# THE FLUCTUATION THEOREM FOR

### STOCHASTIC SYSTEMS

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### ABSTRACT

The Fluctuation Theorem describes the probability ratio of observing trajectories that satisfy or violate the second law of thermodynamics. It has been proved in a number of different ways for thermostatted deterministic nonequilibrium systems. In the present paper we show that the Fluctuation Theorem is also valid for a class of stochastic nonequilibrium systems. The Theorem is therefore not reliant on the reversibility or the determinism of the underlying dynamics. Numerical tests verify the theoretical result.

#### 1. INTRODUCTION

The Fluctuation Theorem (FT) [1-6] states that the ratio of the probability of observing nonequilibrium trajectory segments of duration  $\tau$  with a time averaged rate of entropy production  $\overline{\sigma}_{\tau}$ , to the probability of observing segments with an average entropy production rate  $-\overline{\sigma}_{\tau}$  is,

$$\ln\left(\frac{p(\overline{\sigma}_{\tau})}{p(-\overline{\sigma}_{\tau})}\right) = \overline{\sigma}_{\tau}\tau \tag{1}$$

There are three approaches that have been used to derive this expression. This relationship was originally derived by Evans, Cohen and Morriss [1] from a natural invariant measure which was proposed heuristically for steady state trajectories [7]. It was shown [1] that the Fluctuation Theorem (1), was consistent with numerical results [1] for a fluid undergoing steady, reversible shear flow far from equilibrium. Gallavotti and Cohen [5, 6] improved this derivation, demonstrating that the FT can be derived from the Sinai-Ruelle-Bowen measure [8], if one employs the so-called Chaotic Hypothesis [5,6].

The second approach to derivating the FT, is applicable to transient trajectories which are initially sampled from an equilibrium microcanonical ensemble. It is valid for **all** trajectory durations,  $\tau$ . This approach is based on the Liouville measure [2-4, 9]. Since, in the limit  $\tau \rightarrow \infty$ , transient trajectory segments become indistinguishable from a steady state segments, this derivation also leads to (1), the asymptotic ( $\tau \rightarrow \infty$ ) steady state FT. The fact that these two measures, Liouville and SRB, lead to the same Theorem, gives credence to these two approaches.

A third approach that has been used to derive the FT is valid only in the linear response regime close to equilibrium. In a footnote to the original paper on the Fluctuation Theorem [1], the authors noted that the FT can be derived using the Green-Kubo relations for the linear response together with an application of the Central Limit Theorem to the distribution of  $\{\overline{\sigma}_{\tau}\}$ , in the  $\tau \rightarrow \infty$  limit. This third approach although limited to the linear response regime, is quite general with respect to the nature of

the thermostatting. In an obvious limit this approach applies to *unthermostatted* systems. This is because the Green-Kubo relations are robust with respect to thermostatting.

The FT is interesting in that it gives an analytic expression for the probability that, for a finite system and for a finite time, the Second Law of Thermodynamics will be violated. This expression has been tested numerically and predicts the expected long time and large system behaviour, that is: Second Law violating trajectories *will not be observed* in the thermodynamic and/or long time limits. Recently the FT has been shown to be valid for various reversible and deterministic systems [1, 2, 10-12].

Theoretical and numerical studies of the FT have concentrated on reversible, deterministic dynamics although recently theoretical studies on stochastic systems have been carried out [13, 14]. In the present paper the derivation of the FT which is based on the Liouville measure, is generalised so that it applies to stochastic systems. Numerical data verifying the FT for these systems are also presented. Since the FT is also valid for some stochastic systems, reversibility and determinism are clearly not prerequisites for the FT.

The derivation of the FT based on the Liouville measure presented previously [2-4, 9], considered the transient response of time-reversible dynamics. Numerical tests of this formulation were carried out using the commonly used deterministic homogeneous Gaussian thermostat, yet there is no reason that this particular thermostat *must* be used or that it should be applied homogeneously. It is trivial to see that an inhomogeneous thermostat - for example a thermostat which only acts on particles in a certain *wall* region - can be treated in exactly the same manner. Here it is shown that the FT is also applicable to some stochastic systems and therefore it is quite general and is not just applicable to a special classes of thermostatted systems.

