, the treatment shows how Observation entropy generalizes and interpolates between classical “Gibbs” and “Boltzmann” entropies. The latter is often thought of as Gibbs entropy where equal probability is attributed to all microstates compatible with a given set of macroscopic constraints. Here, we see Boltzmann entropy as a limit of Observational entropy in which all probability is attributed to a single microstate, while Gibbs entropy appears in the limit in which the coarse-graining is as fine as possible so that each microstate constitutes a macrostate.

Second, Observational entropy has both an information-theoretic and a thermodynamic interpretation. Every additional measurement on a system – corresponding to an additional coarse-graining – that better pins down a particular subset of phase-space yields more information in a clear and quantifiable way. At the same time, here and in previous work we have shown that with an appropriate choice of coarse-graining, Observational entropy corresponds thermodynamic entropy in equilibrium.

Third, this work demonstrates a quite elegant and direct correspondence between the quantum and classical cases. By defining projection operators that on Hilbert space and classical phase-space, respectively, carefully defining volume units for classical phase-space, and suitably defining quantum and classical density operators, we show that formulas and most theorems concerning Observational entropy carry over directly between the classical and quantum case. The only key fundamental difference arises in non-commuting projection operators in the quantum case (though there are subtleties in translating between quantum states and regions of classical phase-space.) In contrast, quantum entanglement has no direct classical analog, so entanglement entropy lacks – to our knowledge – a clear correspondence with a classical quantity that behaves similarly.

Thus we view Observational entropy as a framework that relates and unifies a number of disparate views and definitions of entropy. We hope that this treatment proves both illuminating and useful in understanding how entropy manifests and operates in a wide range of physical systems.

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Appendix A: Proofs

We are going to use Jensen’s inequality:

**Theorem 6.** (Jensen) Let \( f \) be a strictly concave function, \( 0 \leq a_i \leq 1, \sum_i a_i = 1 \). Then for any \( b_i \in \mathbb{R}, \)
\[
f\left( \sum_i a_ib_i \right) \geq \sum_i a_if(b_i). \tag{A1}\]
\( f(\sum_i a_ib_i) = \sum_i a_if(b_i) \) if and only if \((\forall i,j) \{ a_i \neq 0, a_j \neq 0 \} (b_i = b_j) \).

**Proof.** (Theorem 1) (Observational entropy is a generalization of the Boltzmann entropy) Clearly, for a single point in phase-space \((x,p) \in P_i\), we have \( p_i = 1 \) and \( p_j = 0 \) for \( j \neq i \). Then from Jensen’s inequality applied on concave function \( f(x) = -x \ln x \), taking \( a_i = \frac{V_i}{V} \) and \( b_i = \frac{p_i}{V} \), we have
\[
S_{O(C)}(\rho) = -\sum_i p_i \ln \frac{p_i}{V} \leq -\sum_i p_i \ln \frac{\sum_{i \in I^{(i)}} p_i}{V_i} = \sum_i V_i \left( -\sum_{i \in I^{(i)}} \frac{V_{i_2}}{V_i} p_{i_2} \ln \frac{V_{i_2}}{V_i} \frac{\sum_{i \in I^{(i)}} p_i}{V_i} \right) = -\sum_i p_i \ln \frac{p_i}{V_i} = S_{O(C_2)}(\rho). \tag{A3}\]

The equality conditions from the Jensen’s inequality show that \( S_{O(C_1)}(\hat{\rho}) = S_{O(C_2)}(\hat{\rho}) \) if and only if \((\forall i_1) [V_{i_1} \neq 0] (\forall i_2, i_2 \in I^{(i)} \mid V_{i_2} \neq 0, V_{i_2} \neq 0) \)
\[
\left( \frac{p_{i_2}}{V_{i_2}} = \frac{p_{i_2}}{V_{i_2}} = c^{(i)} \right). \tag{A4}\]

To determine the constant \( c^{(i)} \) we multiply the equation by \( V_{i_2} \) and sum over all \( i_2 \in I^{(i)} \), which gives
\[
c^{(i)} = \frac{p_{i_1}}{V_{i_1}}. \tag{A5}\]

