

Fluctuation Theorem and Central Limit Theorem for the Time-Reversible Nonequilibrium Baker Map

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Abstract

The nonequilibrium Time-Reversible Baker Map provides simple illustrations of the Fluctuation Theorem, the Central Limit Theorem, and the Biased Random Walk. This is material in preparation for the Book form of Carol's and my 2016 Kharagpur Lectures. Comments welcome.

Keywords: Fluctuation Theorem, Chaos, Lyapunov Exponents, Irreversibility, Second Law, Baker Map

I. INTRODUCTION

In 1993 Denis Evans, Eddie Cohen, and Gary Morriss discovered an interesting symmetry, by now “well-known”, in their studies of the periodic shear flow of 56 hard disks¹. They kept track of the time-averaged Gibbs’ entropy changes associated with the flow as a function of the averaging time τ . At a strainrate $\dot{\epsilon}$ and over a time window τ the distribution of entropy production rates approaches a smooth curve with a mean value, $\langle (\dot{S}/k) = (V/T)\eta\dot{\epsilon}^2 \rangle_\tau$. The fluctuations about this mean necessarily satisfy the Central Limit Theorem for large τ .

Evans, Cohen, and Morriss stressed that both positive and *negative* values of the entropy production can be observed if the system is not too small (56 soft disks in their case) and τ is not too large (a few collision times). At equilibrium the positive and negative values even out over time. Away from equilibrium the positive values win out. The relatively few time intervals with negative values correspond to periods of entropy decrease. These unlikely fluctuations are reflected in the title of their paper, “Probability of Second Law Violations in Shearing Steady Flows”. Their key insight was the definition of a nonequilibrium measure in terms of the local Lyapunov exponents.

I expected that an analog of their shear-stress fluctuations could be found in the qualitatively simpler dynamics of a nonequilibrium Baker Map.²⁻⁴ The simplicity of the map provides a worthwhile pedagogical approach to understanding the Evans-Cohen-Morriss “Fluctuation Theorem”. The “Theorem” is not quite an identity. It relates the probability of phase-space trajectory fragments forward-in-time for a time interval τ to the less-likely probability of observing these same fragments with the time order reversed :

$$[\text{prob}_{\text{forward}}(\tau)/\text{prob}_{\text{backward}}(\tau)] \simeq e^{\tau\dot{S}/k} \simeq e^{\Delta S/k} [\text{Fluctuation Theorem}] .$$

I have used \simeq rather than $=$ as reminders that the equalities describe limiting cases and are not valid for short sampling times, $\tau \simeq 0$.

For long times the theorem corresponds to a comparison of the zero-probability unstable repeller to the probability-one strange attractor generated by the forward mapping. It is interesting that Reference 7 of Evans-Cohen-Morriss’ paper describes the measurement of fluctuations for a (fractal) “Skinny Baker Map”⁵. The classic Baker Map maps the unit square ($0 < x, y < 1$) onto itself with no change in area (a caricature of Liouville’s phase

volume conservation at equilibrium. We consider a generalization of that map to a 2×2 square, centered on the origin and rotated 45° so as to fit the conventional definition of time reversibility for the coordinate q and momentum p :

$$q = (\sqrt{1/2})(dx + dy) ; p = (\sqrt{1/2})(dx - dy) \text{ for}$$

$$dx = 2x - 1 ; dy = 2y - 1 ; -1 < (dx, dy) < +1 .$$

The expansion and rotation, together with defining (q, p) coordinates relative to the center of the square, gives a diamond-shaped time-reversible ergodic dissipative map B :

$$B(q, p) = (q_{\text{new}}, p_{\text{new}}) \longleftrightarrow B(q_{\text{new}}, -p_{\text{new}}) = (q, -p) .$$

