Ergodicity, non-ergodicity and aging processes

Amir Golan

Department of Physics, Ben-Gurion University, Beer Sheva 84105, Israel

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Abstract:

This paper is intended to clarify and explain the meaning of ergodicity in physical systems as well as non-ergodic processes and the aging phenomena. The first approach to ergodicity is done by introducing a general setup of "particles in a box", with emphasis on different boxes that result both ergodic outcome and non-ergodic one. Following this "graphical" introduction a mathematical view on ensemble vs. time average will show through equations how a stationary system implies "ergodic system". I then show a theoretical model with some examples of aging as an introduction to real, physical, non-ergodic systems that demonstrate the aging process. The systems shown here are simple glass and a more modern topic, of spin-glasses. Many experiments have been done in the last couple of decades in the spin-glasses field, this paper show only one experiment that, in a way, summarize many of the experiments in spin-glasses that exhibit aging and non-ergodicity.

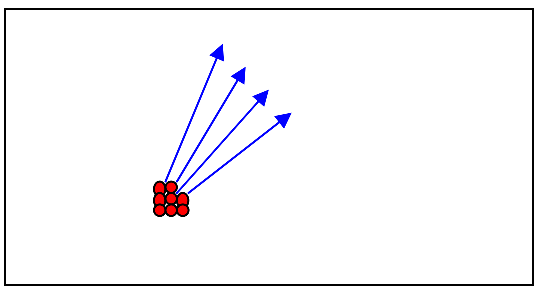
Ergodization:

If we take a system with some d-dimensions (d>1) with energy

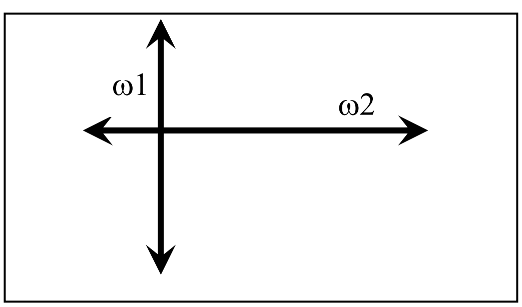
$H(x_i,p_i) = E$, $i = 1,2,3\ldots d$,

The system will fill all of its "energy envelope" within some typical time.

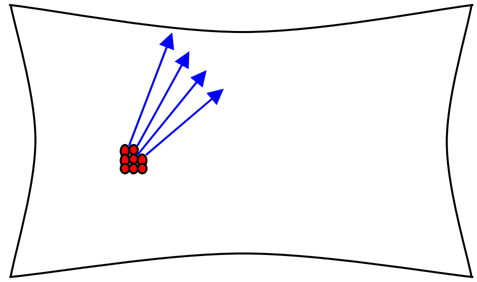
Rectangular Box



If we put some particles in a specific location and with some specific momentum, with in a short time the system will have d frequencies for the system:

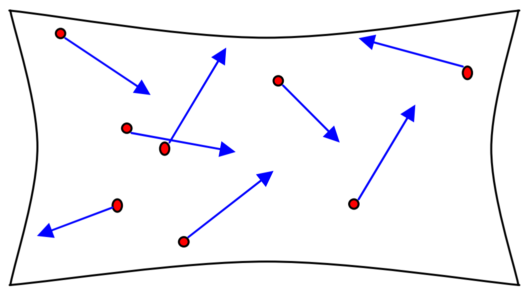


Sinai Billiard:



In a more complex surface, the system will not remain with its two basic frequencies, but will fill the entire space randomly.

In some computer simulation it was shown that within 6 hits with the walls, we have complete chaos.

