What is Geometric Entropy, and does it really increase?

József Beck

Rutgers

Wednesday, July 3^{rd} 2013.

What is spatial equilibrium? How long does it take to reach spatial equilibrium?

Simplest model: N point billiards move in a cube container $[0,1]^3$.

Let

$$\mathcal{Y} = (\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_N)$$

denote the initial point configuration, and let

$$\mathcal{M} = (\mu_1, \mu_2, \ldots, \mu_N)$$

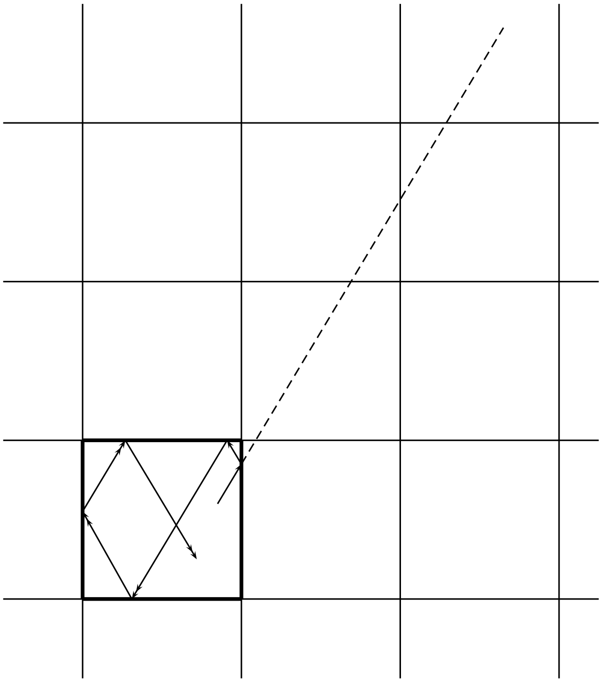
be the corresponding mass distribution.

For convenience, assume that the average mass is 1:

$$\frac{1}{N}\sum_{k=1}^{N}\mu_k = 1, \quad \text{or equivalently,} \quad \sum_{k=1}^{N}\mu_k = N.$$

An important special case is $1 = \mu_1 = \mu_2 = \ldots = \mu_N$.

The trick of Unfolding reduces the cube to the torus:



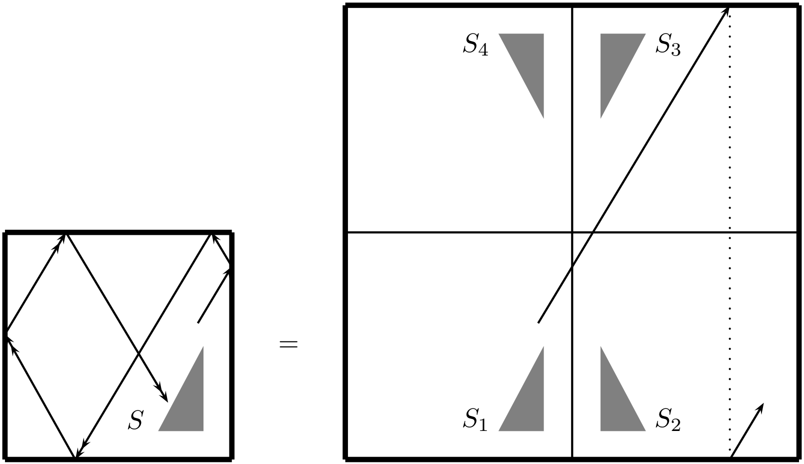
Unfolding of the billiard path in the d-dimensional unit cube

$[0, 1]^d$ can be defined in the analog way. Formally, unfolding means the map

$$2||x/2|| \to \{x\} \text{ applied to each coordinate,}$$

where $0 \le \{x\} < 1$ denotes the fractional part of a positive real x,

and $||x||$ is the distance of x from the nearest integer.