And considering that for all \( V_{i_2} = 0 \) also \( p_{i_2} = 0 \), we can simplify Eq. (A4), and obtain that \( S_{O(C_1)}(\hat{\rho}) = S_{O(C_2)}(\hat{\rho}) \) if and only if
\[
(\forall i_1) [V_{i_1} \neq 0] (\forall i_2 \in I^{(i)} \mid V_{i_2} \neq 0, V_{i_2} \neq 0) \)
\[
\left( p_{i_2} = V_{i_2} p_{i_1} \right). \tag{A6}\]

**Proof.** (Theorem 3) (Observational entropy with multiple coarse-grainings is bounded) Since Observational entropy with multiple coarse-grainings can be rewritten as Observational entropy with a joint coarse-graining,
\[
S_{O(c_1,\ldots,c_n)}(\rho) = S_{O(c_1,\ldots,c_n)}(\rho), \tag{A7}\]
it is enough to prove the inequalities just for a single coarse-graining \( C \),
\[
S_C(\rho) \leq S_{O(C)}(\rho) \leq \ln V. \tag{A8}\]

For the second inequality we define coarse-graining with a single element – the entire phase-space – \( C_\Gamma = \{ \Gamma \} \). Clearly, this coarse-graining is coarser than any other coarse-graining, therefore from Theorem 2 we have
\[
S_{O(C)}(\rho) \leq S_{O(C_1)}(\rho) = -p_\Gamma \ln \frac{p_\Gamma}{V_\Gamma} = -1 \ln \frac{1}{V} = \ln V. \tag{A9}\]

The first inequality comes from the fact that one can choose a coarse-graining where macrostates are single points in phase-space. This coarse-graining is finer than any other coarse-graining, and one can easily derive that the Observational entropy is then equal to the Gibbs entropy. By the same argument we can therefore obtain the first inequality. However, this argument does not give us the equality conditions, for which we will have to make a more elaborate derivation:

To prove the first inequality and the equality conditions, we define the spectral decomposition of the phase-space density in its eigenvector projectors \( \rho = \sum_{(x,p)} \rho(x,p) \tilde{P}(x,p) \) (meaning \( \rho(\tilde{x},\tilde{p}) = \sum_{(x,p)} \rho(x,p) \tilde{P}(\tilde{x},\tilde{p}) \)), where eigenvalues \( \rho(x,p) \) do not have to be different for different \( (x,p) \). The eigenvector projectors project onto infinitesimal regions surrounding \( (x,p) \) are defined as
\[
\tilde{P}(x,p)(\tilde{x},\tilde{p}) = \begin{cases} 1, & (\tilde{x},\tilde{p}) \in [x, x + dx] \times [p, p + dp], \\ 0, & \text{otherwise}. \end{cases} \tag{A10}\]

We also define spectral decomposition of the density matrix in a form where the eigenvector projectors associated with the same eigenvalue are now grouped together,
\[
\rho = \sum_{\lambda} \lambda \tilde{P}_\lambda, \tag{A11}\]
where eigenvalues \( \lambda \) are now different from each other. This decomposition is unique. It follows that for each \( (x,p) \) there exists \( \lambda \) such that \( \rho(x,p) = \lambda \).

We remind Eq. (9): the probability of a state being in a macrostate \( i \) of volume \( V_i = (\tilde{P}_i, \mu) \) is \( p_i = (\tilde{P}_i, \rho) \).

Defining
\[
\hat{c}^{(i)}_{(x,p)} = \frac{\mu(\tilde{P}_i, \tilde{P}(x,p))}{V_i}, \tag{A12}\]
for $V_i \neq 0$ and $a^{(i)}_{(x,p)} \equiv 0$ for $V_i = 0$, and then using the spectral decomposition of $\rho$ we have

$$p_i \frac{V_i}{V} = \frac{\rho_i}{\rho} \frac{\rho(x,p)}{\rho(x,p)} = \sum_{(x,p)} \rho(x,p) \frac{a^{(i)}_{(x,p)}}{\mu}.$$ (A13)

Since $\sum_{(x,p)} \hat{P}(x,p) = 1$,

$$\sum_{(x,p)} a^{(i)}_{(x,p)} = 1,$$ (A14)

and since $\sum \hat{P}_i = 1$, also

$$\sum_{i} V_i a^{(i)}_{(x,p)} = (\mu, \hat{P}(x,p)) = \mu \int dxdp.$$ (A15)

