## Evolution of phase space probability distributions/H-Theorem

Systems of $N$ real particles occupy domains in $6N$-dimensional ***phase space***, rather than cells of a CA. Phase space is a product space described by continuous $3N$ spatial $\{\vec{q}_i,\ i=1,\ldots,N\}$ and $3N$ momentum $\{\vec{p}_i,\ i=1,\ldots,N\}$ coordinates. Therefore, the probabilities $p_i$ of discrete cells $i$ discussed previously is replaced by continuous, time dependent ($t$) distribution functions $\{f(\vec{q}_i,\vec{p}_i,t),\ i=1,\ldots,N\}$ for the $N$ particles. These functions are probability densities normalized to unity when integrated over the entire phase space,

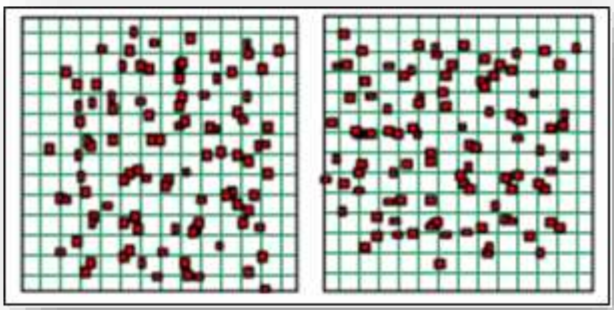

**Figure 1:** Two possible 2-dim systems of 100 particles each distributed differently over the available space.

$$\int d^3\vec{q}_i \int d^3 f(\vec{q}_i,\vec{p}_i,t) \equiv 1 \qquad \{i=1,\ldots,N\} \tag{1}$$

Following the same line of arguments as before, the time dependent information content of an occupied multi-particle state is contained in the ***Boltzmann H-function*** (*eta*-function)

$$H(t) := \sum_{i=1}^{N} \int d^3\vec{q}_i \int d^3\vec{p}_i \ \{f(\vec{q}_i,\vec{p}_i,t)\cdot \ell n f(\vec{q}_i,\vec{p}_i,t)\} \le 0 \tag{2}$$

The $H$ function is obviously equivalent to the negative of the information $S$ given by the statistical entropy (cf. Equ.**Error! Reference source not found.**). It is negative since the distribution functions are probability densities.

Based on very general principles, predictions can be made as to the spontaneous time evolution of the $H$ function, or the equivalent statistical entropy function *S.* In the following, the entropy *S(t)* is expressed as

$$S(t) = -H(t) = -k_B \sum_{n=1}^{\Omega} p_n(t) \ell n\left(p_n(t)\right) \geq 0 \qquad \sum_{n=1}^{\Omega} p_n(t) \equiv 1 \tag{3}$$

in terms of time dependent (normalized) probabilities for discrete system states numbered by $n$.

This time dependence of the entropy function reflects an underlying dynamics, a transport process, which tends to redistribute the importance (or population) of the microscopic states and all of its attributes. The trend is equivalent to an entropy flux or current

$$j_s := \frac{dS}{dt} \tag{4}$$

If $j_s$ has a finite magnitude, it defines a direction of increasing or decreasing diversity or spread in *a priori probabilities.*

The *a priori* probabilities $p_n$ can be regarded as populations of these states which can be queried in experimental observations. If these populations are time dependent, there have to be microscopic transition probabilities $w_{nm}$ connecting any state $n$ and $m$. The transition probabilities describe the rate of change in the population of state $n$ due to gain and loss from and to state $m$ according to a balance "Master Equation,"

$$\frac{dp_n(t)}{dt} = \sum_m \left\{ \underbrace{w_{mn} \cdot p_m(t)}_{Gain} - \underbrace{w_{nm} \cdot p_n(t)}_{Loss} \right\} \tag{5}$$

For microscopic, quantal reasons, the transition probabilities are symmetric, $w_{nm} = w_{mn}$, which ensures time reversal invariance (detailed balance). Obviously, the Master Equation (5) is a classical approximation in that it neglects quantal interference terms involving transition amplitudes, rather than probabilities.

Now, the time derivative of the entropy function in Equ. (3), the entropy flux (Equ. (4)), can be calculated:

$$\frac{dS(t)}{dt} = -k_B \sum_{n=1}^{\Omega} \left\{ \left( \frac{dp_n(t)}{dt} \right) \ell n\left(p_n(t)\right) + p_n(t) \left( \frac{d \ell n\, p_n(t)}{dt} \right) \right\}; \qquad \frac{d}{dt} \sum_{n=1}^{\Omega} p_n(t) \equiv 0 \quad (6)$$

