A∀$_{60}$

GRUPPO T.N.T.

...

1992 ....TNT group

Aging Fluctuation Relations
and
Fluctuation Dissipation Theorem:
a Possible Relation

(Long-lasting) Collaboration with:
- Marco Picco (CNRS, LPTHE-UPMC Paris)
- Felix Ritort (U Barcelona)

Fluctuations Relations
why?

Microscopic vs Macroscopic

Fluctuations Relations
why?

Microscopic vs Macroscopic

Microscopic variables: trajectories

Difficult
Too fine

Fluctuations Relations
why?

Microscopic vs Macroscopic

Microscopic variables: trajectories

Difficult
Too fine

Global variables: averages

Physical quantities undergo random fluctuations

Statistical properties described by Statistical Mechanics

Microscopic dynamics → Restrictions on the PDF of fluctuating quantities

Fluctuations Relations

X: Macroscopic (extensive) variable

$$\frac{{}^{F}P(X)}{{}^{R}P(-X)} = \exp\left[a(X-b)\right]$$

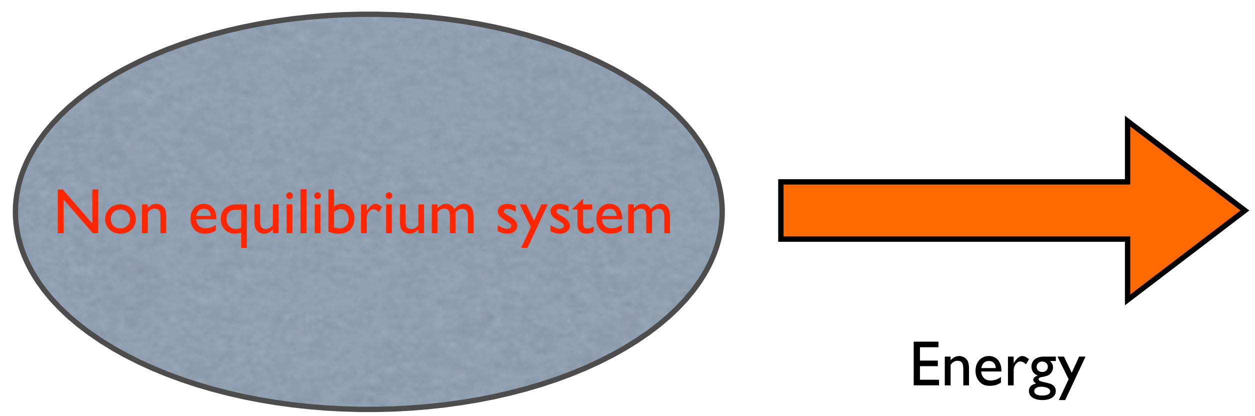
Fluctuation Relation (FT)

F: "Forward" process

R: "Reversed" process

Non-Equilibrium Systems

Non equilibrium systems → Net energy flux with environment



Fluctuation Relations → Relate Probability of Absorbing / Releasing a given amount of energy

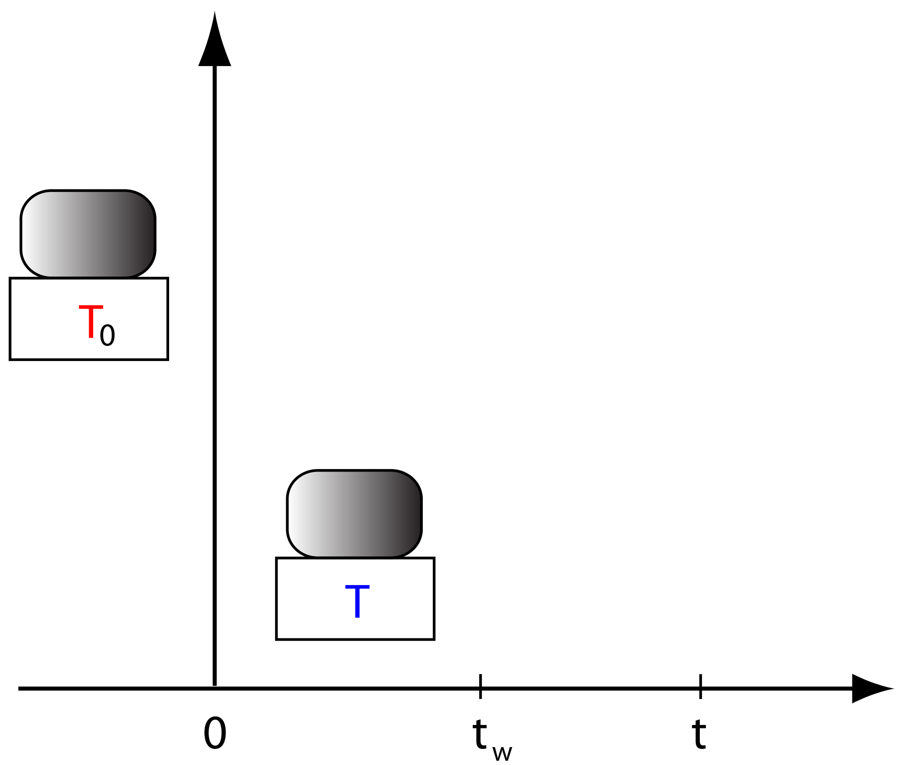
Aging Systems
(Quench)

Aging systems are characterized by two time-scales

The age or waiting time t_w

The time $t > t_w$ of measurement

Quench Protocol



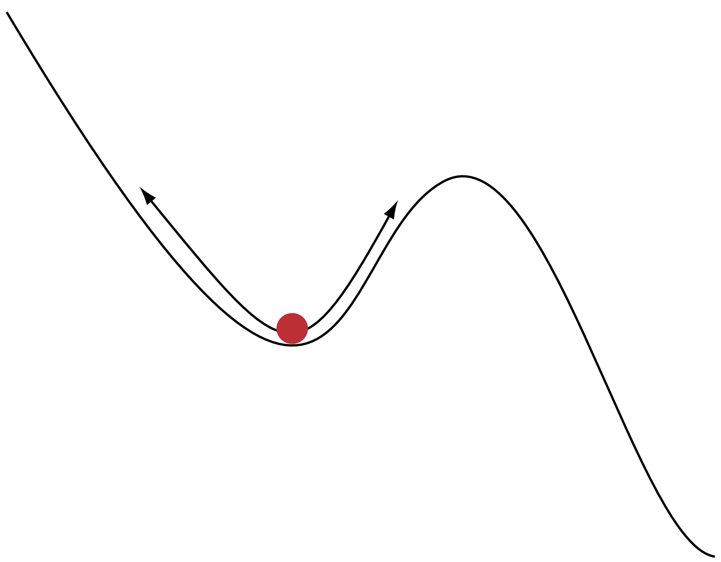
At time $t=0$ the systems is quenched from high temperature T_0 down to low temperature T

Non equilibrium (relaxation) state characterized by a net energy flux

Measurements between t and t_w depends on both t and t_w

Energy Fluctuations: Stimulated Process

- Times $t - t_w << t_c - t_w$



The heat Q is exchanged back and forth but the the net flux is vanishingly small

On these time-scales the system looks as equilibrated at the bath temperature T

The PDF of Q is a Gaussian of zero mean and T-dependent width

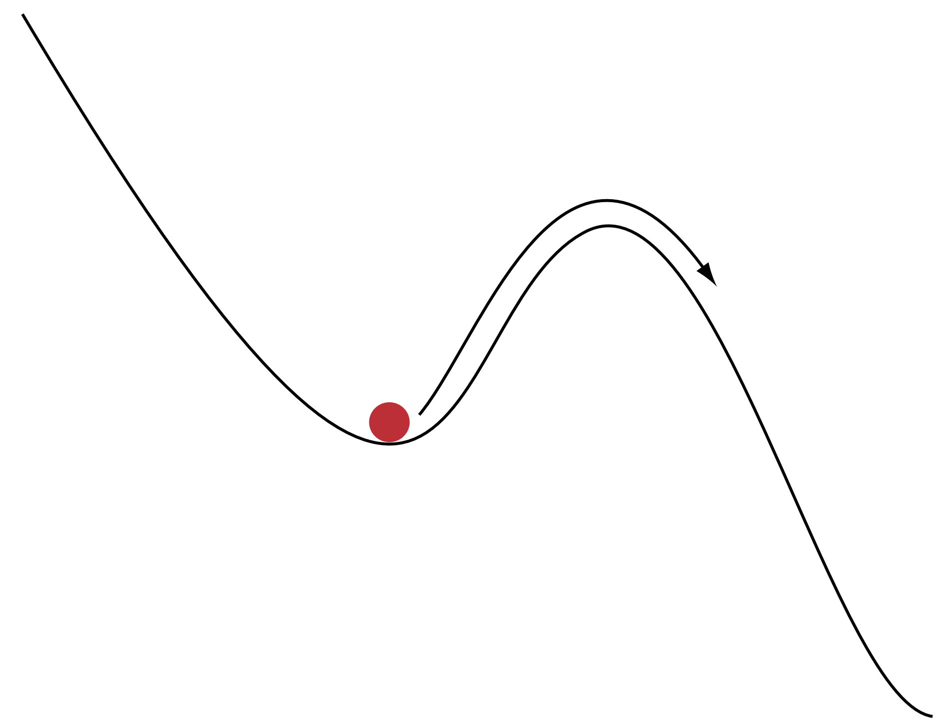
Stimulated Process → Originates from thermally activated processes