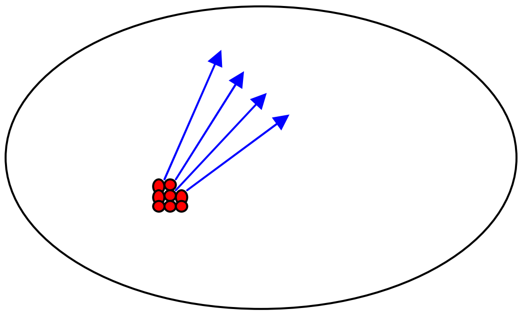


If we define $\theta = \arctan\left(\frac{V_x}{V_y}\right)$, where

$V_x^2 + V_y^2 = 2E/m$

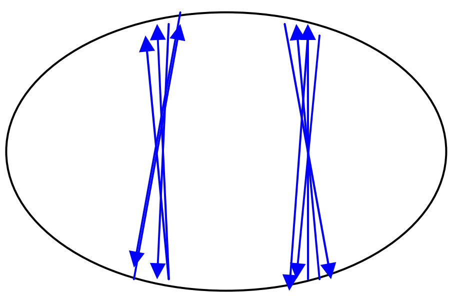
Ergodicity is reached when θ has covered all angles.

Ellipsoid:

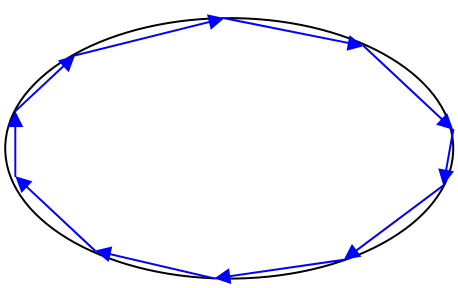


In this special shape there are ergodic and non-ergodic areas:

Focusing areas:

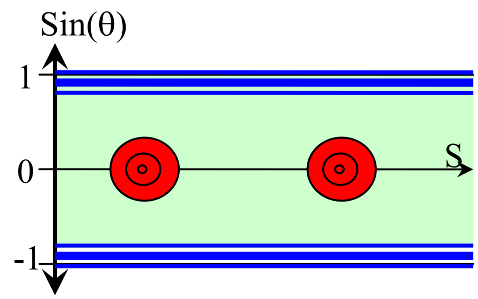


Whispering Gallery:



We can define Puankare sections if we call the angle of impact as θ and the location along the circumference S and than plot the locations where there is no ergodicity, on an axis of S versus sinθ.

These sections denote specific areas where there is no ergodicity.



In the green section, there is complete ergodization.

In that case, all measurement of the system will yield the same result.

This can be described as a stationary state, another characteristic of ergodicity.

As we know stationary state is defined by that that it does not change it time, or in other words that it commute with the Hamiltonian.

$$\frac{\partial \rho}{\partial t} = [H, \rho] = 0$$

Ensemble and time averages

There are two types of averages that are of interest. The first of these is the ordinary average of y at a given time over all systems of the ensemble.

This ensemble average which we denote by $\langle y \rangle$, is defined by:

$$\overline{y(t)} \equiv \langle y(t) \rangle \equiv \frac{1}{N}\sum_{k=1}^{N} y^{(k)}(t)$$

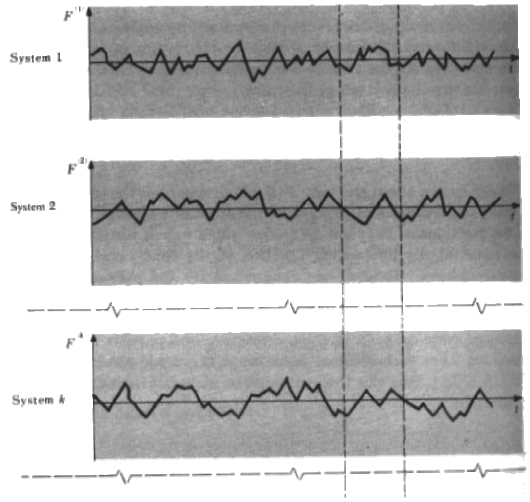
Where $y^{(k)}(t)$ is the value assumed by $y(t)$ in the kth system of the ensemble and where N is the very large total number of systems in the ensemble.

