Ensembles and distributions on energy shells

General considerations and terminology

A *statistical ensemble* can loosely be viewed as infinitely many hypothetical copies, or *realizations*, of a system. Each realization represents the system in one of its possible states. Here the terms "system" and "state" are taken very generally. For instance our system might be a flipped coin, in which case:

- the possible states are `heads` and `tails`
- each realization represents the outcome of one hypothetical coin flip, and
- the statistical ensemble is a collection of infinitely many coin flips.

We often talk about "drawing a sample from the ensemble", which should be interpreted as choosing one member at random from the infinite collection of realizations; in the coin example this would correspond to flipping the coin once. The space of all possible states can be discrete or continuous, and we can represent the ensemble in terms of a probability distribution on this state space.

Ensembles and probability distributions on energy shells

For Hamiltonian systems, the state of the system is specified by a point in phase space, and often the term *microstate* is used rather than "state" or "point in phase space". When considering an ensemble that is restricted to a single energy shell, E, the state space is the set of all microstates x satisfying $H(x) = E$. It is convenient to picture the ensemble as a collection of N dots that are sprinkled over the energy shell (not necessarily uniformly!), with the understanding that the limit $N \to \infty$ will be taken. In what follows, I will use the notation $\mathcal{E}$ to denote one such ensemble.

The ensemble $\mathcal{E}$ can be represented by a probability distribution $f_{\mathcal{E}}(x)$, which is defined with respect to the measure μ discussed in class. We can construct this probability distribution using a familiar "box counting" procedure. Imagine dividing the energy shell E into a number of cells ("boxes") of equal measure ϵ, and let $n(x; \epsilon, N)$ denote the number of dots found inside the cell that contains the point x. This depends on the total number of dots

(N) and on the measure of the cells (ϵ). We then have

$$f_{\mathcal{E}}(x) = \lim_{\epsilon \to 0} \frac{1}{\epsilon} \lim_{N \to \infty} \frac{n(x; \epsilon, N)}{N} \quad . \tag{1}$$

The ordering of limits is important here. The quantity $\lim_{N\to\infty}(n/N)$ represents the fraction of the ensemble that is found in the cell that contains x. Dividing this quantity by the measure of the cell and then letting that measure go to zero, we get the desired probability distribution. This distribution is properly normalized:

$$\int_E \mathrm{d}\mu \, f_{\mathcal{E}}(x) = 1 \quad . \tag{2}$$

The microcanonical ensemble is a special case of such an ensemble, and is represented by a uniform probability distribution with respect to the measure μ:

$$f^E_{\mu c}(x) = \frac{1}{\Sigma} \quad , \tag{3}$$

where $\Sigma = \int_E \mathrm{d}\mu$ is the measure of the entire energy shell. In the notation $f^E_{\mu c}$, the subscript is an abbreviation of "microcanonical" and the superscript specifies the energy.

Ensemble averages

We can define the ensemble average of an observable $A(x)$ in terms of samples $x_1, x_2, \cdots$ drawn randomly from the ensemble $\mathcal{E}$:

$$\langle A \rangle_{\mathcal{E}} = \lim_{M \to \infty} \frac{1}{M} \sum_{i=1}^{M} A(x_i) \quad , \tag{4}$$

In terms of the probability distribution $f_{\mathcal{E}}$, this average is given by the expression

$$\langle A \rangle_{\mathcal{E}} = \int_E \mathrm{d}\mu \, f_{\mathcal{E}}(x) \, A(x) \quad . \tag{5}$$

Time-dependent probability distributions

To discuss dynamics, imagine an ensemble of microstates at time $t = 0$, specified by an probability distribution $f(x, 0)$. Picturing this ensemble as a collection of dots sprinkled over the energy shell E, let us take each of these dots to represent the initial conditions for a single Hamiltonian trajectory. This collection of initial conditions gives rise to a swarm of trajectories evolving on the energy shell, and $f(x, t)$ is the time-dependent probability distribution that describes the evolution of this swarm. A *stationary distribution* $\pi(x)$ is one that remains unchanged under this evolution:

$$\text{if} \quad f(x,0) = \pi(x) \quad \text{then} \quad f(x,t) = \pi(x) \quad , \quad t > 0 \quad . \tag{6}$$