S
=
S_4
S_3
S_1
S_2

Let

$$\mathcal{R} = (\mathbf{r}_1(t), \mathbf{r}_2(t), \ldots, \mathbf{r}_N(t))$$

be a family of N continuous rectifiable parametrized space curves with $\mathbf{r}_k(0) = \mathbf{0}$.

General Torus Model:

the trajectory of the kth point particle is

$$\mathbf{y}_k + \vartheta_k(\rho_k \mathbf{r}(t)) \text{ modulo one}: \ 1 \leq k \leq N,$$

where the initial velocity space is either the first type (Maxwellian distribution)

$$\omega = (\rho_1, \vartheta_1, \rho_2, \vartheta_2, \ldots, \rho_N, \vartheta_N) \in \Omega_1 = ([0, \infty) \times SO(3))^N$$

equipped with the product measure, where $[0, \infty)$ has the probability measure

$$\Pr[\rho_j \leq u] = \sqrt{\frac{2}{\pi}} \int_0^u y^2 e^{-y^2/2}\, dy,$$

or the second type

$$\omega = (\vartheta_1, \vartheta_2, \ldots, \vartheta_N) \in \Omega_2 = (SO(3))^N$$

(i.e., $1 = \rho_1 = \rho_2 = \ldots = \rho_N$), or the third type

$$\omega = (\rho_1, \vartheta_1, \rho_2, \vartheta_2, \ldots, \rho_N, \vartheta_N) \in \Omega_3 = ([0,1] \times SO(3))^N$$

with

$$\Pr[\rho_k \le u] = 3 \int_0^u y^2\, dy = u^3 \quad \text{for } 0 \le y \le 1, \text{ and } 1 \text{ for } u \ge 1.$$

Metatheorem:

Consider a general 3-dimensional N-particle torus model with initial point configuration $(\mathcal{Y}, \mathcal{M})$ where each point particle has the same space curve

$$\mathbf{r} = \mathbf{r}_1(t) = \mathbf{r}_2(t) = \ldots = \mathbf{r}_N(t).$$

Then the typical time evolution of the system (representing the majority of $\omega \in \Omega_i$, $i = 1, 2, 3$) is described by the negative entropy

$$\mathrm{Negentropy}_i(t) = \mathrm{Negentropy}_i(\mathcal{Y}, \mathcal{M}; \mathbf{r}; t),$$

where

$$\mathrm{Negentropy}_1(\mathcal{Y}, \mathcal{M}; \mathbf{r}; t) =$$

$$= \max \left\{ \sup_{\mathbf{n} \in \mathbb{Z}^d \setminus \mathbf{0}} \left| \sum_{k=1}^{N} \mu_k e^{2\pi \mathbf{i} \mathbf{n} \cdot \mathbf{y}_k} \right|^2 \exp\left(-(2\pi |\mathbf{r}(t)| \; |\mathbf{n}|)^2 \right), \sum_{k=1}^{N} \mu_k^2 \right\}$$

for the first type (Maxwellian initial velocity distribution),

$$\mathrm{Negentropy}_2(\mathcal{Y}, \mathcal{M}; \mathbf{r}; t) =$$

$$= \max \left\{ \sup_{\mathbf{n} \in \mathbb{Z}^3 \setminus \mathbf{0}} \left| \sum_{k=1}^{N} \mu_k e^{2\pi i \mathbf{n} \cdot \mathbf{y}_k} \right|^2 \min \left\{ \frac{1}{20(2\pi |\mathbf{r}(t)| \; |\mathbf{n}|)^2}, 1 \right\}, \sum_{k=1}^{N} \mu_k^2 \right\}$$