Energy Fluctuations: Spontaneous Process

- Times $t - t_w >> t_w$

Intermittent exchange of larger than typical amount of heat Q

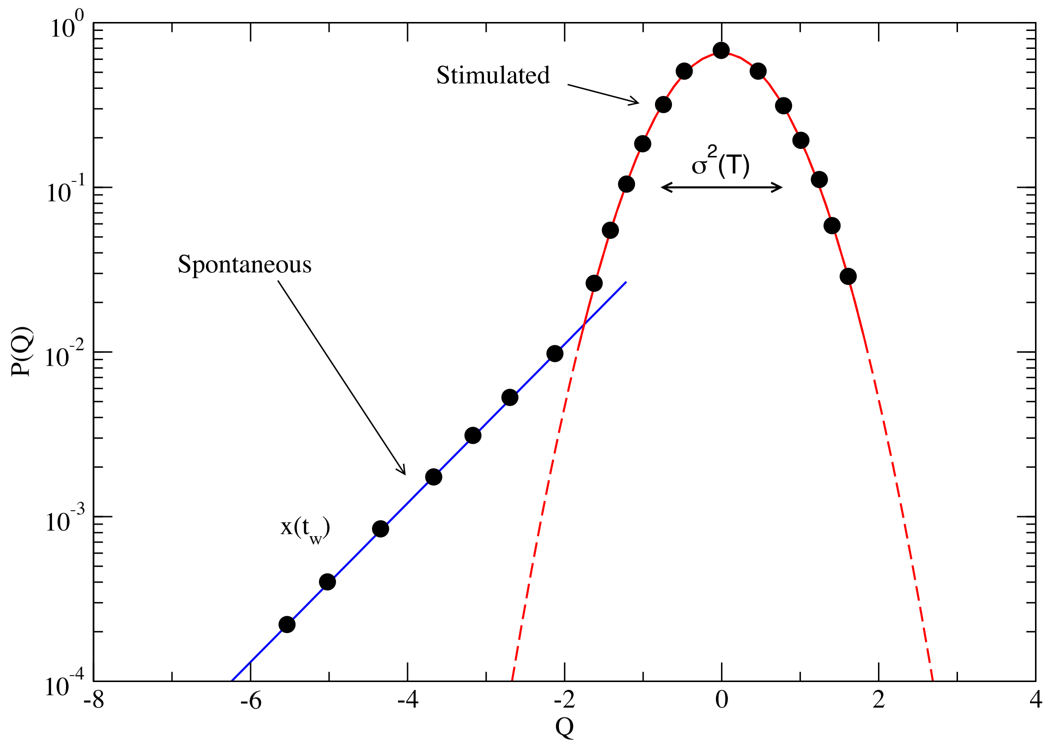
Finite net heat flow

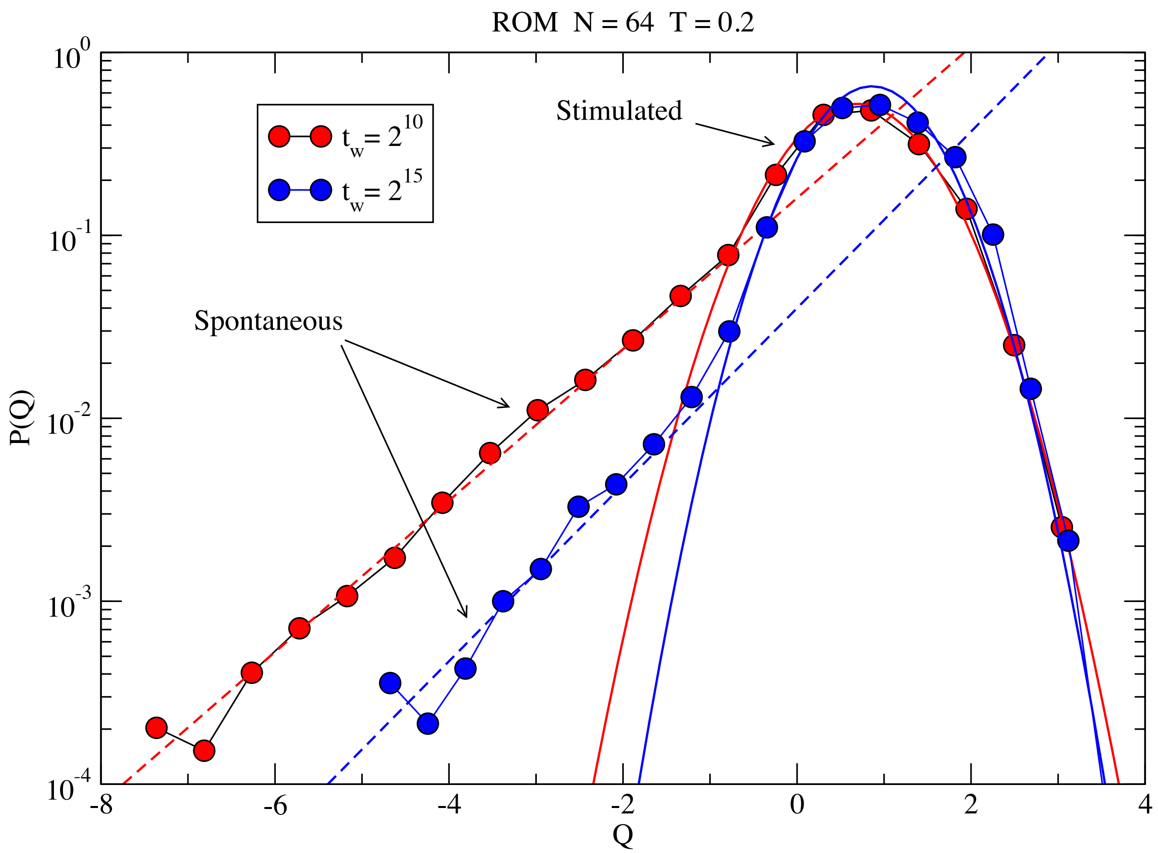


The PDF of Q has a t_w-dependent exponential tail

Spontaneous Process → Originates because the system was not in equilibrium at t_w.