# 2. DERIVATION OF THE FT FROM THE LIOUVILLE MEASURE FOR A CLASS OF STOCHASTIC SYSTEMS

Consider the equations of motion for a stochastic system given by:

$$\dot{\mathbf{\Gamma}} = \mathbf{G}(\mathbf{\Gamma}) + \boldsymbol{\xi}(\mathbf{t}) \tag{2}$$

where  $\boldsymbol{\xi}(t)$  is a random variable. The first term on the right hand side  $G(\boldsymbol{\Gamma})$ , is deterministic and assumed to be reversible. As an example, consider the transient response of a system, initially at equilibrium, to an applied field with a random term,  $\boldsymbol{\xi}_i$ , contributing to the equations of motion for the momenta. The system is thermostatted to ensure a steady state can be reached and the equations of motion are:

$$\dot{\mathbf{q}}_{i} = \frac{\mathbf{p}_{i}}{m} + \mathbf{C}_{i}(\mathbf{\Gamma})F_{e}$$

$$\dot{\mathbf{p}}_{i} = \mathbf{F}_{i}(\mathbf{q}) + \mathbf{D}_{i}(\mathbf{\Gamma})F_{e} + \boldsymbol{\xi}_{i}(t) - \alpha \mathbf{p}_{i}$$
(3)

where  $\mathbf{q}_i$  and  $\mathbf{p}_i$  are the coordinates and momenta of the ith particle, respectively,  $\mathbf{F}_i$  is the interparticle force on that particle,  $F_e$  is an external field applied to the system,  $\mathbf{C}_i$  and  $\mathbf{D}_i$  describe the coupling of the system to the field, and  $\alpha$  is a Gaussian thermostat multiplier that fixes the internal energy:

$$\alpha = \frac{\sum_{i=1}^{N} F_{e} \mathbf{D}_{i}(\mathbf{\Gamma}) \cdot \mathbf{p}_{i} / m + \mathbf{\xi}_{i} \cdot \mathbf{p}_{i} / m - F_{e} \mathbf{C}_{i}(\mathbf{\Gamma}) \cdot \mathbf{F}_{i}(\mathbf{q})}{\sum_{i=1}^{N} \mathbf{p}_{i} \cdot \mathbf{p}_{i} / m}.$$
(4)

To ensure that the system remains on a constant energy, zero total momentum, hypersurface, the thermostat multiplier contains the random term and the restriction,  $\sum_{i=1}^{N} \xi_i = \mathbf{0}$ , is imposed. The phase space of the nonequilibrium system is therefore is a subset of that of the initial equilibrium ensemble. In equation (3) the stochastic term can be regarded either as a random force that is added to the equation for the rate of change of momentum, or it can be regarded as contributing a random term to

the thermostat. The difference between these two interpretations is purely semantic.

If the adiabatic incompressibility of phase space (AI $\Gamma$ ) condition is satisfied, then the Liouville equation for this system reads:

$$\frac{\mathrm{d}f(\boldsymbol{\Gamma},t)}{\mathrm{d}t} = -f(\boldsymbol{\Gamma},t)\partial\dot{\boldsymbol{\Gamma}} \bullet_{\partial\boldsymbol{\Gamma}} = \mathrm{d}\mathbf{N}\alpha(\boldsymbol{\Gamma})f(\boldsymbol{\Gamma},t) + O(1)f(\boldsymbol{\Gamma},t)$$
(5)

where d is the number of Cartesian coordinates considered. In the following, terms of O(1) are neglected as they are not important to the theoretical arguments. However note that incorporation of these terms poses no difficulty and in Section 3, where small systems are examined, the consequences of these terms are indicated. The solution of equation (5) can be written [3]

$$f(\mathbf{\Gamma}(t),t) = \exp[dN \int_{0}^{t} \alpha(s) ds] f(\mathbf{\Gamma},0).$$
(6)

The FT considers the probabilities of observing trajectories with entropy production rates which are equal in magnitude but opposite in sign. In the proof of this theorem using the Liouville measure [2-4, 9] it was necessary, for every possible trajectory, to identify a conjugate trajectory which had this property: that is all trajectories were sorted into conjugate pairs. In a reversible, deterministic system this identification was straightforward and was accomplished by carrying out time reversal mappings [2-4, 9]. It is now shown how this procedure can be modified for stochastic systems.