for the second type, and finally,

$$\text{Negentropy}_2(\mathcal{Y}, \mathcal{M}; \mathbf{r}; t) =$$

$$= \max\left\{ \sup_{\mathbf{n}\in\mathbb{Z}^3\setminus\mathbf{0}} \left| \sum_{k=1}^{N} \mu_k e^{2\pi \mathbf{i}\mathbf{n}\cdot\mathbf{y}_k} \right|^2 \min\left\{ \frac{1}{20(2\pi|\mathbf{r}(t)|\ |\mathbf{n}|)^2}, 1 \right\}, \sum_{k=1}^{N} \mu_k^2 \right\}$$

for the second type, and finally,

$$\text{Negentropy}_3(\mathcal{Y}, \mathcal{M}; \mathbf{r}; t) =$$

$$= \max\left\{ \sup_{\mathbf{n}\in\mathbb{Z}^3\setminus\mathbf{0}} \left| \sum_{k=1}^{N} \mu_k e^{2\pi \mathbf{i}\mathbf{n}\cdot\mathbf{y}_k} \right|^2 \min\left\{ \frac{1}{2(2\pi|\mathbf{r}(t)|\ |\mathbf{n}|)^4}, 1 \right\}, \sum_{k=1}^{N} \mu_k^2 \right\}$$

for the third type.

The function $\mathrm{Negentropy}_i(t) = \mathrm{Negentropy}_i(\mathcal{Y}, \mathcal{M}; \mathbf{r}; t)$ describes the total "order" (microscopic and macroscopic) for the typical time evolution of the system, starting from $(\mathcal{Y}, \mathcal{M}; \mathbf{r})$, at time t.

The function $\text{Negentropy}_i(t) = \text{Negentropy}_i(\mathcal{Y}, \mathcal{M}; \mathbf{r}; t)$ is monotone decreasing in terms of the drifting distance $|\mathbf{r}(t)|$; the function $\text{Negentropy}_i(t)$ is N^2 at the start $t = 0$, and the system reaches Average Square-Root Equilibrium when $\text{Negentropy}_i(t)$ attains its minimum $\sum_{k=1} \mu_k^2$ (which is N if every mass μ_k is one).

We have similar formulas in every dimension.

For a given initial condition $(\mathcal{Y}, \mathcal{M}; \mathcal{R}; \omega)$, let $N(\mathcal{Y}, \mathcal{M}; \mathcal{R}; \omega; S; t)$ denote the mass-counting function in a given test set S at time t:

$$\text{MassCounting} = N(\mathcal{Y}, \mathcal{M}; \mathcal{R}; \omega; S; t) = \sum_{\substack{1 \le k \le N: \\ \mathbf{x}_k(t) \in S}} \mu_k,$$

where $\mathbf{x}_k(t) = \mathbf{y}_k + \vartheta_k(\rho_k \mathbf{r}_k(t))$ modulo one is the trajectory of the kth particle.

In general, for an arbitrary complex valued Lebesgue square integrable (in the unit torus) test function $f \in L^2$, we write

$$N(\mathcal{Y}, \mathcal{M}; \mathcal{R}; \omega; f; t) = \sum_{1 \le k \le N} f(\mathbf{x}_k(t))\mu_k.$$

Let

$$\sigma_0^2(f) = \int_{I^3} \left| f - \int_{I^3} f \, dV \right|^2 \, dV = \int_{I^3} |f|^2 \, dV - \left| \int_{I^3} f \, dV \right|^2$$

denote the “variance” of the given test function f.

Uniformity means

$$N(\mathcal{Y}, \mathcal{M}; \mathcal{R}; \omega; f; t) \approx N \int_{I^3} f \, dV,$$

where I^3 is the 3-dimensional unit torus ($N = \sum_{k=1}^{N} \mu_k$ is the total mass, and V indicates volume). So we study the discrepancy

$$N(\mathcal{Y}, \mathcal{M}; \mathcal{R}; \omega; f; t) - N \int_{I^3} f \, dV.$$