Energy Fluctuations PDF





Aging Fluctuation Relation

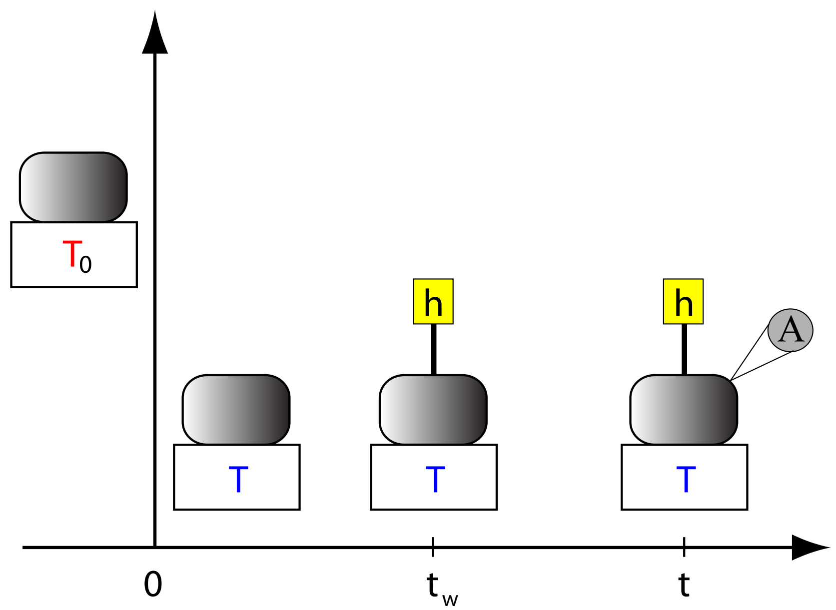
Protocol:

- $t = 0$ quench to low temperature
- t_w apply a constant external perturbation h coupled to the macroscopic variable (observable) A
- $t = t_w + \Delta t$ measure the entropy production ΔS during Δt

$$\Delta S_{t_w,t} = Q_{t_w,t}/T$$

$$= \beta h \big[A(t) - A(t_w)\big]$$

$$= \beta \mathcal{W}_0(t_w, t) \quad \text{(Exclusive Work)}$$



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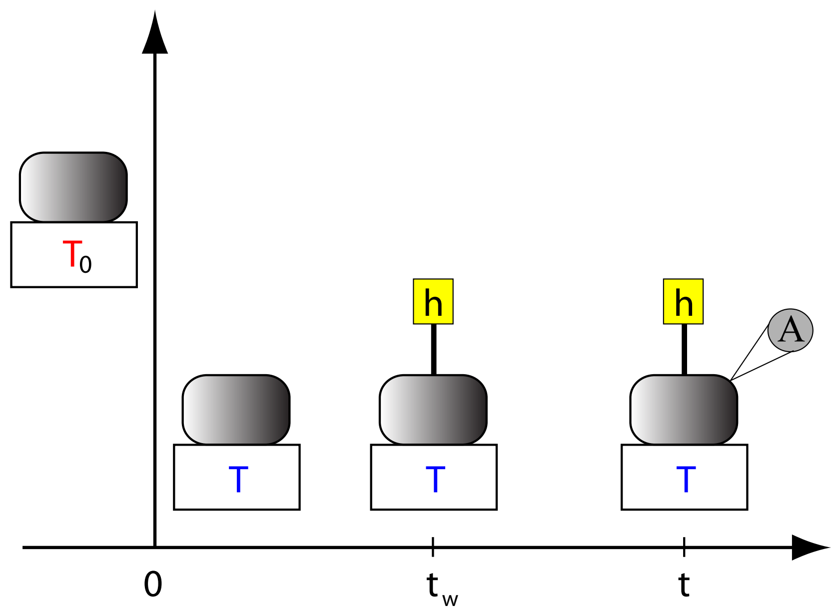
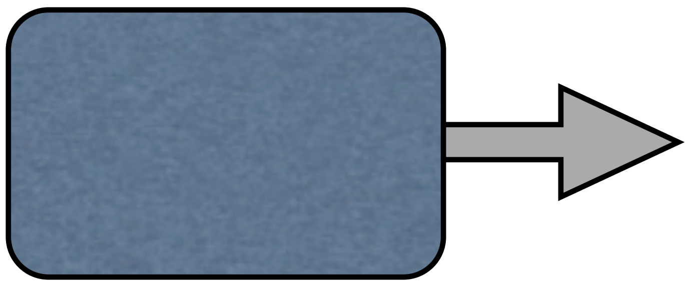


- Build the PDF: $P_{t_w,t}(\Delta S)$

$$\frac{{}^F P_{t_w,t}(\Delta S)}{{}^R P_{t_w,t}(-\Delta S)} = ?$$

Reversed Path Protocol

- After a time t_w the systems will *output a sequence of* "$t - t_w$" states (Forward Path)



$011011 \cdots 001$

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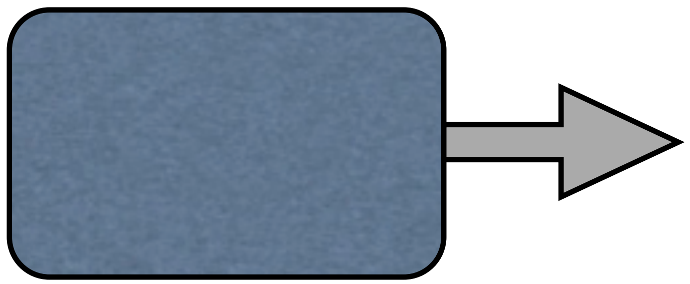

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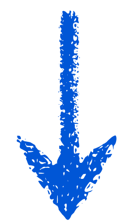
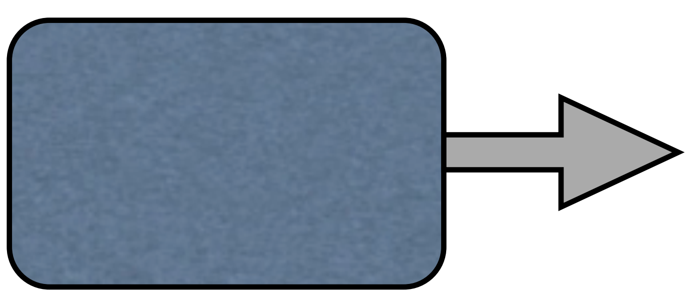


We consider the probability that the system after the time t_w (Reversed Path)

will output the same sequence in the reversed order



$$100\cdots110110$$

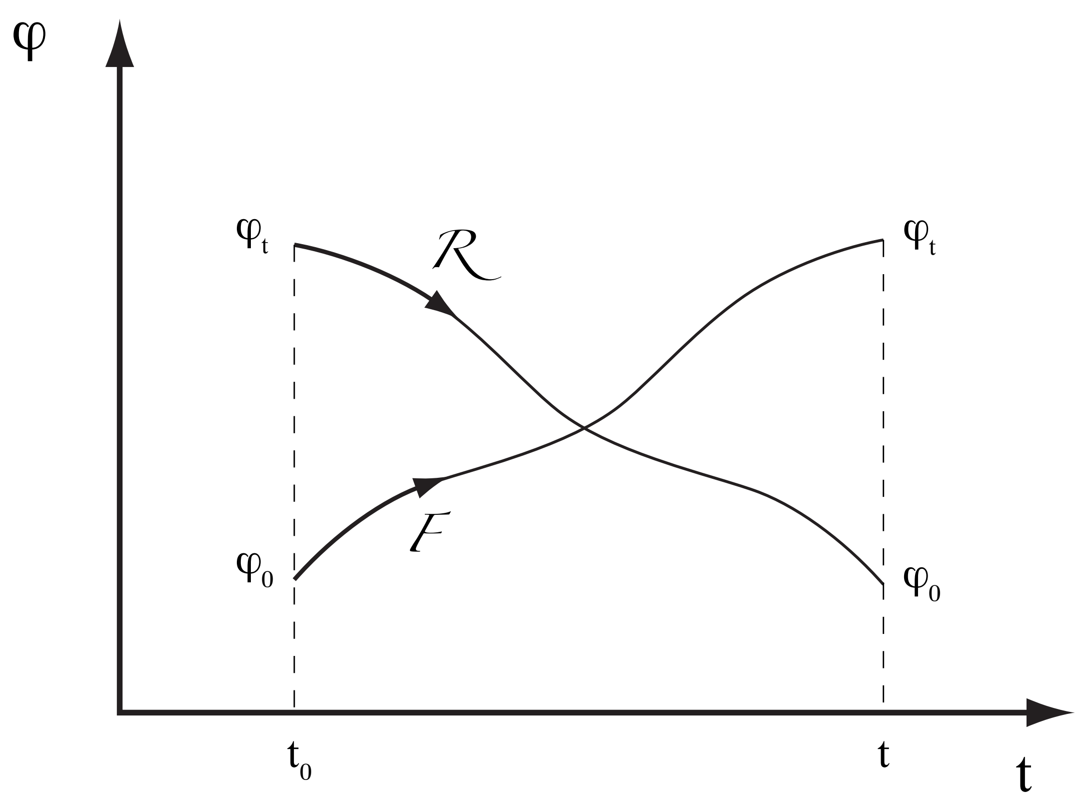
A Model

Langevin Dynamics

$$\frac{d\varphi}{dt} = F(\varphi) + h + \xi$$

$$\langle \xi(t)\, \xi(t') \rangle = 2T\delta(t - t')$$

$$F(\varphi) = -\frac{\delta H(\varphi)}{\delta\varphi} \longrightarrow \lim_{t\to\infty} P(\varphi, t) = P^{\mathrm{eq}}(\varphi) = \frac{e^{-\beta H(\varphi)}}{Z}$$