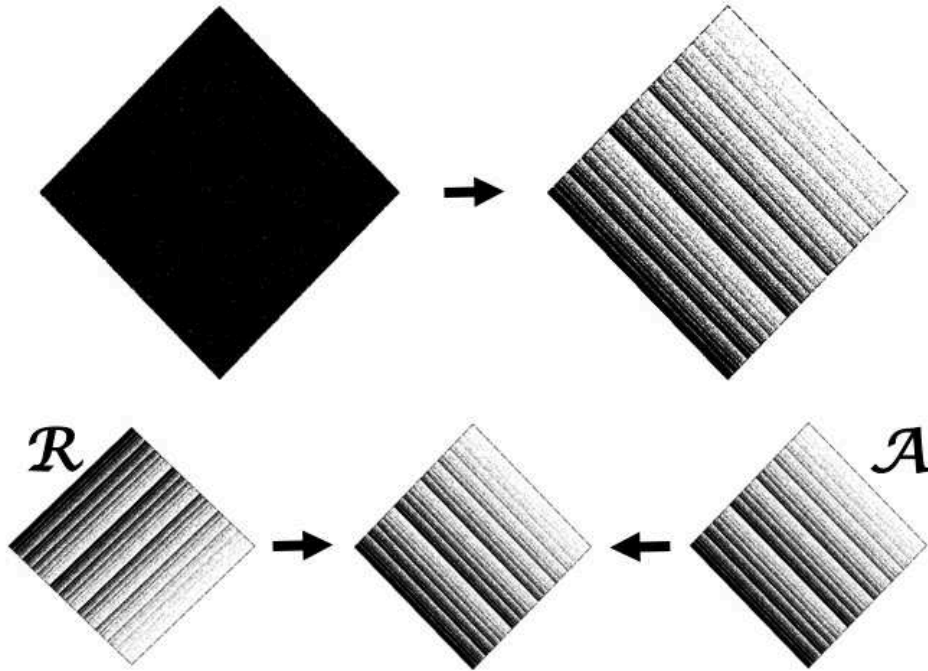


FIG. 1: Here I show (at top left) 250,000 points generated for the equilibrium Baker Map in which areas are unchanged by the mapping. On the right are 250,000 points generated with the *nonequilibrium* map $B(q, p)$ where the comoving area changes by a factor of 2, increasing about $(1/3)$ of the time and decreasing about $(2/3)$ of the time. The repeller (shown at bottom left) is a mirror image of the attractor ($\pm p \rightarrow \mp p$). Whether one starts with the attractor or repeller the final distribution of points invariably produces the attractor (shown in the center and top right). The tops and the bottoms of the diamond domains correspond to unstable fixed points.

See **Figure 1** for the steady-state distribution corresponding to the mapping $B(q, p)$. Here we consider a particular special case different to both the skinny and the classic maps. In our case the comoving density is doubled two-thirds of the time and halved one-third. The single-step dynamics of the time-reversible nonequilibrium Baker Map B converts a (q, p) phase point to a new one, $(q_{\text{new}}, p_{\text{new}})$ always with a factor-of-two change in the comoving area. The domain of the map is diamond-shaped with a sidelength of 2, centered on the origin, $(q = 0 ; p = 0)$. The FORTRAN programming necessary to each iteration of the map $B(q, p \rightarrow q_{\text{new}}, p_{\text{new}})$ is as follows :

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if(q.lt.p-sqrt(2.0/9)) then ! [ expanding ]
    qnew = +(11.0/6)*q - (7.0/6)*p + sqrt(49.0/18)
    pnew = +(11.0/6)*p - (7.0/6)*q - sqrt(25.0/18)
endif

if(q.gt.p-sqrt(2.0/9)) then ! [ contracting ]
    qnew = +(11.0/12)*q - (7.0/12)*p - sqrt(49.0/72)
    pnew = +(11.0/12)*p - (7.0/12)*q - sqrt( 1.0/72)
endif

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In 1991, Bill Vance was interested in computing the relative probability of forward and reversed trajectories using unstable periodic orbits⁶. He showed me that it is easy to confirm the time-reversibility of the “rotated” Baker map $B(q, p \rightarrow q_{\text{new}}, p_{\text{new}})$. First, choose the point (q, p) within the 2×2 diamond-shaped domain of **Figure 1** and compute $(q_{\text{new}}, p_{\text{new}})$ using B . Then compute $B(q_{\text{new}}, -p_{\text{new}}) \rightarrow (q, -p)$ and confirm that the resulting point $(q, -p)$ is indeed the time-reversed image of the original (q, p) point.