Series of equalities and inequalities follow

$$S_{O(C_1,...,C_n)}(\rho) = -\sum_{i} p_i \ln \frac{p_i}{V_i}$$

$$= -\sum_{i} V_i \frac{p_i}{V_i} \ln \frac{p_i}{V_i}$$

$$= \sum_{i} V_i \left( -\sum_{(x,p)} \frac{\rho(x,p)}{\mu} \frac{a^{(i)}_{(x,p)}}{\mu} \ln \frac{\rho(x,p)}{\mu} \frac{a^{(i)}_{(x,p)}}{\mu} \right)$$

$$\leq \sum_{i} V_i \left( -\sum_{(x,p)} \frac{\rho(x,p)}{\mu} a^{(i)}_{(x,p)} \ln \frac{\rho(x,p)}{\mu} \right)$$

$$= -\sum_{(x,p)} \sum_{i} V_i a^{(i)}_{(x,p)} \frac{\rho(x,p)}{\mu} \ln \frac{\rho(x,p)}{\mu}$$

$$= -\int_{\Gamma} \frac{\rho(x,p)}{\mu} \ln \frac{\rho(x,p)}{\mu} \mu dxdp \equiv S_{O}(\rho).$$ (A16)

Where we have used Eqs. (A13) and (A15) for the equalities, and applied Jensen’s Theorem 6 on function $f(x) = -x \ln x$ to derive the inequality. We have chosen $a^{(i)}_{(x,p)} \equiv a^{(i)}_{(x,p)}$ and $b_{(x,p)} \equiv \frac{a^{(i)}_{(x,p)}}{\mu}$ for the Theorem.

According to the Jensen’s Theorem, the inequality becomes equality if and only if

$$\forall i(V_i \neq 0) \forall (x,p), (\hat{x}, \hat{p})((\hat{P}_i, \hat{P}(x,p)) \neq 0, (\hat{P}_i, \hat{P}(x,p)) \neq 0)$$

$$((\rho(x,p) = \rho(\hat{x}, \hat{p})).$$ (A17)

To explain, the inequality becomes equality when for a given index $i$, all eigenvector projectors $\hat{P}_{(x,p)}$ of the phase-space density such that $(\hat{P}_i, \hat{P}(x,p)) \neq 0$ have the same associated eigenvalue $\rho(x,p)$ with them. In other words, we can associate this unique eigenvalue to the index $i$ itself, $\rho_i \equiv \rho(x,p)$, where $\rho(x,p)$ is given by any representative $(x,p)$ such that $(\hat{P}_i, \hat{P}(x,p)) \neq 0$. Realizing that $(\hat{P}_i, \hat{P}(x,p)) \neq 0$ is the same as saying $P_i \cap P(x,p) \neq 0$, or $P_i \cap P(x,p) \neq 0$ we can rewrite Eq. (A17) as

$$\forall i(V_i \neq 0) \forall (x,p), (\hat{x}, \hat{p})((\hat{P}_i, \hat{P}(x,p)) \neq 0, (\hat{P}_i, \hat{P}(x,p)) \neq 0)$$

$$((\rho(x,p) = \rho(\hat{x}, \hat{p})).$$ (A18)

Assuming that this holds, we can write

$$\rho \hat{P}_i = \sum_{(x,p)} \rho(x,p) \hat{P}(x,p) \hat{P}_i = \rho_i \sum_{(x,p)} \hat{P}(x,p) \hat{P}_i = \rho_i \hat{P}_i,$$ (A19)

where we have used $\sum_{(x,p)} \hat{P}(x,p) = 1$. Summing the above equation over $i$, and using $\sum_i \hat{P}_i = 1$, we obtain

$$\rho = \sum_i \rho_i \hat{P}_i,$$ (A20)

i.e., $\rho$ can be decomposed using coarse-graining $C = \{ \hat{P}_i \}$. Defining sets $I^{(\lambda)} = \{ i | \rho_i = \lambda \}$, we can rewrite this equation as

$$\rho = \lambda \sum_{i \in I^{(\lambda)}} \hat{P}_i,$$ (A21)

and since decomposition Eq. (A11) is unique, it must be that

$$\hat{P}_\lambda = \sum_{i \in I^{(\lambda)}} \hat{P}_i,$$ (A22)

which by definition means $C_\rho \rightarrow C$. For multiple coarse-graining this then means that $C_\rho \rightarrow C_{1,...,n}$.