Forward Path:

$$\{\varphi_s\}_{s\in[t_0,t]}$$

Reverse Path:

$$\{\widetilde{\varphi}_s\}_{s\in[t_0,t]} =^R \{\varphi_s\}_{s\in[t_0.t]} \equiv \{\varphi_{t+t_0-s}\}_{s\in[t_0,t]}$$

Path Integral Formulation

$$P(\varphi_t, t|\varphi_0, t_0) = \int_{\varphi_0}^{\varphi_t} \mathcal{D}\varphi \, \exp\left[\int_{t_0}^{t} ds\, \mathcal{L}(\dot{\varphi}, \varphi; h)\right]$$

Probability Forward Process

$$P(\varphi_0, t|\varphi_t, t_0) = \int_{\varphi_0}^{\varphi_t} \mathcal{D}\varphi \, \exp\left[\int_{t_0}^{t} ds\, \mathcal{L}(-\dot{\varphi}, \varphi; h)\right]$$

Probability Reverse Process

$$\mathcal{L}(\dot{\varphi}, \varphi; h) = -\frac{\beta}{4}\Big[\dot{\varphi} - F(\varphi) - h\Big]^2.$$

External perturbation h
not reversed

$$\int_{t_0}^{t} ds\, \mathcal{L}(-\dot{\varphi}, \varphi; h) = \int_{t_0}^{t} ds\, \mathcal{L}(\dot{\varphi}, \varphi; h)$$
$$+\beta\big[H(\varphi_t) - H(\varphi_0)\big] - \beta\mathcal{W}_0(\varphi_t, \varphi_0; h),$$

$$\mathcal{W}_0(\varphi_t, \varphi_0; h) = \int_{t_0}^{t} ds\, h\, \dot{\varphi} = h\,(\varphi_t - \varphi_0)$$

(Exclusive Work)

Forward / Reverse

Probability ratio Forward/Reverse Process:

$$\frac{P^{(h)}(\varphi_t, t|\varphi_0, t_0)\, P_0(\varphi_0)}{P^{(h)}(\varphi_0, t|\varphi_t, t_0)\, P_1(\varphi_t)} = e^{\Delta S_{\rm tot}(\varphi_t, \varphi_0)}$$

$P_{0,1}(\varphi)$ Probability initial/final states

Entropy production or information gain

$$\Delta S_{\rm tot}(\varphi_t, \varphi_0) = \Delta S_{\rm m}(\varphi_t, \varphi_0) + \Delta S_{\rm b}(\varphi_t, \varphi_0)$$

Medium

$$\Delta S_{\rm m}(\varphi_t, \varphi_0) = \beta \mathcal{Q}(\varphi_t, \varphi_0)$$

Dissipated Heat

$$= \beta \int_{t_0}^{t} ds \big[F[\varphi(s)] + h\big]\, \dot{\varphi}(s)$$

$$= -\Delta S^{\rm eq}(\varphi_y, \varphi_0) + \beta \mathcal{W}_0(\varphi_t, \varphi_0; h)$$

$$\Delta S^{\rm eq}(\varphi_t, \varphi_0) = -\ln \frac{P^{\rm eq}(\varphi_t)}{P^{\rm eq}(\varphi_0)} = \beta\big[H(\varphi_t) - H(\varphi_0)\big]$$

Boundary

$$\Delta S_{\rm b}(\varphi_t, \varphi_0) = -\ln \frac{P_1(\varphi_t)}{P_0(\varphi_0)}$$

Integral Fluctuation Relation

$$\left\langle F(\varphi_t,\varphi_0)\, e^{-\Delta S_{\rm tot}(\varphi_t,\varphi_0)} \right\rangle_{t,t_0} = {}^{R}\langle F(\varphi_t,\varphi_0)\rangle_{t,t_0}$$

$F(\varphi_t,\varphi_0)$ generic functional of (φ_t,φ_0)

Integral Fluctuation Relation

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$F(\varphi_t, \varphi_0)$ generic functional of (φ_t, φ_0)

- If $F(\varphi_t, \varphi_0) = \delta(W_0 - \mathcal{W}_0(\varphi_t, \varphi_0; h))$

$$\rightarrow \quad P(-W_0; t, t_0) = \left\langle \delta(W_0 - \mathcal{W}_0(\varphi_t, \varphi_0; h))\, e^{-\Delta S^{\rm tot}(\varphi_t, \varphi_0)} \right\rangle_{t,t_0}$$

Equilibrium

In <u>equilibrium</u>

$$P_0(\varphi) = P_1(\varphi) = P^{\rm eq}(\varphi)$$

$$\downarrow$$

$$\Delta S_{\rm tot} = \beta \mathcal{W}_0 - \Delta S^{\rm eq} + \Delta S_{\rm b} = \beta \mathcal{W}_0$$

$$\Rightarrow \quad \frac{P(W_0; t, t_0)}{P(-W_0; t, t_0)} = e^{\beta W_0}$$

$$\Rightarrow \quad \left\langle e^{-\beta W_0} \right\rangle = 1$$

Bochkov - Kuzovlev
Sov. Phys. JEPT 45, 125 (1977)

Aging Fluctuation Relation

Aging (Glassy) System

- Phase space made of a set of disjoint subsets (cages)
- Number of cages depends on the age t_0 (waiting time)
- At the initial time t_0 the system is inside one cage
- It is trapped into the cage for a typical time $t_c \sim t_0$
- Microscopic relaxation time $<< t_c$ (local equilibrium)

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$$\frac{P(\Delta S; t, t_0)}{P(-\Delta S; t, t_0)} = e^{\Delta S} \qquad t - t_0 \ll t_c \sim t_0$$

$$\Delta S = \beta W_0$$

Aging Fluctuation Relation

What about $t - t_0 \gg t_c \sim t_0$?

Aging Fluctuation Relation

What about $t - t_0 \gg t_c \sim t_0$?

- The exclusive work depends on macroscopic quantities

$$\mathcal{W}_0(\varphi_t, \varphi_0; h) = h\,(\varphi_t - \varphi_0) \equiv h\left(\sum_i \varphi_{t,i} - \sum_i \varphi_{0,i}\right)$$

$$P(-W_0; t, t_0) = e^{-\beta W_0} \int d\psi_0 \int d\psi_t\, \delta\big(W_0/h - \psi_t + \psi_0\big)$$

$$\times \left\langle e^{\Delta S^{\mathrm{eq}}(\varphi_t,\varphi_0) - \Delta S_{\mathrm{b}}(\varphi_t,\varphi_0)} \right\rangle_{\psi_t,t;\psi_0;t_0}$$

Only states with fixed $\psi = \sum_i \varphi_i$

Aging Fluctuation Relation

In local equilibrium

$$P(\varphi|\psi) \propto P^{\rm eq}(\varphi)\,\frac{\Omega_T(\psi)}{\Omega(\psi)}$$