The second average of interest is the average of y for a given system of the ensemble over some very large time interval 2θ (where $\theta \to \infty$). We shall denote this time average by $\{y\}$ and define it for the kth system of the ensemble by

$$\left\{ y^{(k)}(t) \right\} \equiv \frac{1}{2\theta}\int_{-\theta}^{\theta} y^{(k)}(t+t')dt'$$

In more pictorial terms illustrated in the following figure (1), the ensemble average is taken vertically for a given t, while the time average is taken horizontally for a given k.

Figure (1)



Let us show that the operations of taking a time average and taking an ensemble average commute.[3]

We can see that:

$$\left\langle \left\{ y^{(k)}(t) \right\} \right\rangle \equiv \frac{1}{N}\sum_{k=1}^{N}\left[\frac{1}{2\theta}\int_{-\theta}^{\theta} y^{(k)}(t+t')dt' \right]$$

$$= \frac{1}{2\theta}\int_{-\theta}^{\theta}\left[\frac{1}{N}\sum_{k=1}^{N} y^{(k)}(t+t') \right]dt' = \frac{1}{2\theta}\int_{-\theta}^{\theta}\langle y(t+t') \rangle dt' =$$

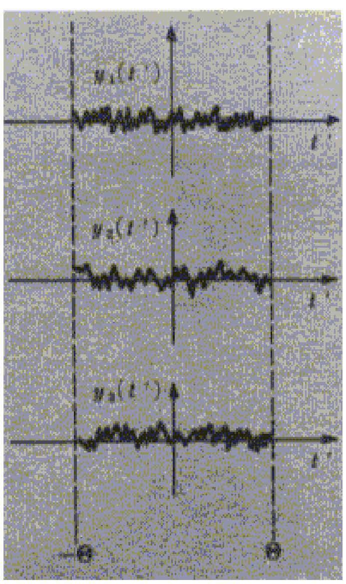
$$\Rightarrow \quad \left\langle \left\{ y^{(k)}(t) \right\} \right\rangle = \left\{ \langle y(t+t') \rangle \right\}$$

Consider now a situation which is "stationary" with respect to y. This means that there is no preferred origin in time for the statistical description of y i.e., the same ensemble ensues when all member functions $y^{(k)}(t)$ of the ensemble are shifted by arbitrary amounts in time. (In an equilibrium situation this would, of course, be true for all statistical quantities.)

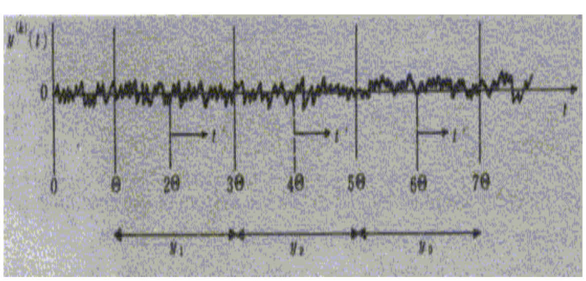
For such stationary ensembles there is an intimate connection between ensemble and time averages if one assumes that (with the possible exception of a negligible number of exceptional systems in the ensemble) the function $y^{(k)}(t)$ for each system of the ensemble will in the course of a sufficiently long time pass through all the values accessible to it. – This is called the "ergodic" assumption.

One can then imagine that one takes, for example, the *k*th system of the ensemble and subdivides the time scale into very long sections (or intervals) of magnitude 2θ, as shown in figure (2,3).

Figure (2)



Figure(3)



Since θ is very large, the behavior of $y^{(k)}(t)$ in each such section will then be independent of its behavior in any other section. Some large number of M such sections should then constitute as good a representative ensemble of the statistical behavior of *y* as the original ensemble average.

More precisely, in such a stationary ensemble the time average of *y* taken over some very long time interval θ must be independent of the time *t*. Furthermore, the ergodic assumption implies that the time average must be the same for essentially all systems of the ensembles.