Consider a trajectory segment,  $\Gamma_+(s)$ ; 0<s<t and its time-reversed trajectory,  $\Gamma_-(s)$ ; 0<s<t which we call an antisegment. The sign in the subscript reflects the sign of the integral of the thermostat multiplier (or entropy production) along the trajectory segment. For a reversible system, these trajectories are simply related by a time reversal mapping: each conjugate trajectory  $\Gamma_-$  is generated from the original trajectory  $\Gamma_+$  by carrying out a time-reversal mapping of the phase at the midpoint of the trajectory and integrating the equations of motion backward and forward in time [2-4, 9]. Without loss of generality if the field is assumed to be even with respect to the time-reversal mapping, then the

flux, entropy production rate and the thermostat multiplier will be odd. We use the notation that the averages of a phase variable, A, along a forward trajectory and its conjugate, time reversed, trajectory are given by:

$$\overline{A}_{+}(t) \equiv \frac{1}{t} \int_{0}^{t} ds \ A(\Gamma_{+}(s))$$
(7)

and

$$\overline{A}_{-}(t) \equiv \frac{1}{t} \int_{0}^{t} ds A(\Gamma_{-}(s))$$
(8)

respectively. Depending on the parity of the phase function  $A(\Gamma)$  under time reversal symmetry, there may be a simple relation between  $\overline{A}_{+}(t)$  and  $\overline{A}_{-}(t)$ .

In a stochastic system the conjugate trajectory can no longer be generated by simply carrying out a time reversal mapping and solving the equations of motion. After the time reversal mapping at the midpoint of the original trajectory, integration of the equations of motion forward and backward in time will with overwhelming probability, result in the observation of a different set of random numbers than were observed for the original trajectory and the trajectories will not be conjugate. Clearly a mapping of the sequence of random numbers observed for the forward trajectory must be carried out for the conjugate trajectory. The necessary mapping of the random numbers will depend on the function  $\xi_i(R)$  where R is a random number. Figure 1 give a diagrammatic representation of the way in which conjugate trajectories are generated for stochastic systems.

If the sequence of random numbers:  $R_1$ ,  $R_2$ ,  $R_3$ ,  $R_4$  is observed for the original trajectory, then this sequence must be appropriately mapped in the conjugate trajectory. For example if the random term contributes only to the equation of motion for  $\dot{p}_{xi}$ , which is even under a time-reversal mapping, then the sequence  $R_4$ ,  $R_3$ ,  $R_2$ ,  $R_1$  must be observed for the conjugate trajectory to be generated. Similarly, if the random term contributes only to  $\dot{q}_{xi}$ , which is odd under time reversal, then the sequence  $-R_4$ ,  $-R_3$ ,  $-R_2$ ,  $-R_1$  must be observed. Provided the mapped sequence is allowed by the random number generator, the antisegment will be a solution of the equations of motion. It should be noted that in the first case no restrictions on the random number generator are required however in the second case, a symmetry restriction on the range of numbers is necessary for this proof to be valid.

It can be observed from Figure 1 that  $M^{(T)}\Gamma_{(3)} = \Gamma_{(4)}$ ;  $M^{(T)}\Gamma_{(1)} = \Gamma_{(6)}$  and  $M^{(T)}\Gamma_{(2)} = \Gamma_{(5)}$  where is  $M^{(T)}$  used to to represent a time-reversal mapping. At all points along the trajectory the fluxes of conjugate trajectories are related by  $J(t;\Gamma_+, 0 < t < \tau) = -J(t;\Gamma_-, 0 < t < \tau)$  and therefore fluxes averaged over the duration of the segment are related by:  $\overline{J}_+ = -\overline{J}_-$ . It is straightforward then to see that in order to divide the trajectories into conjugate pairs, the equations of motion do not have to be reversible (that is  $M^{(T)} \cdot e^{iL(\Gamma)t} \cdot M^{(T)} \cdot e^{iL(\Gamma)t} \cdot \Gamma(0) = \Gamma(0)$  where  $M^{(T)} \cdot M^{(T)} = 1$ ), but it is necessary that *the antisegment is a solution of the equations of motion.* 