Evaluating the derivatives one obtains

$$\begin{aligned} \frac{dS(t)}{dt} &= -k_B \sum_{n=1}^{\Omega} \left\{ \left( \frac{dp_n(t)}{dt} \right) \ell n\left(p_n(t)\right) + p_n(t) \left( \frac{1}{p_n(t)} \frac{dp_n(t)}{dt} \right) \right\} = \\ \frac{dS(t)}{dt} &= -k_B \sum_{n=1}^{\Omega} \left( \frac{dp_n(t)}{dt} \right) \ell n\left(p_n(t)\right) - k_B \underbrace{\sum_n \frac{dp_n(t)}{dt}}_{=0} \end{aligned} \quad (7)$$

The last term drops out because of the conservation of total probability implied by Equ. (6). Now, inserting for $dp_n/dt$ the expression given by the Master Equation (5), the second row in (7) reads,

$$\frac{dS(t)}{dt} = -k_B \sum_{n,m=1}^{\Omega} w_{mn} \cdot \left\{ p_m(t) - p_n(t) \right\} \ell n\left(p_n(t)\right) \quad (8)$$

Here, use has been made of the symmetry of the transition probabilities $w_{mn}$. Since the two indices $n$ and $m$ run over the same range, this expression can also be written as,

$$\frac{dS(t)}{dt} = -k_B \sum_{n,m=1}^{\Omega} w_{mn} \left\{ p_n(t) - p_m(t) \right\} \ell n\left(p_m(t)\right) \quad (9)$$

Taking the average of Equs. (8) and (9), a more symmetric expression is obtained fro the time rate of change of the entropy function:

$$\frac{dS(t)}{dt} = \frac{k_B}{2} \sum_{n,m=1}^{\Omega} w_{mn} \left\{ p_n(t) - p_m(t) \right\} \left[ \ell n\left(p_n(t)\right) - \ell n\left(p_m(t)\right) \right] \quad (10)$$

However, since $d\ell n(p)/dp > 0$, all terms in the sum are non-negative and therefore,

$$j_s = \frac{dS(t)}{dt} = -\frac{dH(t)}{dt} \geq 0 \tag{11}$$

According to this derivation, the entropy *S* increases and the *H* function decreases in time, as long as the transition probabilities are finite, $w_{nm} = w_{mn} > 0$. The larger the differences between the populations $p_i$ of different states are, the higher is the rate of entropy changes. When

$$p_n \approx const.; \quad n = 1, \ldots.., \Omega \tag{12}$$

the *S* (or *H*) functions no longer change. The system described by such function has reached its asymptotic stationary state, also known as equilibrium state. ***This equilibrium state is characterized by maximum entropy corresponding to equal a priori probabilities $p_n$ and chaotic dynamics***. While for a given theoretic model the expectation values of the functions *S* and *H* can be calculated exactly, there are also higher moments (fluctuations) to consider, since they depend on stochastic parameters, the probabilities $p_n$.

### 1. Gibbs stability criterion for random states

The situation of maximum entropy, where all accessible states are uniform and have equal *a priori* probabilities, is called "***equilibrium***." It will be shown further below how these information/entropy functions change in complex dynamical processes.

***All systems where accessible states are not uniformly populated are in states of disequilibrium and have statistical entropies less than the maximum possible:***
The equilibrium state is therefore defined by the variational condition

$$S(\vec{q}_i,\vec{p}_i) = S_{max}(\vec{q}_i,\vec{p}_i) =: S_{equ} \rightarrow \delta S(\vec{q}_i,\vec{p}_i) = 0 \qquad (13)$$

Here, $\delta$ stands for a variation with respect to the individual probability densities. Once a multi-particle system is in such an equilibrium state of maximum entropy, there is conceptionally ***no net driving force*** that would force it out of this state in one direction or another. However, such an equilibrium state can be either stable or unstable. Microscopically, there are always quantal fluctuations in all coordinates. Even systems presumably at rest show "zero-point fluctuations." In addition, physical particles move even classically from phase space cell to phase space cell, changing individual occupation probabilities ($p_i$ or $f(\vec{q}_i,\vec{p}_i,t)$) instantaneously away from their respective equilibrium values. The magnitude of these fluctuations depend on their origin in classical or quantum dynamics. They may vary in size and follow a distribution in time or frequency (chance of occurrence). Therefore, the actual entropy at a given instant will reflect these fluctuations.

Connecting to discussions of stability in previous sections, one can obtain a stability criterion by studying the expansion of the entropy $S$ of an actual system state about the equilibrium state ($\delta S = 0$),

$$S = S_{equ} + \delta S + \frac{1}{2}\delta^2 S + .... \approx S_{equ} + \frac{1}{2}\delta^2 S \qquad (14)$$

From this relation it simply follows that the state of maximum entropy is stable, only if fluctuations away from this state reduce the entropy,

$$\delta^2 S < 0 \qquad (15)$$

This “Gibbs” stability criterion has to be applied in specific cases to identify the stable equilibrium. Stable equilibrium states are attractors of complex system, as will be demonstrated in later sections.