→ Probability of $\psi = \sum_i \varphi_i$ in a cage

$\Omega_T(\psi)$ Number of states with $\psi = \sum_i \varphi_i$ in a cage

$\Omega(\psi)$ Number of accessible states with $\psi = \sum_i \varphi_i$

$\ln \Omega_T(\psi) = S_T(\psi)$ local equilibrium

Aging Fluctuation Relation

$$\frac{P(W_0;t,t_0)}{P(-W_0;t,t_0)} = e^{\beta x W_0}$$

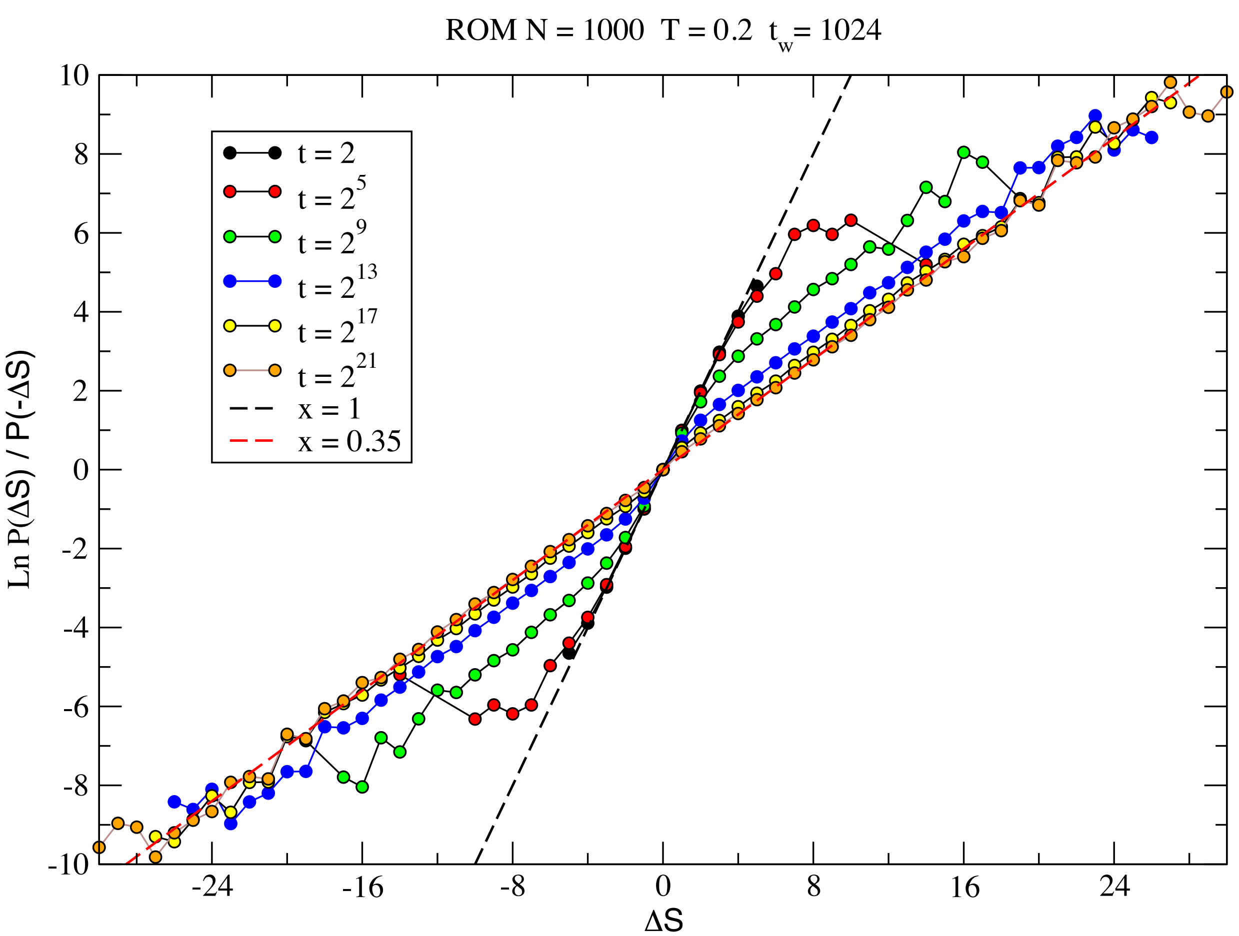
$$t - t_0 \gg t_0$$

(AFR)