Conversely, we assume that Eq. (A22) holds. Points $(x,p), (\hat{x}, \hat{p})$ such that $(\hat{P}_i, \hat{P}(x,p)) \neq 0, (\hat{P}_i, \hat{P}(x,p)) \neq 0$ belong into the same macrostate $\hat{P}_i$, and therefore by Eq. (A22) they must have the same associated eigenvalue,

$$\rho(x,p) = \rho_\lambda = \rho(\hat{x}, \hat{p}),$$ (A23)

which means that Eq. (A18) holds, thus inequality in (A16) becomes equality.

Proof. (Theorem 4) (Observational entropy is non-increasing with each added coarse-graining.) Since joint coarse-graining $C_{1,...,n}$ is finer than joint coarse-graining $C_{1,...,n-1}$, from Theorem 2 we have

$$S_{O(C_1,...,C_n)}(\rho) \leq S_{O(C_1,...,C_{n-1})}(\rho).$$ (A24)

Statement of the theorem then follows from Eq. (A7).

Proof. (Theorem 5) Using $\hat{P}_E \hat{P}_{n \hat{E}} = \delta_{E \hat{E}} \hat{P}_{n \hat{E}}$ we have

$$p_{n \hat{E}}(\rho) = \mu \int_{(x,p)} \sum_{E} f(E) \hat{P}_E(x,p) \hat{P}_{n \hat{E}}(x,p) dxdp$$

$$= \mu \int_{(x,p)} \left( \sum_{E} f(E) \delta_{E \hat{E}} \right) \hat{P}_{n \hat{E}}(x,p) dxdp$$

$$= f(\hat{E}) \int_{(x,p)} \mu_\hat{E} \hat{P}_{n \hat{E}}(x,p) dxdp$$

$$= f(\hat{E}) V_{n \hat{E}}.$$ (A25)
from which
\[
S_{x,E}(t) = -\sum_{n,E} f(E) V_{n,E} \ln \frac{f(E) V_{n,E}}{V_{n,E}}
= -\sum_E \left( \sum_n V_{n,E} \right) f(E) \ln f(E)
= -\sum_E V_{E} f(E) \ln f(E).
\] (A26)

Appendix B: Details for dynamics of \(S_{x,E}\) for a microcanonical ensemble

Here we provide details for the calculation done in subsection VII B, showing that \(S_{x,E} = S_{O(C_x,H_{\nu})}\) of a microcanonical state of particles confined in the left part of the box is equal to the microcanonical entropy of this left part.

The initial state is a microcanonical state of \(N\) particles contained in the left part of the box. It can be written in two ways as
\[
\rho_0 \equiv \rho_{E,\Delta E}^{(\text{micro}; H_1)} = \frac{\mu \tilde{P}_{E,\Delta E}^{(H_1)}}{V_{E,\Delta E}} = \frac{\mu \tilde{P}_{E,\Delta E}^{(H_2)}}{V_{E,\Delta E}}.
\] (B1)

\(\tilde{P}_{E,\Delta E}^{(H_1)}\) and \(\tilde{P}_{E,\Delta E}^{(H_2)}\) denote projectors onto energy macrostates given by the first and the second Hamiltonian, and \(\tilde{P}_{E,\Delta E}^{(N,0)}\) is the projector onto a positional macrostate, corresponding to a statement that \(N\) particles are in the left side of the box, and zero on the right.

We take \(S_{x,E} = S_{O(C_x,H_{\nu})}\) with positional coarse-graining that halves the box \(\langle n = (n_1, n_2), L_1 = 0, \Delta x = \frac{L}{2}\rangle\), and which has energy macrostates given by the second Hamiltonian, \(H_2\). Using
\[
\tilde{P}_{E,\Delta E}^{(H_1)} \equiv \delta_{n_1,N} \tilde{P}_{E,\Delta E}^{(N,0)},
\] (B2)
\[
\tilde{P}_{E,\Delta E}^{(H_2)} \equiv \begin{cases} \tilde{P}_{E,\Delta E}^{(N,0)}, & E \in [E, E + \Delta E] \\ 0, & \text{otherwise} \end{cases}
\] (B3)

where \(\delta_{n_1,N}\) denotes Kronecker delta, we have
\[
p_{n,E}(\rho_0) = \begin{cases} \frac{V_{E,\Delta E}^{(N,0)}}{V_{E,\Delta E}^{(\text{micro}; H_1)}}, & n_1 = N \wedge \tilde{E} \in [E, E + \Delta E] \\ 0, & \text{otherwise} \end{cases}
\] (B4)

from which we obtain
\[
S_{x,E}(\rho_0) = \ln V_{E,\Delta E}^{(H_1)} = S_{\text{micro}}^{(H_1)}(E).
\] (B5)

In other words, \(S_{x,E}\) of the initial state is equal to the microcanonical entropy of the first half of the box.

