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# 1 Ensembles and Replicas

A replica is a single system and an ensemble is collection of systems. Every replica obeys the same evolutions equations (Hamilton's equations). In general, every element of the ensemble can be in a different state. The state of a system is given by specifying the positions and momenta of all the particles that make up a system:

$$y = (q, p) = (q_1, q_2, \cdots, p_1, p_2, \cdots), \tag{1}$$

where for most of our cases we can assume that $y = (q, p) \in \Gamma$ will represent a point in a $6N$ dimensional phase space $\Gamma$ when there are $N$ particles in a given system. Here I have assumed that the motion takes place in 3-dimensions.

If I have a very large collection of systems, i.e. my ensemble consists of very many systems then I can I speak of a distribution of replicas in phase space. The distribution $\rho(q, p, t)$ will depend upon the location $y \in \Gamma$ and generally upon time. In physical terms, at this stage, you can think of $\rho(q, p, t)dqdp$ as giving the fraction of replicas contained in the volume $dy = dqdp$ at the point $y = (q, p)$ at time $t$.

Remarks:

1. At this stage $\rho(q, p, t)$ can be anything. The only restriction is that it be a properly defined probability distribution; i.e. that, $\int_\Gamma \rho(y, t)\, dy = 1$ and $\rho(q, p, t) \geq 0$.

2. $\rho$ is often referred to as the phase space density.

# 2 Governing Equation

Every replica is required to obey the same evolution equations – in our case Hamilton's equations. The Hamiltonian is a map from phase space to the real numbers:

$$H : \Gamma \times [0, T] \to \mathbb{R}, \tag{2}$$

where $H(q, p, t)$ represents the total energy of a system in state $(q, p)$ at time $t$. The evolution of the state is given as:

$$\dot{q} = \frac{\partial H}{\partial p} \tag{3}$$

$$\dot{p} = -\frac{\partial H}{\partial q}\,. \tag{4}$$

## 3 Liouville's Theorem

There are two forms to Liouville's Theorem. The first form is a global statement and the second is a local statement. In its global form, this theorem states:

> The volume occupied by any collection of replicas, vol($D_t$), remains constant in time, where $D_t \subset \Gamma$.

The essential fact/assumption used to prove this statement is that every replica obeys Hamilton's equations.

The second form of Liouville's Theorem, the local form, states:

> The total time derivative of the phase space density is zero; i.e. $\frac{d\rho}{dt} = 0$.

To prove this form of the relation, one only needs to use Hamilton's equations. In class, I used the additional assumption of Ergodicity, but this is not needed. Why? Consider a fix collection of replicas occupying a region $D_o$ at time $t_o$ with coordinates $Y = y(t_o)$. At a later time $t$, these replicas will occupy the region $D_t$ with coordinates $y(t)$. Note that at both times they represent the same fraction of replicas of the entire ensemble. Thus

$$
\begin{aligned}
0 &= \frac{d}{dt}\int_{D_t} \rho(q,p,t)\, dy && (5)\\
&= \frac{d}{dt}\int_{D_o} \rho(q,p,t)\det\left(\frac{\partial y}{\partial Y}\right)\, dY && (6)\\
&= \int_{D_o} \frac{d\rho}{dt}(q,p,t)\det\left(\frac{\partial y}{\partial Y}\right) + \rho(q,p,t)\frac{d}{dt}\det\left(\frac{\partial y}{\partial Y}\right)\, dY && (7)\\
&= \int_{D_o} \frac{d\rho}{dt}(q,p,t)\det\left(\frac{\partial y}{\partial Y}\right)\, dY && (8)\\
&= \int_{D_t} \frac{d\rho}{dt}(q,p,t)\, dy. && (9)\\
& && (10)
\end{aligned}
$$

Since $D_t$ was arbitrary, we have that

$$
\begin{aligned}
0 = \frac{d\rho}{dt}(q,p,t) &= \frac{\partial \rho}{\partial t} + \sum_i \frac{\partial \rho}{\partial q_i}\frac{\partial q_i}{\partial t} + \frac{\partial \rho}{\partial p_i}\frac{\partial p_i}{\partial t}\\
&= \frac{\partial \rho}{\partial t} + \sum_i \frac{\partial \rho}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial \rho}{\partial p_i}\frac{\partial H}{\partial q_i}\,.
\end{aligned} \qquad (11)
$$

Remarks:

1. The summation term on the right-hand side of the evolution equation for the phase density is known as a Poisson bracket. The Poisson bracket of any two functions over phase space is abbreviated as $\{F, G\}$, where

$$\{F, G\} = \sum_i \frac{\partial F}{\partial q_i}\frac{\partial G}{\partial p_i} - \frac{\partial F}{\partial p_i}\frac{\partial G}{\partial q_i}. \qquad (12)$$

Note that the Poisson bracket is skew-symmetric; i.e. $\{F, G\} = -\{G, F\}$.

2. For a function over the phase space which does not explicitly depend upon time, $F : \Gamma \to \mathbb{R}$, one has the result

$$\frac{dF}{dt} = \{F, H\} \tag{13}$$

3. If the Hamiltonian does not explicitly depend on time, i.e. $H(q, p, t) = H(q, p)$, then we have the result

$$\frac{dH}{dt} = \{H, H\} = 0. \tag{14}$$

Thus we can conclude that the energy of a replica/system in the ensemble is constant.

# 4 Statistical Equilibrium

Equilibrium or more precisely statistical equilibrium of an ensemble is defined to be the condition where

$$\frac{\partial \rho}{\partial t} = 0\,. \tag{15}$$

In other words, one has statistical equilibrium of an ensemble when the phase density at any point in phase space remains constant. From above we have that

$$\frac{\partial \rho}{\partial t} = -\{\rho, H\}\ . \tag{16}$$

Thus for an ensemble to be in a state of (statistical) equilibrium we must have the condition that

$$\{\rho, H\} = 0\,. \tag{17}$$

Remark:

1. Not every possible distribution $\rho$ will satisfy Eq. (17). Thus if one creates any arbitrary distribution $\rho$, it will in general change in time.

2. If the Hamiltonian depends explicitly on time, then it is not clear that Eq. (17) has any solutions.

3. If the phase density can be expressed as function solely of the energy of the system, $\rho(q, p, t) = \rho(H(q, p))$, then one has automatic satisfaction of Eq. (17).

## 5 Micro-canonical Ensemble

If the energy is of all elements of the ensemble are required to have a fixed constant energy, say $H(q,p) = E$ with no explicit time dependence, then evolution of the ensemble will also be required to remain within the hyper-surface $S(E) = \{(q,p)|H(q,p) = E\}$. Let us now assume further assume the ensemble is in equilibrium. If the hyper-surface $S(E)$ is metrically indecompossible and we assume that $\rho$ is continuous on $S(E)$, we can then conclude that $\rho = C$ a constant on $S(E)$ and zero otherwise.

## 6 Ergodic Assumption

Note that all of the above results are completely independent of the ergodic hypothesis. The results are valid for all Hamiltonian systems (time dependent or not). The requirement that time averages are equal to phase averages is a completely separate issue and one that we will always assume but one that is not needed for many of the results which we have derived so far.