$$\frac{d \ln \Omega(\psi_0)}{d\psi_0} = x\beta h$$

→ $x < 1$ Phase space contraction factor

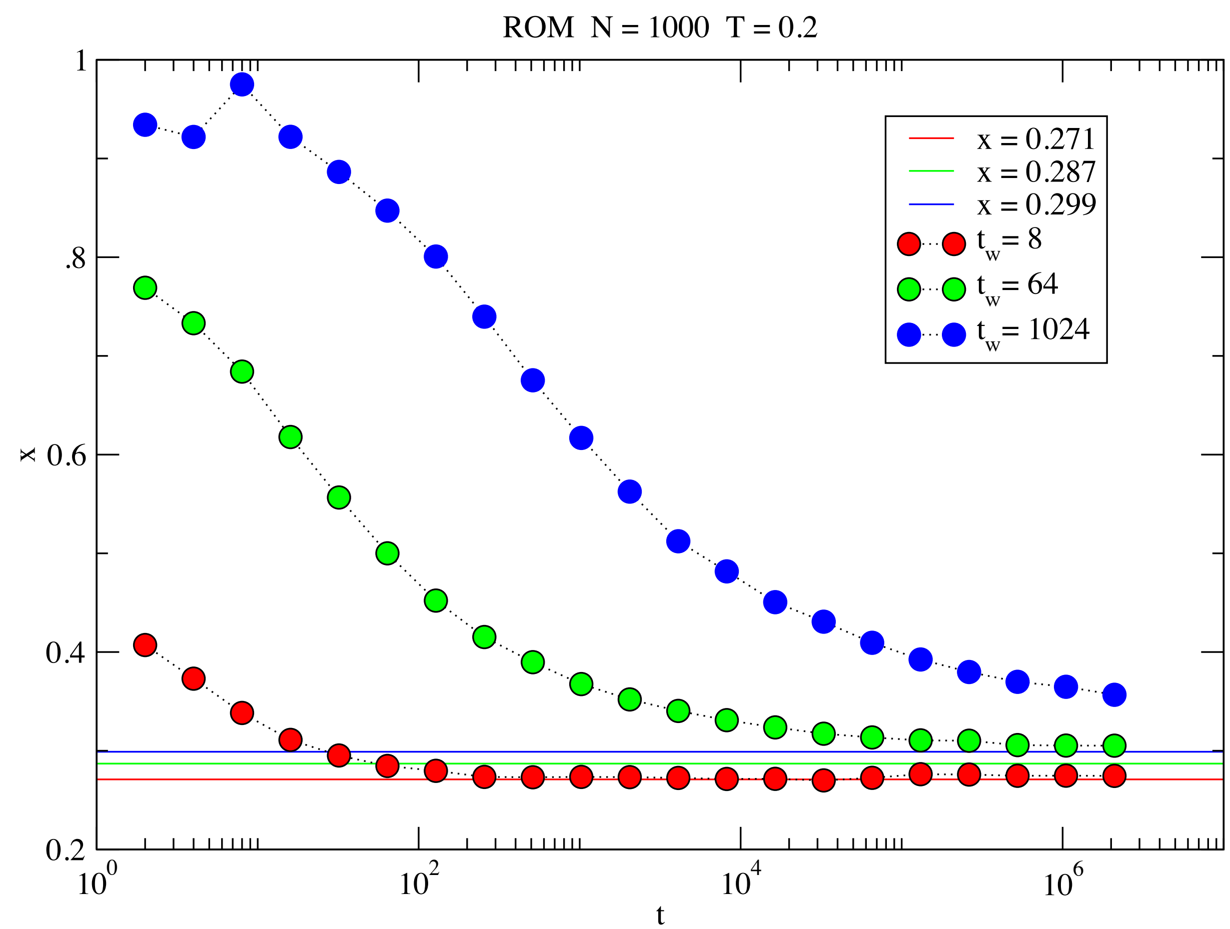
Numerical Test
ROM



$$H = -\sum_{i,j}^{1,N} J_{i,j}\,\sigma_i\,\sigma_j$$

$$\sigma = \pm 1$$

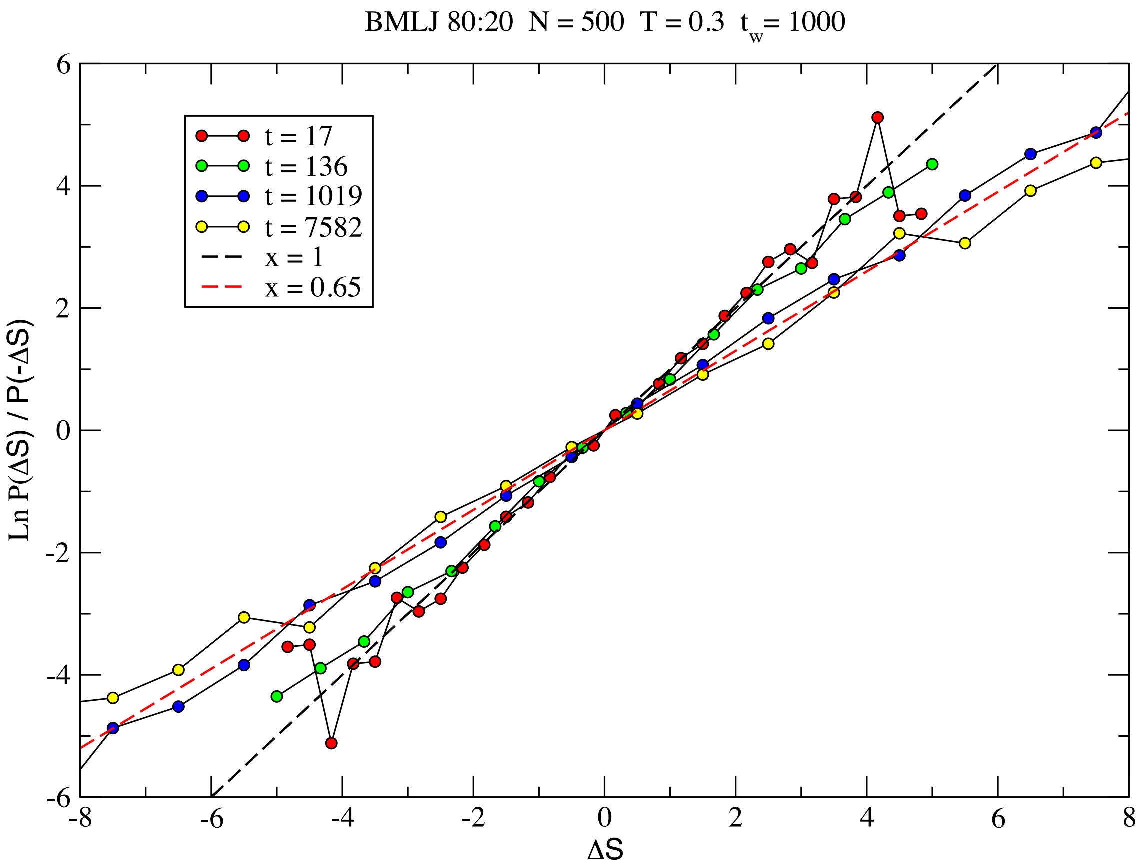
$J_{i,j}$ Random orthogonal



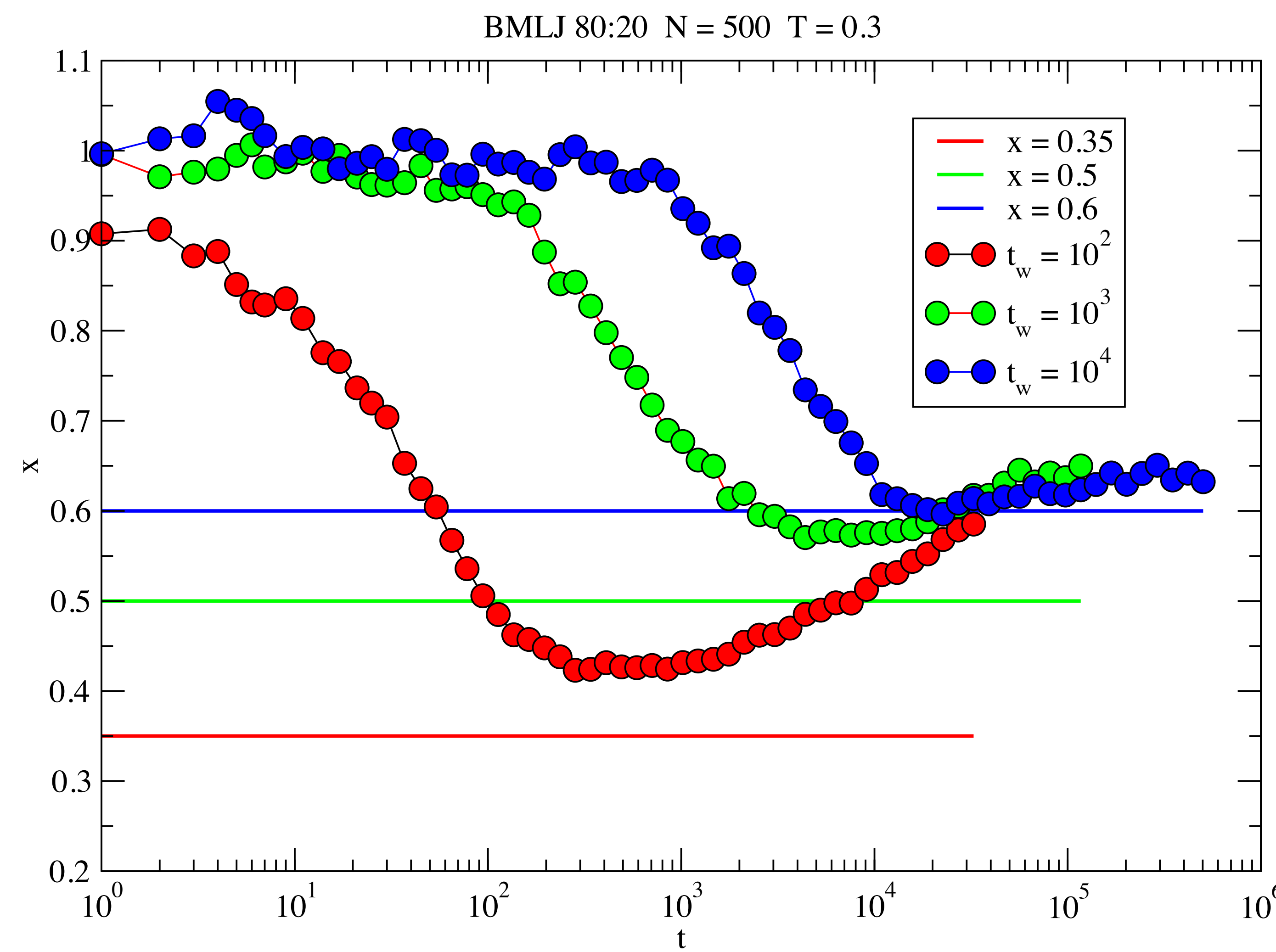
$x \sim 1$ $\quad t \ll t_w$ Short time

$x < 1$ $\quad t \gg t_w$ Long time

Numerical Test
BMLJ 80:20



$$V_{\alpha\beta}(r) = 4\epsilon_{\alpha\beta}\left[\left(\frac{\sigma_{\alpha\beta}}{r}\right)^{12} - \left(\frac{\sigma_{\alpha\beta}}{r}\right)^{6}\right]$$



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Numerical Test
BMLJ 80:20

$\Delta S_{t_0,t}$ Strongly Intermittent

$\Delta S_{t_0,t} = \Delta S \quad \Leftrightarrow \quad$ broad time interval $t - t_0$