Appendix C: Dynamics of \(S_{x,E}\) for a single point in phase-space

Here we provide calculation on the long-time limit of \(S_{x,E}\) in the case of an initial single point in phase-space. We note that derivation of \(S_{x,E}\) of an initial state follows exactly the same pattern as in Appendix B, with the only difference that we have \(dE\) instead of \(\Delta E\).

We now focus on calculating microcanonical entropy of the largest macrostate of phase-space jointly coarse grained by \(C_X\) and \(C_{H_2}\) (we will further denote \(H \equiv H_2\)).

Consider \(N\) identical classical particles in \(d\) dimensions evolving through a Hamiltonian \(H\). Their positions and momenta are described by a point in phase-space \(\Gamma \equiv (x_1, \ldots, x_N, p_1, \ldots, p_N)\). They are confined to a box of dimensions \(L^d\), where \(L\) is a linear dimension. We subdivide the box into smaller ones of linear dimensions \(\Delta x\), so that there are \(m \equiv \left(\frac{L}{\Delta x}\right)^d\) boxes. An arbitrary \(\Gamma\) will be in some coarse grained region \(P_{n,E}\), and this will have \(n_1\) particles in the first box, \(n_2\) in the second, and in general \(n_i\) in the \(i\)th box. We would like to know how many distinct ways, \(\mathcal{N}\), there are of arranging the \(N\) particles having precisely these \(n = (n_1, \ldots, n_m)\). The answer is the multinomial distribution
\[
\mathcal{N}(n_1, \ldots, n_m) = \frac{N!}{\prod_{i=1}^{m} n_i!},
\] (C1)

where \(\sum_{i=1}^{m} n_i = N\).

\(\mathcal{N}\) is maximized when the \(n_i\)'s are uniformly distributed, that is, for large \(\frac{N}{m}\), \(n_i = \frac{N}{m}\).

The spatial volume of a coarse grained region is \(\Delta x^d \mathcal{N}(\{n_1, \ldots, n_m\})\). If we fine grain in energy, we can write the (phase-space) volume of the \(i\)th region for which \(\Gamma\) is in,
\[
V_{n,E} = \int dp^{Nd} \int_{x \in x_{n,E}} dx^{Nd} \delta\left(E - H(\{x_i\}, \{p_i\})\right).
\] (C2)

\(P_{n,E}\) contains all permutations of particles. This means that if we consider a single \(\Gamma\) in this region, \(P_{n,E}\) will also contain other \(\Gamma\)’s with all of particle permutations consistent the same particle numbers, \(n = (n_1, \ldots, n_m)\), and the same energy \(E\).

1. Case of dilute gas

Consider the case where the interaction between the particles is small. We can also take the particles to be indistinguishable, meaning all phase-space volumes are divided by \(N!\). In the limit of small interactions, the Hamiltonian only depends on the \(p\)'s and we can integrate over \(x\), and write
\[
V_{n,E} = \frac{N!}{\prod_{i=1}^{m} n_i!} \Delta x^d \mathcal{N}(\{n_1, \ldots, n_m\}) \int dp^{Nd} \frac{1}{N!} \delta\left(E - H(\{p_i\})\right).
\] (C3)

The right part is equal to the microcanonical phase-space volume, the logarithm of which is equal to the microcanonical entropy of all \(N\) particles in a box of spatial
volume $\Delta x^d$, at total energy $E$ (we remind that the microcanonical entropy is defined as by the right hand side of Eq. (36)). We can therefore write
\[
\exp (S_{\text{micro}}(E, \Delta x^d)) = \Delta x^N \int dp \frac{N_d}{N} \delta (E - H(\{p\}))).
\]
(C4)

This gives
\[
V_{nE} = N(n_1, \ldots, n_m) \exp (S_{\text{micro}}(E, \Delta x^d)).
\]
(C5)

$S_{\text{micro}}(E, V)$ is the microcanonical entropy of a system of energy $E$ in a spatial volume $V$ (setting $k_B = 1$). In the limit of large $N$, this is given by the Sackur-Tetrode equation [36],
\[
S_{\text{micro}}(E, V) = N \left( \ln \left( \frac{V}{N} \right) \left( \frac{4\pi m E}{Nd} \right)^\frac{d}{2} \right) + 1 + \frac{d}{2} \left( \ln 2 \pi N \right).
\]
(C6)