Now it is shown how the probability of observing the conjugate trajectories can be determined. For the system considered, the initial phases are distributed microcanonically, so the probability of observing an initial phase inside a small phase volume,  $\delta V(\Gamma(0))$  about  $\Gamma(0)$  is proportional to  $\delta V(\Gamma(0))$ . It is assumed that our universe is causal: the probability of observing a trajectory segment is proportional to the probability of observing the *initial* phase that generates the segment. Using the fact that for sufficiently small volumes,  $\delta V(\Gamma(t) \sim 1/f(\Gamma(t))$  and that the Jacobian for the time reversal mapping is unity, the solution the Liouville equation given by equation (5) allows the expansion or contraction of a phase volume along a trajectory to be determined. This is illustrated in Figure 2.

The ratio of volumes the  $\delta V_1$  and  $\delta V_4$  gives the ratio of the probability of observing *initial phase points*. The probability of observing a *trajectory* is equal to the product of the probability of observing the initial phase point and the probability of observing the sequence of random numbers:

$$\operatorname{prob}(\Gamma(s); 0 < s < t) = \operatorname{prob}(\delta V(0))\operatorname{prob}(R_1 \dots R_n)$$
(9)

The probability of observing a trajectory segment with a particular time-averaged value of  $\alpha$  is then given by the sum over all trajectories with that value, and the probability ratio is given by:

$$\frac{p(\overline{\alpha}_{+}(\tau))}{p(\overline{\alpha}_{-}(\tau))} = \frac{\sum_{i \mid \int \alpha(\Gamma_{i}) = \overline{\alpha}_{+}(\tau)} \delta V(\Gamma_{i+}(0)) p(R_{1}...R_{n})_{i}}{\sum_{i \mid \int \alpha(\Gamma_{i}) = \overline{\alpha}_{-}(\tau)} \delta V(\Gamma_{i+}(0)) p(R_{1}...R_{n})_{i}}$$

$$= \frac{\sum_{i \mid \int \alpha(\mathbf{G}_{i}) = \overline{\alpha}_{+}(\tau)} \delta V(\mathbf{\Gamma}_{i-}(0)) p(\mathbf{R}_{1} \dots \mathbf{R}_{n})_{i}}{\sum_{i \mid \int \alpha(\mathbf{\Gamma}_{i}) = \overline{\alpha}_{+}(\tau)} \delta V(\mathbf{\Gamma}_{i-}(0)) p(\mathbf{M}^{(T)}(\mathbf{R}_{1} \dots \mathbf{R}_{n})_{i})}$$

$$= \frac{\sum_{i \mid \int \alpha(\mathbf{\Gamma}_{i}) = \overline{\alpha}_{+}(\tau)} \delta V(\mathbf{\Gamma}_{i+}(0)) p(\mathbf{R}_{1} \dots \mathbf{R}_{n})_{i}}{\sum_{i \mid \int \alpha(\mathbf{\Gamma}_{i}) = \overline{\alpha}_{+}(\tau)} \exp[-dN\tau \overline{\alpha}_{+i}(\tau)] \delta V(\mathbf{\Gamma}_{i+}(0)) p(\mathbf{M}^{(T)}(\mathbf{R}_{1} \dots \mathbf{R}_{n})_{i})}$$

$$(10)$$

$$= \exp[dN\tau\overline{\alpha}_{+}(\tau)]$$

where the notation:  $i|\int \alpha(\Gamma_i) = \overline{\alpha}_+(\tau)$  is used to represent all trajectories, i, for which the time averaged value of the thermostat multiplier is equal to  $\overline{\alpha}_+$ ; and it is assumed that  $p(R_1,...R_n) = p(M^{(T)}(R_1...R_n))$ . The resulting fluctuation formula given by equation (10) for this stochastic system is identical to that for the deterministic, reversible systems [1-3, 5, 9]. As in the deterministic case there may be many different pairs of conjugate trajectories which each have the same value for  $\overline{\alpha}_+(\tau)$ .

The FT derived above is valid for *transient* trajectory segments of arbitrary length. Steady state trajectory segments can be considered as the long time limit of transient trajectory segments and therefore the stochastic FT will also apply to steady state systems.