Thus,

$$\left\{y^{(k)}(t)\right\} = \{y\} \quad \text{independent of } k\,.$$

Similarly, it must be true that in such a stationary ensemble the ensemble average of *y* must be independent of time.

Thus,

$$\langle y(t) \rangle = \langle y \rangle \quad \text{independent of } t\,.$$

The general relation regarding the commutation of the two averages leads then immediately to an interesting conclusion, by taking the ensemble average (independent of k), we can get the relation:

$$\left\langle \left\{ \mathrm{y}^{(\mathrm{k})}(\mathrm{t}) \right\} \right\rangle = \{ y \}$$

and if we take the time average of the second we will get:

$$\left\{ \left\langle \mathrm{y}^{(\mathrm{k})}(\mathrm{t}) \right\rangle \right\} = \langle y \rangle$$

Hence from the above we can conclude that for a stationary ergodic ensemble we have:

$$\{ y \} = \langle y \rangle$$

Aging – History-dependent relaxation

Aging in an infinite-range Hamiltonian system of coupled rotators

The Hamiltonian of the system is:

$$H = \frac{1}{2}\sum_i L_i^2 + \frac{1}{2N}\sum_{i,j}\left[1 - \cos\left(\theta_i - \theta_j\right)\right] = K + U$$

Aging can be characterized by measuring the two-time autocorrelation function along the system trajectories. If the state of the system in phase space can be completely characterized giving a state vector $\vec{x}$, then the two-time autocorrelation function is defined as follows: [1]

$$C(t + t_w, t_w) = \frac{\langle \vec{x}(t + t_w) \cdot \vec{x}(t_w) \rangle - \langle \vec{x}(t + t_w) \rangle \cdot \langle \vec{x}(t_w) \rangle}{\sigma_{t+t_w} \sigma_{t_w}}$$

where σ_t' are standard deviations and the symbol <...> stands for average over several realizations of the dynamics. In the case of a Hamiltonian system with *N* degrees of freedom the state vector is decomposed in coordinates and their conjugate momenta, therefore we establish the following notation: $\vec{x} \equiv (\vec{\theta}, \vec{L})$

The difference between the experiments was the waiting time (t_w) in which the system was held "frozen" before letting it evolve with time. In this case, these initial conditions where keeping all angles at zero while giving the system a random momenta form a uniform distribution, such that the system has a total energy K+U.

In the following example we can see the autocorrelation versus the time. (log-log graph)

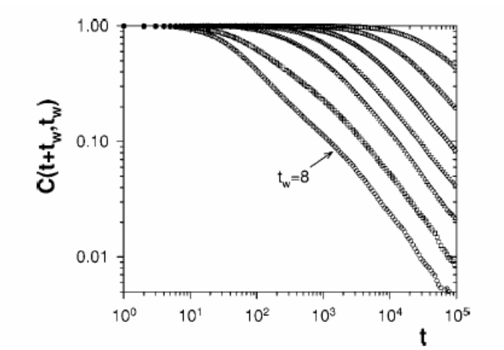


FIG. 2. Two-time autocorrelation function $C(t+t_w,t_w)$ vs t for systems of size $N=1000$ and energy per particle $U=0.69$. The data correspond to an average over 200 trajectories initialized in water-bag configurations. The waiting times are $t_w=8$, 32, 128, 512, 2048, 8192, and 32 768.

We can see that the autocorrelation function obeys a power law – but for every waiting time we have a different decay factor – the system "remembers" the waiting time.

This is the aging phenomena.

Let us now look at the graph with "scaled" time axis, the scaling is done to the system's "own time" – the waiting time.