Fixed time statistics mixes different regimes

Numerical Test
BMLJ 80:20

$\Delta S_{t_0,t}$ Strongly Intermittent

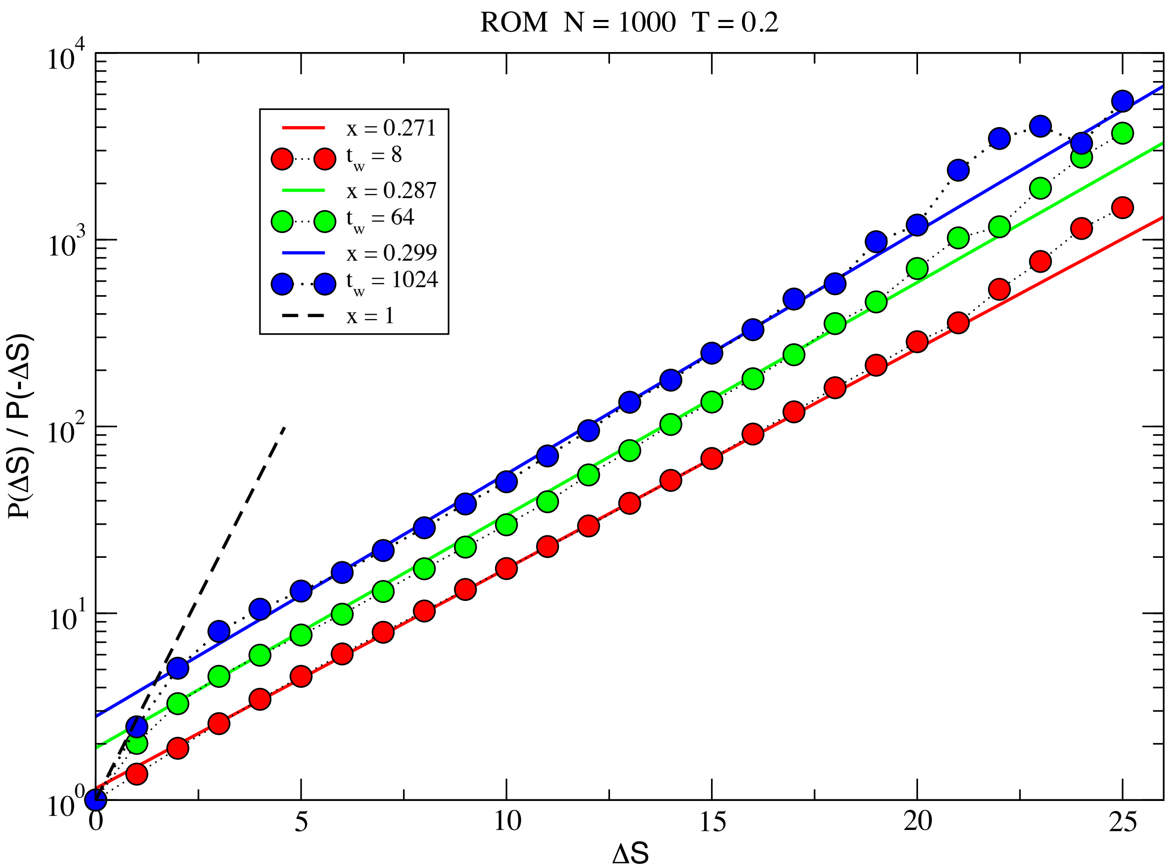
$P_{\Delta t}(\Delta S; t_0)$ = Probability of $\Delta S_{t_0,t} = \Delta S$

in the time interval $[t_0, t_0 + \Delta t]$

$$\ln \frac{P_{\Delta t}(\Delta S; t_0)}{P_{\Delta t}(-\Delta S; t_0)} \simeq \Delta S$$ $|\Delta S| < \Delta S^*$ Stimulated process

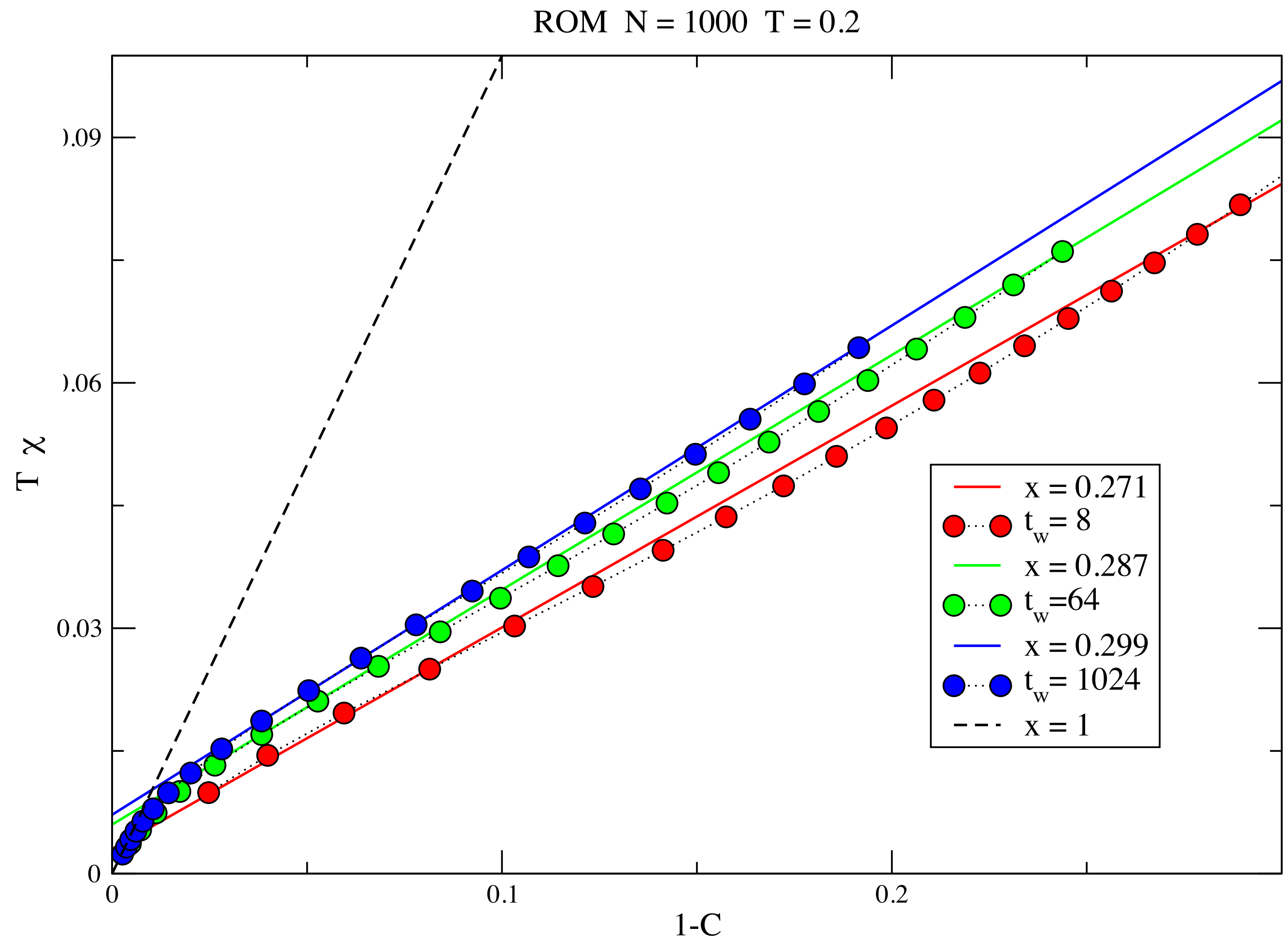
$$\ln \frac{P_{\Delta t}(\Delta S; t_0)}{P_{\Delta t}(-\Delta S; t_0)} \simeq x\Delta S$$ $|\Delta S| > \Delta S^*$ Spontaneous process