Another point of view from which to analyze the rotated map B is “statistical”, based on distributions rather than on a single long dynamical trajectory. The statistical viewpoint describes the evolution of the phase-space probability density due to transformations of the comoving *area*, $dqdp \xrightarrow{B} dq_{\text{new}}dp_{\text{new}}$. The map *doubles* the comoving area whenever $q < p - \sqrt{(2/9)}$. B *halves* the area when $q > p - \sqrt{(2/9)}$:

$$(11/6)^2 - (7/6)^2 = 2 ; (11/12)^2 - (7/12)^2 = (1/2) .$$

The probability of observing k expansions with $N - k$ contractions (in any order) in a total

of N iterations of the map is the same as the biased random walk probability :

$$(1/3)^k(2/3)^{N-k} \binom{N}{k} .$$

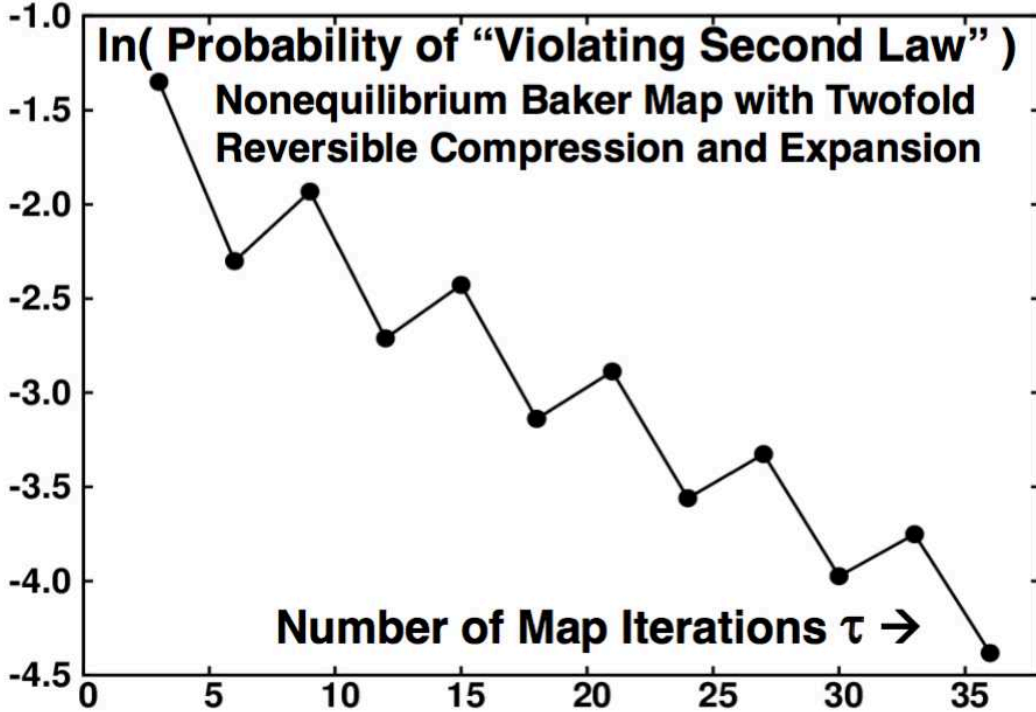


FIG. 2: Iterations of the Baker map with twofold compression or expansion can yield negative entropy production. Here I show the probability of these “Second Law Violations” for from 3 to 36 iterations of the map, where all possible 2^τ combinations of compressions and expansions have been included and properly weighted.

For the most likely 12-step example the probability is $(1/3)^4(2/3)^8 \binom{12}{4}$ while the probability of the *reversed* walk, $(1/3)^8(2/3)^4 \binom{12}{4}$ is sixteen times smaller. For the $2^{36} = 68,719,476,736$ 36-step walks the probability of finding expansion rather than contraction is still readily observable, and happens about one percent of the time. In **Figure 2** we plot the probability of finding expansion, corresponding to negative entropy production, as a function of the length of the observation window. For windows evenly divisible by six the probability varies roughly as $(2/3)^{(\tau/6)}$.

If we associate the logarithm of phase-space area with Gibbs’ entropy the entropy changes by $\pm k \ln(2)$ with each iteration of the map. Because the region subject to halving is twice as large as that subject to doubling, the *net* effect is an entropy *decrease* averaging $-(k/3) \ln(2)$

per iteration. Let us apply some steady-state thermodynamics. We imagine a heat reservoir that extracts the entropy produced by an iteration of the map and note that in the steady state that reservoir's entropy (external to the map) increases at a nearly constant rate, $\simeq (k/3)\ln(2)$ per iteration of the map. Although this idea (based on continuity) might seem a bit suspect for a fractal distribution it appears to be fully consistent with the ideas and results of Evans, Cohen, and Morriss.