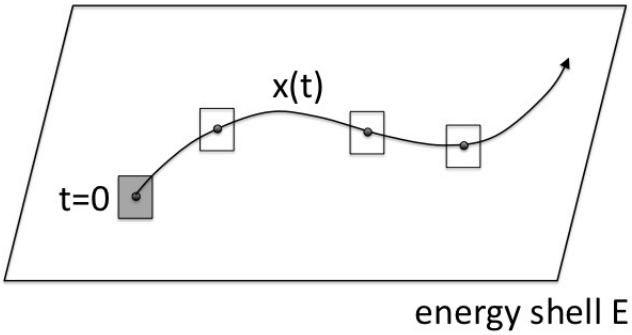

FIG. 1: Four points along a Hamiltonian trajectory $x(t)$. The shaded box represents a tiny cell that contains the initial point $x(t)$. This cell evolves to later times as illustrated. Since the measures of all four cells are equal (because the measure μ is preserved under Hamiltonian evolution), it follows that the probability density is the same at each of the four points.

Since Hamiltonian dynamics preserves the measure μ, **the probability density along any trajectory** $x(t)$ **remains constant**:

$$\frac{\mathrm{d}}{\mathrm{d}t} f(x(t), t) = 0 \quad , \tag{7}$$

as illustrated schematically in Fig. 1. This holds for both stationary and non-stationary distributions $f(x, t)$.

The unique stationary distribution for ergodic systems

We can use this result to establish that **if the system is ergodic, then the micro-canonical distribution is the unique stationary distribution**. [1] Consider a trajectory $x(t)$ that evolves ergodically from a microstate $x(0) = x_1$, and consider a tiny cell σ that contains some other microstate x_2 on the same energy shell. Let t^* denote a time at which the trajectory is found within this cell, $x(t^*) \in \sigma$, as illustrated in Fig. 2. By Eq. 7 we have

$$f(x_1, 0) = f(x(t^*), t^*) \approx f(x_2, t^*) \quad . \tag{8}$$

The approximation becomes an equality as we take $|\sigma| \to 0$, therefore we simply write

$$f(x_1, 0) = f(x_2, t^*) \quad , \tag{9}$$

[1] More precisely, it is the unique *smooth* stationary distribution.

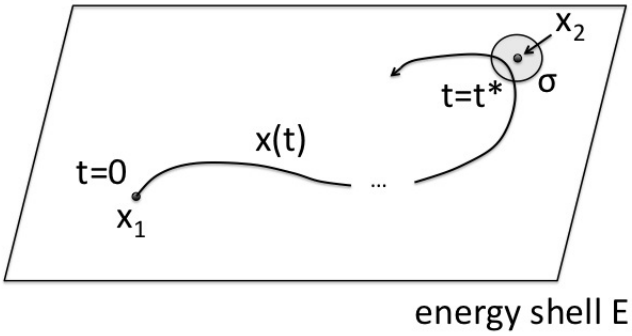

FIG. 2: The trajectory $x(t)$ wanders ergodically over the energy shell, starting from initial conditions x_1. Eventually it will pass through a cell σ containing the point x_2. Let t^* denote a time at which the trajectory finds itself within this cell.

with the understanding that the smaller the value of $|\sigma|$, the longer we will have to wait for the trajectory to find this cell.

Eq. 9 is valid for an arbitrary time-dependent ensemble $f(x,t)$. Now consider the case of a stationary ensemble, $f(x,t) = \pi(x)$ (Eq. 6). Eq. 9 then gives us

$$\pi(x_1) = \pi(x_2) \quad . \tag{10}$$

But x_1 and x_2 were chosen arbitrarily, so we conclude that $\pi(x)$ must be independent of x, in other words it is the microcanonical distribution.