What we actually study is the *square* of the discrepancy:

$$\mathbf{H}(\mathcal{Y}, \mathcal{M}; \mathcal{R}; \omega; f; t) = \left| N(\mathcal{Y}, \mathcal{M}; \mathcal{R}; \omega; f; t) - N \int_{I^3} f \, dV \right|^2.$$

Definition

We study the time evolution of an N-element torus model of the first type $(\mathcal{Y}, \mathcal{M}; \mathcal{R}; \omega)$, $\omega \in \Omega_1$. We say that the system is in Square-Root Equilibrium with parameters $0 < \varepsilon < 1$ and $C < \infty$ at time t, if for every square-integrable test function $f \in L^2$ there exists a subset $\Omega_1(\varepsilon; f) \subset \Omega_1$ of the initial velocity space with measure at least $1 - \varepsilon$ such that, for every $\omega \in \Omega_1(\varepsilon; f)$

$$\mathbf{H}(\mathcal{Y}, \mathcal{M}; \mathcal{R}; \omega; f; t) \leq C \cdot \sigma_0^2(f) \sum_{k=1}^{N} \mu_k^2.$$

The term $\sigma_0^2(f) \sum_{k=1}^{N} \mu_k^2$ represents "randomness" (="equilibrium").

We emphasize that Square-Root Equilibrium is not the only important equilibrium concept: see *Utmost Equilibrium*.

Utmost Equilibrium is about uniformity in the high-dimensional configuration space, and Square-Root Equilibrium is about uniformity in the cubic container (containing the point particles).

When the system reaches Utmost Equilibrium, it exhibits full-blown randomness!

We take average over the concrete initial velocity space Ω_1:

$$\mathbf{H}_1(\mathcal{Y}, \mathcal{M}; \mathcal{R}; f; t) = \int_{\Omega_1} \mathbf{H}(\mathcal{Y}, \mathcal{M}; \mathcal{R}; \omega; f; t)\, d\omega.$$

We call it the *Big Square-Error* of the first type (relative to f); it is the big quadratic average of the discrepancy with respect to the given square integrable test function $f \in L^2$ at time t, assuming the given initial point configuration $\mathcal{Y}$ with mass distribution $\mathcal{M}$.

Since the torus I^3 is translation invariant, any translated copy $S + \mathbf{w} \pmod 1$, $\mathbf{w} \in \mathbb{R}^3$ is just as good of a test set as S itself. In general, any translation of f by $\mathbf{w}$ modulo one is just as good:

$$f_{\mathbf{w}}(\mathbf{x}) = f(\mathbf{x} - \mathbf{w}).$$

Let

$$\mathbf{AH}(\mathcal{Y}, \mathcal{M}; \mathcal{R}; \omega; f; t) = \int_{I^3} \mathbf{H}(\mathcal{Y}, \mathcal{M}; \mathcal{R}; \omega; f_{\mathbf{w}}; t)\, d\mathbf{w} =$$

$$= \int_{I^3} \left| N(\mathcal{Y}, \mathcal{M}; \mathcal{R}; \omega; f_{\mathbf{w}}; t) - N \int_{I^3} f \, dV \right|^2 d\mathbf{w}$$

Definition

Again we study the time evolution of an N-element torus model of the first type $(\mathcal{Y}, \mathcal{M}; \mathcal{R}; \omega)$, $\omega \in \Omega_1$. We say that the system is in Average Square-Root Equilibrium with parameters $0 < \varepsilon < 1$ and $C < \infty$ at time t, if for every square-integrable test function $f \in L^2$ there exists a subset $\Omega_1(\varepsilon; f) \subset \Omega_1$ of the initial velocity space with measure at least $1 - \varepsilon$ such that, for every $\omega \in \Omega_1(\varepsilon; f)$

$$\mathbf{AH}(\mathcal{Y}, \mathcal{M}; \mathcal{R}; \omega; f; t) \leq C \cdot \sigma_0^2(f) \sum_{k=1}^{N} \mu_k^2.$$