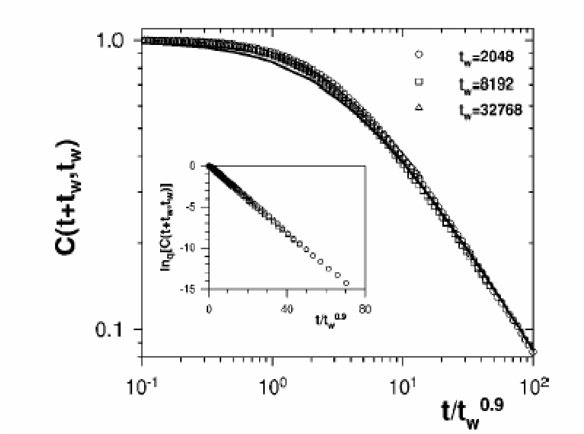


FIG. 3. Data collapse for the long-time behavior of the autocorrelation function $C(t+t_w,t_w)$. The data are the same shown in Fig. 2 for the three largest t_w. The gray solid line corresponds to $e_q(-0.2t/t_w^{\beta})$. Inset: $\ln_q$-linear representation of the same data, with $q\simeq 2.35$.

In the new, scaled graph we can see that the autocorrelation for all different waiting times behaves the same.

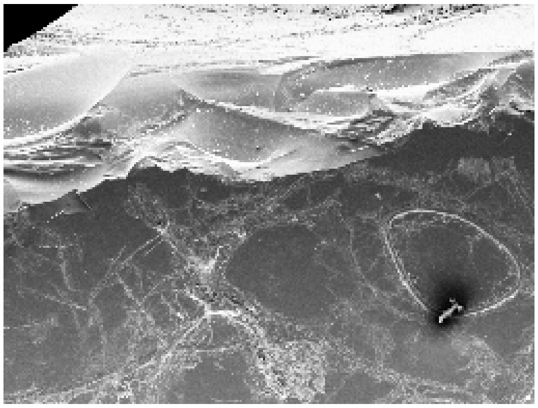
Note that the scaling is not "simple division" but has some power factor to it. Now we can fit the graph to some power law function to analyze the autocorrelation function:

$$C(t+t_w,t_w) = f\left(\frac{t}{t_w}\right) \propto \left(\frac{t}{t_w^{\beta}}\right)^{-\lambda}$$

In this case the constants came out to be:

$\lambda = 0.74$ and $\beta = 0.90$

Simple-glass:



Glass as we know it is an amorphous SiO_2 which would, according to its lowest free energy be in a crystalline shape (like sand) although it is "frozen" in a *metastable state*, which is in a higher free energy level.

This state will, in a finite (but VERY long) time decay into crystalline state by nucleating sufficiently large domains of the crystalline phase, which will then grow and cover all the material. [2]

This system is none ergodic since it has not yet reached its equilibrium.

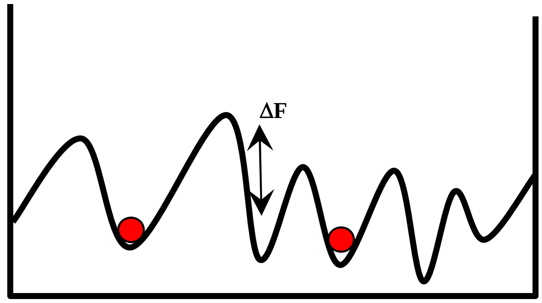
Helmholtz's free energy: $\boldsymbol{F = E - TS}$

Spin-glass:

Non-ergodic process with aging (Ising model)

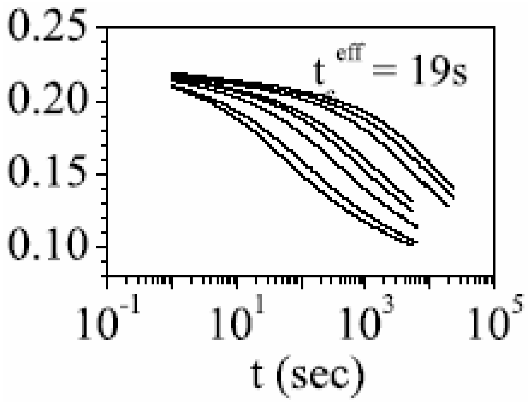
In this equilibrium picture the spin-glass phase is believed to be an ensemble of randomly oriented spins, which are frozen due to short and infinite-range correlations.