In the Baker-Map case where the probability density is asymptotically uniform in the direction parallel to the line $(q + p) = 0$ and fractal in the perpendicular direction, parallel to the line $(q - p) = 0$, the southwest third of the diamond necessarily comes to include $(2/3)$ of the natural measure. The southwest third of the remainder (see **Figure 2**) is a scale model of the larger northeast third and contains $(2/3)$ of the remaining measure, that is $(2/9)$ of the total. This scaling in the northeast direction continues on with each image of the original smaller by a factor of $(2/3)$ while containing $(1/3)$ of the remaining measure. Thus the total area of $2 \times 2 = 4$ is divided up as follows :

$$(4/3) + (4/3)(2/3) + (4/3)(2/3)^2 + (4/3)(2/3)^3 + (4/3)(2/3)^4 + \dots = \frac{(4/3)}{1 - (2/3)} \equiv 4 .$$

The total “natural measure” is unity and corresponds to the following sum where the first term corresponds to the southwest third of the domain :

$$(2/3) + (2/3)(1/3) + (2/3)(1/3)^2 + (2/3)(1/3)^3 + (2/3)(1/3)^4 + \dots = \frac{(2/3)}{1 - (1/3)} \equiv 1 .$$

In our Baker Map $(2/3)$ of the measure expands to the northwest, with a Lyapunov expansion of $(3/2)$, while being squeezed threefold in the perpendicular direction. Simultaneously $(1/3)$ of the measure expands to the southeast, moving mainly mostly east, with a Lyapunov expansion of 3. In the steady state the $(2/3)$ of the measure halving in area perfectly balances the northeastern motion of the remaining $(1/3)$ which is doubling in area.

The fluctuation theorem for a window of τ steps states that the probability of converting work to heat, divided by the (illegal, according to the Second Law) reversed process, is the exponential of the entropy produced going forward in time :

$$\ln [\text{prob}_{\text{forward}} / \text{prob}_{\text{backward}}] = e^{+\sigma\tau} .$$

For the Baker Map the probabilities $\text{prob}_{\text{forward}}(\tau)$ and $\text{prob}_{\text{backward}}(\tau)$ can be worked out analytically by noting that a sequence of steps forward in time is more probable than its reverse by a factor of $e^{\sigma\tau}$. There is an isomorphism linking the comoving expansions and contractions of the Baker Map to a random walk in which steps to the right (corresponding to compression) are twice as likely as steps to the left (corresponding to expansion). Let us look at the details of a single example.

Consider the case $\tau = 6$ with 2^6 outcomes for the entropy production ranging from $(\Delta S/k) = -6\ln(2)$ with probability $(1/3)^6$ to $(\Delta S/k) = +6\ln(2)$ with probability $(2/3)^6$. Because this six-step mapping is equivalent to a random walk problem with left and right probabilities of $(1/3)$ and $(2/3)$ the distribution for $(\Delta S/k)$ approximates a Gaussian with mean value $\langle(\Delta S/k)\rangle = (\tau/3)\ln(2)$ and mean squared value $[(\tau/3)^2 + (8\tau/9)][\ln(2)]^2$:

$$P_{-6} = \frac{1}{729}; P_{-4} = \frac{6 \cdot 2}{729}; P_{-2} = \frac{15 \cdot 4}{729}; P_0 = \frac{20 \cdot 8}{729}; P_{+2} = \frac{15 \cdot 16}{729}; P_{+4} = \frac{6 \cdot 32}{729}; P_{+6} = \frac{64}{729},$$

the binomial distribution for a biased random walk. In the general case with a window τ the mean entropy production is $\sigma = (\tau/3)$ and the mean of the squared entropy production is

$$\langle\sigma\rangle/(k\ln(2)) = (\tau/3) ; \langle\sigma^2\rangle/[(k\ln(2))^2] = (\tau/3)^2 + (8\tau/9) = \langle\sigma\rangle^2 + (8/3)\langle\sigma\rangle .$$

From the Central Limit Theorem we see that the distribution approaches a Gaussian for large values of the entropy production

$$\text{prob}(\sigma) \propto e^{(-3/16)(\sigma-\langle\sigma\rangle)^2/\langle\sigma\rangle}$$

The biased random walk problem, which satisfies the Fluctuation Theorem precisely, is a useful model for introducing students to the voluminous literature on this subject.⁷

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