# 3. NUMERICAL TESTS OF THE FLUCTUATION THEOREM APPLIED TO TRANSIENT STOCHASTIC SYSTEMS

Transient NEMD simulations of Couette flow using the SLLOD algorithm and the usual Lees-Edwards periodic boundary conditions, were carried out employing a *stochastic* force in the xdirection and the corresponding Gaussian isoenergetic thermostat. The equations of motion for this system are:

$$\dot{\mathbf{q}}_{i} = \mathbf{p}_{i} + \mathbf{i}\gamma\mathbf{y}_{i}$$

$$\dot{\mathbf{p}}_{i} = \mathbf{F}_{i} - \mathbf{i}\gamma\mathbf{p}_{yi} + \mathbf{i}\boldsymbol{\xi}_{i} - \alpha\mathbf{p}_{i}$$
(11)

with the thermostat multiplier given by,

$$\alpha = \frac{\sum_{i=1}^{N} \xi_i p_{xi} - \gamma(p_{xi} p_{yi} + F_{xi} y_i)}{\sum_{i=1}^{N} \mathbf{p}_i \cdot \mathbf{p}_i}$$
(12)

The system consisted of N = 32 particles in 2 Cartesian dimensions and the particles interacted with the WCA short ranged, repulsive pair potential [15]. Lennard-Jones units are use throughout. The internal energy per particle was set at E/N = 1.56032 (*i.e.* T~1.0) and the particle density at n = N/V = 0.8. A strain rate of  $\gamma = 0.5$  was applied.

The stochastic term is of the simplest kind: the sequence of random numbers that must be observed in order to generate a conjugate trajectory are the same numbers that are observed for the forward trajectory, but they must occur in the reverse order. This means that no restrictions on the distribution of the random numbers are required to obtain equation (10). In the simulations, the stochastic term,  $\boldsymbol{\xi}_i$ , was the product of a random number and a delta function at each time step. The random numbers were selected from a Gaussian distribution with zero mean, a standard deviation of 1.0 and were

restricted within the range [-10.0,10.0].

Figure 3 shows the ensemble averaged response of the flux which indicates that a steady state is approached and the initial transient response has a Maxwell time of approximately  $\tau_M = 0.07$ .

In the transient response simulations, many initial equilibrium phases were generated and the response to an applied strain rate was monitored for various trajectory segment lengths. Histograms of  $\overline{\alpha}_{+}(\tau) \equiv \frac{1}{\tau} \int_{0}^{\tau} ds \,\alpha(\Gamma_{+}(s))$  were obtained with  $\tau = 0.1, 0.4$  and 0.6. These histograms are shown in Figure 4. The FT predicts that a plot of  $\ln(p(\overline{\alpha}_{+}(\tau))/p(-\overline{\alpha}_{+}(\tau)))$  versus  $\overline{\alpha}_{+}(\tau)$  should give a straight line of unit slope. For each of the trajectory segment lengths considered in Figure 3 the FT was tested with O(1/N) corrections included. The normalised probability ratios are shown in Figure 5. In each case a slope of unity is obtained and the FT is verified.

These results show that the FT is valid for finite averaging times of this transient, stochastic system.

# 4. NUMERICAL TESTS OF THE FLUCTUATION THEOREM APPLIED TO STEADY STATE STOCHASTIC SYSTEMS

The FT was also examined for steady state systems evolving with the stochastic equations of motion considered in Section 3. Histograms of  $\overline{\alpha}_{+}(\tau) \equiv \frac{1}{\tau} \int_{0}^{\tau} ds \, \alpha(\Gamma_{+}(s))$  for steady state trajectory segments of length  $\tau = 0.05$ , 0.1, 0.2, 0.3 and 0.4 were calculated. The results for  $\tau = 0.05$ , 0.2 and 0.4 are shown in Figure 6.

For steady state trajectories, the FT predicts that a plot of  $\ln(p(\overline{\alpha}_+(\tau))/p(-\overline{\alpha}_+(\tau)))$  vs  $\overline{\alpha}_+(\tau)$  gives a straight line of unit slope *in the limit*  $\tau \rightarrow \infty$ . Figure 7 shows the results and figure 8 plots the slope as a function of  $\tau$ , indicating that it approaches unity in the long time limit.