In other words, in order for the system to get to "ergodization" it has to move though all its possible states, and in this case the glass – structure is making this process very long.

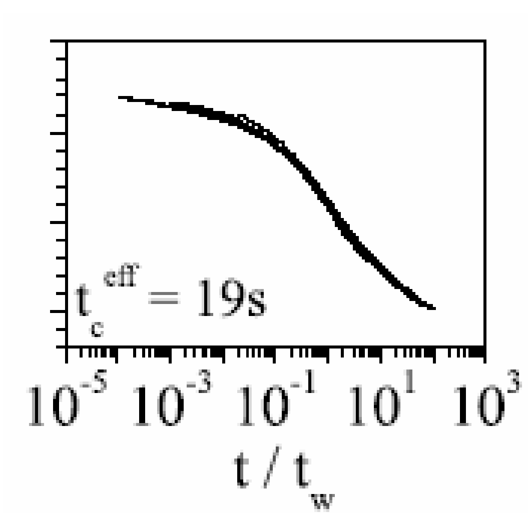


Since the discovery of aging effects in spin glasses approximately 20 years ago, much effort has gone into determining the exact time dependence of the memory decay functions. In particular, memory effects show up in the thermoremagnet magnetization (TRM) (or zero-field cooled magnetization), where the sample is cooled through its spin glass transition temperature in a small magnetic field (zero field) and held in that particular field and temperature configuration for a waiting time tw. At time t_w, a change in the magnetic field produces a very long time decay in the magnetization. The decay is dependent on the waiting time. Hence, the system has a memory of the time it spent in the magnetic field. [4,5]

A rather persuasive argument suggests that, for systems with infinite equilibration times, the decays must scale with the only relevant time scale in the experiment, tw. This would imply that plotting the magnetization on a $t=tw$ axis would collapse the different waiting time curves onto each other. This effect has not been observed.



In these two examples (above and below) we can see an experiment result [4], that show relaxation with time of a sample that was cooled for different periods of times prior to the measurement. This experiment was done with several cooling sequences (not shown here) that show more or less the same results, although the article [4] elaborates more about the different cooling techniques used and their effect on the aging process.



The free energy barrier (for a spin to flip) is ΔF, it is in the order the sample volume, i.e. it is proportional to L^d .

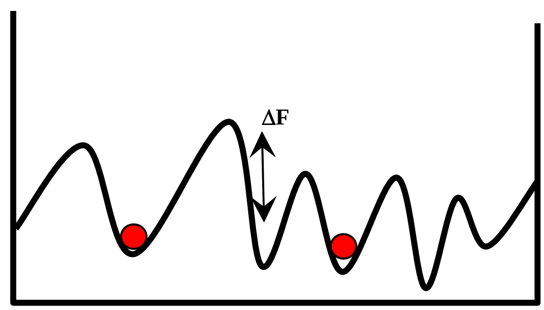
The time needed for such a transition to take place is the ratio of the boltsman factors of the transition: (initial/final)

$$\tau \propto e^{\Delta F / KT}$$

From this relation we can see that the time to cross the barrier between the two phases diverges exponentially as

$$N(or\ L^d) \to \infty$$

The name we call such systems that for them $\tau_{max} \to \infty$ as $N \to \infty$, nonergodic. [6,7]



A mathematical analysis:

Final remarks - conclusion:

Over the last two decades and still today, a lot of work is being done in research, both theoretical and experimental, in the area of long and short range correlations. Many of these works deal with the non-ergodic and aging processes as been shown above. This paper gave both conceptual idea through "particles in a box" models and a mathematical one of ergodicity and the lack of it in physical systems through time and ensemble averages. Stationarity of a system has been shown to imply ergodicity by its nature. The last examples show that many physical systems can be simulated and analyzed by a relatively simple Hamiltonian, although in many cases, full understanding and correct predictions are not always reached.

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