$N$ is maximized with $n_i = \frac{N}{m}$. In this case, using Stirling’s approximation,
\[
\ln(N_{\text{max}}) = \ln \left( \frac{N^N}{m^m} \right) = \frac{1}{2} \ln(2\pi N) - \frac{m}{2} \ln \left( \frac{2\pi N}{m} \right).
\]
(C7)

Combining Eqs. (C5), (C6), and (C7), and realizing that $\Delta x^d = \frac{N}{m}$ (where $V$ denotes the full spatial volume), we obtain $S_{X^d}$ for the point in phase-space $\Gamma$ which wandered into the largest macrostate,
\[
S_{X^d} = \ln(V_{nE}^{(\text{max})}) = \ln(N_{\text{max}}) + S_{\text{micro}}(E, \Delta x^d)
\]
≈ $N \ln(m) + \frac{1}{2} \ln(2\pi N) - \frac{m}{2} \ln \left( \frac{2\pi N}{m} \right)
\]
\[
+N \left( \ln \left( \frac{V}{N} \right) \left( \frac{4\pi m E}{Nd} \right)^\frac{d}{2} \right) + 1 + \frac{d}{2} \left( \ln 2 \pi N \right)
\]
\[
= S_{\text{micro}}(E, V) + \frac{1}{2} \ln(2\pi N) - \frac{m}{2} \ln \left( \frac{2\pi N}{m} \right)
\]
\[
= \ln V_{E}^{(H_2)} + \frac{1}{2} \ln(2\pi N) - \frac{m}{2} \ln \left( \frac{2\pi N}{m} \right)
\]
\[
= S_{\text{micro}}(E) + \frac{1}{2} \ln(2\pi N) - \frac{m}{2} \ln \left( \frac{2\pi N}{m} \right),
\]
(C8)

since terms $N \ln(m)$ cancelled each other, and by definition, $S_{\text{micro}}(E, V) = \ln V_{E}^{(H_2)}$.

If the point in phase-space did not wander into the largest macrostate, but, let’s say, the second largest (given by $n_1 = \frac{N+1}{m} - 1, n_i = \frac{N+1}{m}$ for $i > 1$), there will be minor modifications to the above formula, which will be negligible compared to the first term - the microcanonical entropy. In the end, it does not matter into which of the large macrostate the particle wanders in, the leading term will be always the microcanonical entropy.

To understand to correction term in more detail, we will be interested in the entropy per particle, which means the relevant quantity to consider here is $\ln(N_{\text{max}})/N$.
\[
\frac{S_{X^d}}{N} = \frac{S_{\text{micro}}(E, V)}{N} + \frac{1}{2N} \ln(2\pi N) - \frac{m}{2N} \ln \left( \frac{2\pi N}{m} \right).
\]
(C9)

We take a limiting process where we fix the particle density, and send $N$ to infinity, while keeping the particle density constant. For large $N$ we can ignore the second term on the right hand side. $N_m \equiv \frac{N}{m}$ is the average number of particles per box. In the limit where we fix the density average number of particles and increase the box length so that $N_m$ becomes large, the last term on the right hand side $-(1/2N_m) \ln(2\pi N_m)$ becomes small, and vanishes as $N_m \to \infty$. This correction term therefore represents a finite size effect.

2. General classical systems

The case of a dilute gas can be extended to a general homogeneous classical system that is extensive. The box with maximum entropy will be the one where the number in each box is the same. This follows from the fact that all boxes must have the same chemical potential in equilibrium. The system is most likely to find itself in this coarse grained region. Logarithm of Eq. (C2) represents the entropy of a system that has been partitioned.

As compared to the entropy of the entire system, each particle is confined to a box of width $\Delta x$. It is as if barriers had been added to prevent the exchange of particles between regions. However energy can still be exchanged, therefore the temperature of each sub-system is the same. If the system has a density $\rho$ and temperature $T$, corresponding to its total energy, then the energy per particles $s(E, T)$ will not depend on system size in the thermodynamic limit. There are correction to this due to finite size effects and are particularly pronounced at critical points [37]. They have the general behavior as above, becoming negligible in the limit of large box size. The actual error will depend on the universality class of the system being studied.

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