#### 5. CONCLUSIONS

The present work shows that the Fluctuation Theorem is quite general and applies to both deterministic and stochastic nonequilibrium systems. As was found to be the case for deterministic systems, the Fluctuation Theorem applies:

• exactly to finite (transient) trajectory segments which are initially sampled from the equilibrium microcanonical ensemble and then move isoenergetically towards a steady state, and,

• asymptotically to long time steady state trajectory segments. In all cases, transient or steady state, stochastic or deterministic, the Fluctuation Theorem applies in both the linear and the nonlinear response regimes.

As a final comment we note that although the theory and simulations presented here apply to systems in which every particle is ergostatted (so-called homogeneous thermostatting), the theory presented here applies equally well to systems were only a subset of the particles are thermostatted. The theory also applies to systems composed of mixtures of particles with different interparticle interactions. We can therefore obviously model boundary thermostatted systems where a fluid obeying Newtonian mechanics (ie no thermostat) flows inside thermostatted solid walls, using the theory presented here. To treat such a system you consider a mixture of two types of particles where at the temperature and density studied one set of particles, the wall particles, are in the solid phase and are thermostatted and the other set of particles are liquid and are not thermostatted. In such cases the only difference to the theory above is that in equations such as (6), above the N, refers to the number of thermostatted particles and not to the total number of particles.

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Figure 1: Searles & Evans

Figure 1. A schematic diagram showing the construction of conjugate trajectories for stochastic systems.



Figure 2: Searles & Evans

Figure 2. A schematic diagram representing the change in phase volume with time along a trajectory and its conjugate.



Figure 3. The ensemble averaged response of the flux for as system of 32 particles in 2 Cartesian dimensions to which a strain rate is applied at time zero and for which the SLLOD algorithm is used to model the shear flow. The internal energy per particle was set at E/N = 1.56032 (*i.e.* T~1.0) and the particle density at n = 0.8. A strain rate of  $\gamma = 0.5$  was applied.







Figure 4. Histograms of  $\overline{\alpha}_{+}(\tau) \equiv \frac{1}{\tau} \int_{0}^{\tau} ds \, \alpha(\Gamma_{+}(s))$  for a system undergoing transient response to an applied strain rate of  $\gamma = 0.5$ . The internal energy per particle was set at E/N = 1.56032 (*i.e.* T~1.0) and the particle density at n = 0.8. Trajectory segments of a)  $\tau = 0.1$ , b)  $\tau = 0.4$  and c)  $\tau = 0.6$  were used.







Figure 5. Plots of  $\ln \frac{p(\overline{\alpha}_{+}(\tau))}{p(-\overline{\alpha}_{+}(\tau))}$  / (2N $\tau$ ) vs  $\overline{\alpha}_{+}(\tau)$  for the system considered in Figure 4 with a)  $\tau = 0.1$ , b)  $\tau = 0.4$  and c)  $\tau = 0.6$ . Order (1/N) corrections are included. The straight line is of unit slope and it is the result predicted from the FT. The slopes obtained from weighted least squares fits are a) 0.98±0.01; b) 1.00±0.02; c) 1.02±0.04.







Figure 6. Histograms of  $\overline{\alpha}_{+}(\tau) \equiv \frac{1}{\tau} \int_{0}^{\tau} ds \, \alpha(\Gamma_{+}(s))$  for a system undergoing steady state shear flow with an applied strain rate of  $\gamma = 0.5$ . The internal energy per particle was set at E/N = 1.56032 (*i.e.* T~1.0) and the particle density at n = 0.8. Trajectory segments of a)  $\tau = 0.05$ , b)  $\tau = 0.2$  and c)  $\tau = 0.4$  were used.



Figure 7. The slope of plots of  $\ln \frac{p(\overline{\alpha}_{+}(\tau))}{p(-\overline{\alpha}_{+}(\tau))} / (2N\tau)$  vs  $\overline{\alpha}_{+}(\tau)$  for various trajectory segment lengths. The result is consistent with a convergence to a value of unity in the long time limit which is the result predicted from the FT.