Numerical Test
ROM



AFR

FDT



Numerical Test
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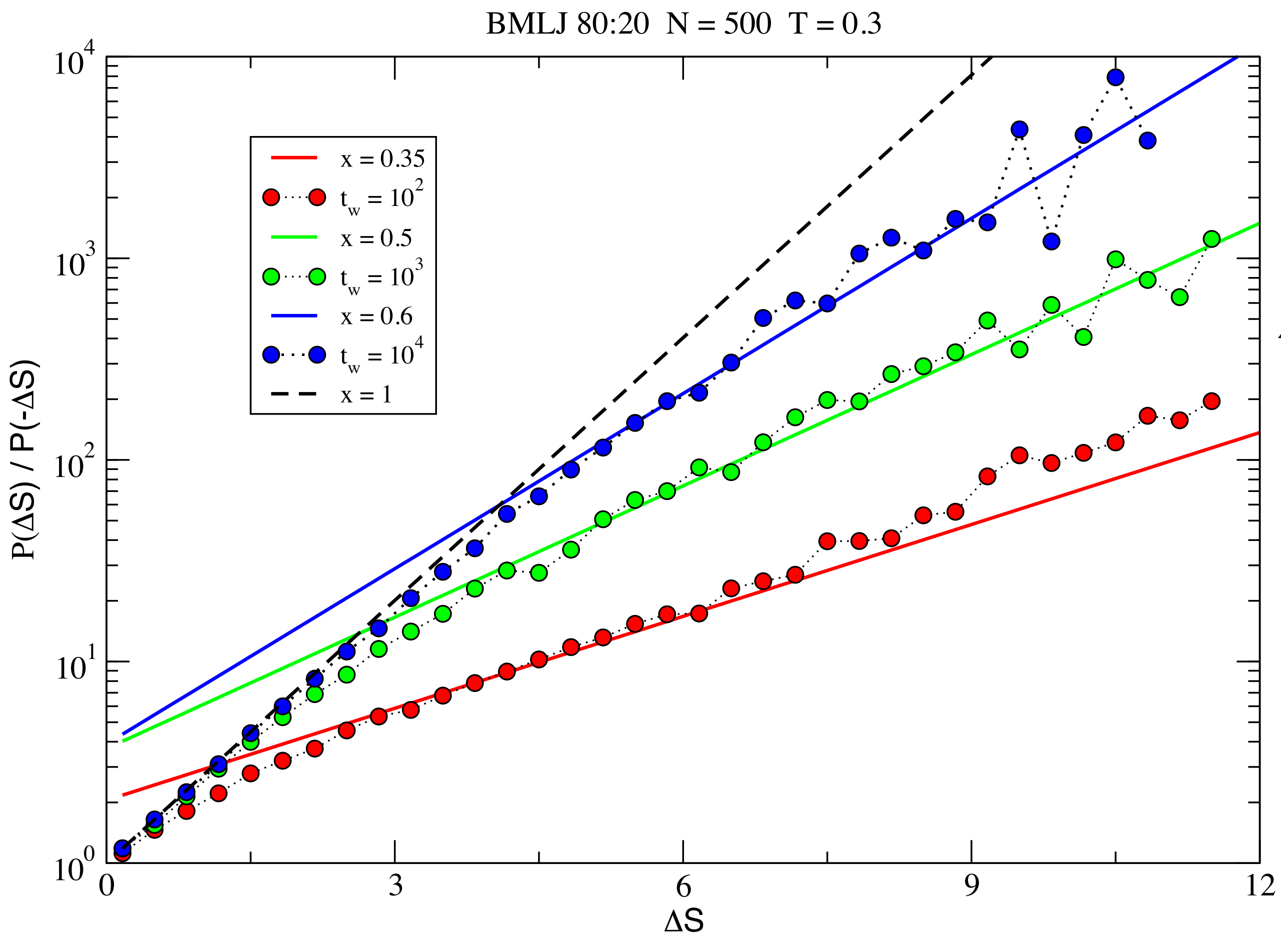
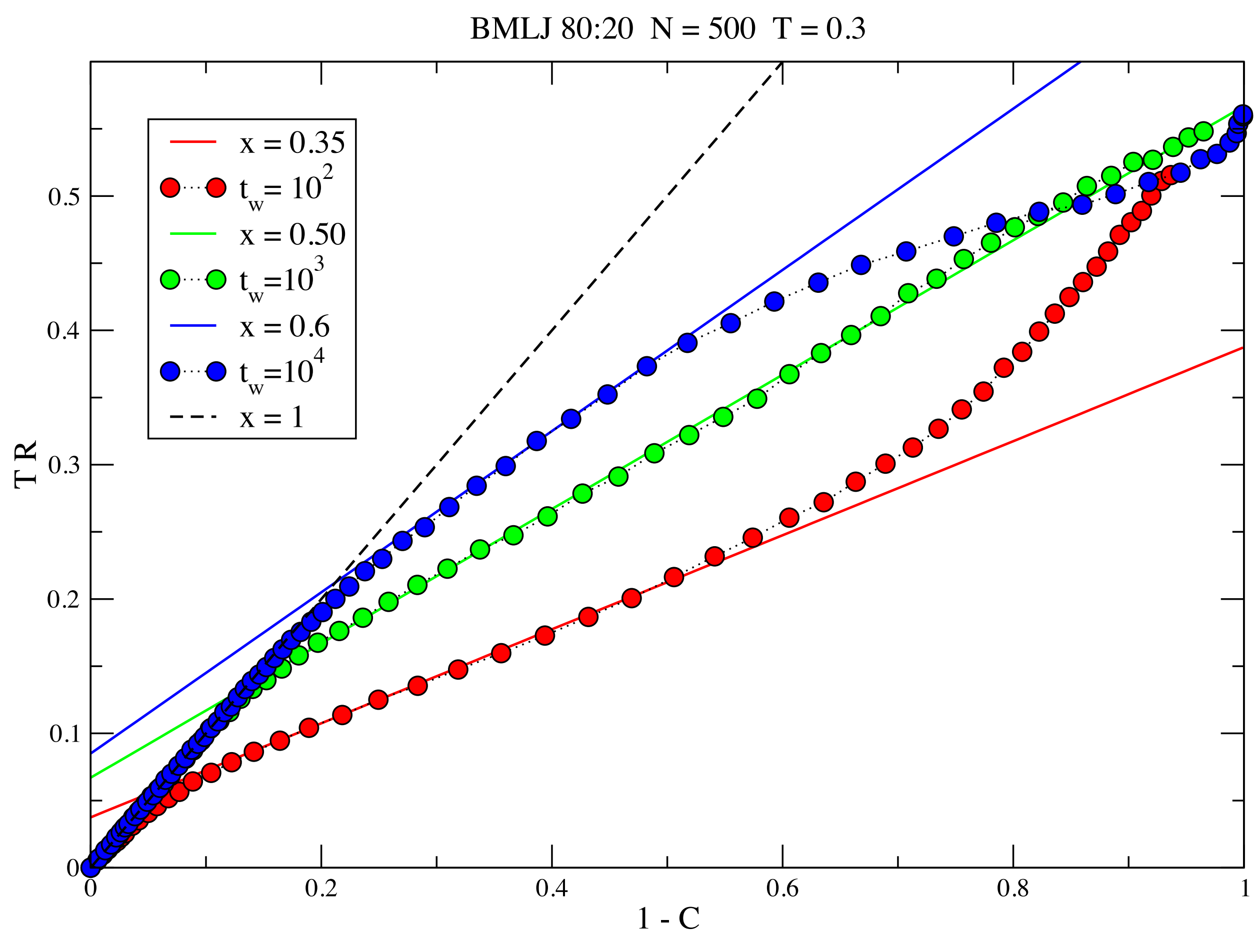


AFR



FDT

Aging Fluctuation Dissipation
and
Fluctuation Dissipation Theorem

$\Delta S = \beta W_0$ Macroscopic (Extensive) quantity

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$$P(\Delta S; t, t_0) \propto \exp\left[-\frac{1}{2\langle \Delta S^2 \rangle_c}\big(\Delta S - \langle \Delta S \rangle\big)^2\right]$$

Aging Fluctuation Dissipation
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Fluctuation Dissipation Theorem

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Reverse Path (Reverse process)

$$P(-\Delta S; t, t_0) = P(\Delta S; t, t_0)|_{\Delta S \to -\Delta S}$$

$$\rightarrow \quad x = \frac{1}{\Delta S} \ln \frac{P(\Delta S; t, t_0}{P(-\Delta S; t, t_0)} = 2\frac{\langle \Delta S \rangle}{\langle \Delta S^2 \rangle_c}$$

AFR

AFR and FDT

Vanishingly small external perturbation $h \ll 0$

FDT

$$\langle \varphi_t \rangle_h = h \int_{t_0}^{t} ds\, R(s, t_0) \qquad [\langle \varphi_0 \rangle_h = \langle \varphi_0 \rangle = 0]$$

$$R(t, t_0) = -\theta(t - t_0) \beta\, x_{\mathrm{FDT}}\, \partial_t \, \langle \varphi(t)\, \varphi(t_0) \rangle .$$

AFR and FDT

Vanishingly small external perturbation $h \ll 0$

FDT

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$$R(t, t_0) = -\theta(t - t_0) \beta\, x_{\mathrm{FDT}}\, \partial_t \left\langle \varphi(t)\, \varphi(t_0) \right\rangle.$$

But: $\Delta S = \beta h \big(\varphi_t - \varphi_0 \big)$

$$x = \frac{2}{\beta h} \frac{\langle \varphi_t \rangle_h}{\left\langle \varphi_t^2 \right\rangle + \left\langle \varphi_0^2 \right\rangle - 2 \left\langle \varphi_t\, \varphi_0 \right\rangle} + O(h)$$

$$x = 2\, x_{\mathrm{FDT}} \frac{\langle \varphi_0^2 \rangle - \langle \varphi_t \varphi_0 \rangle}{\left\langle \varphi_t^2 \right\rangle + \left\langle \varphi_0^2 \right\rangle - 2 \left\langle \varphi_t\, \varphi_0 \right\rangle} + O(h)$$

AFR and FDT

Vanishingly small external perturbation $h \ll 0$

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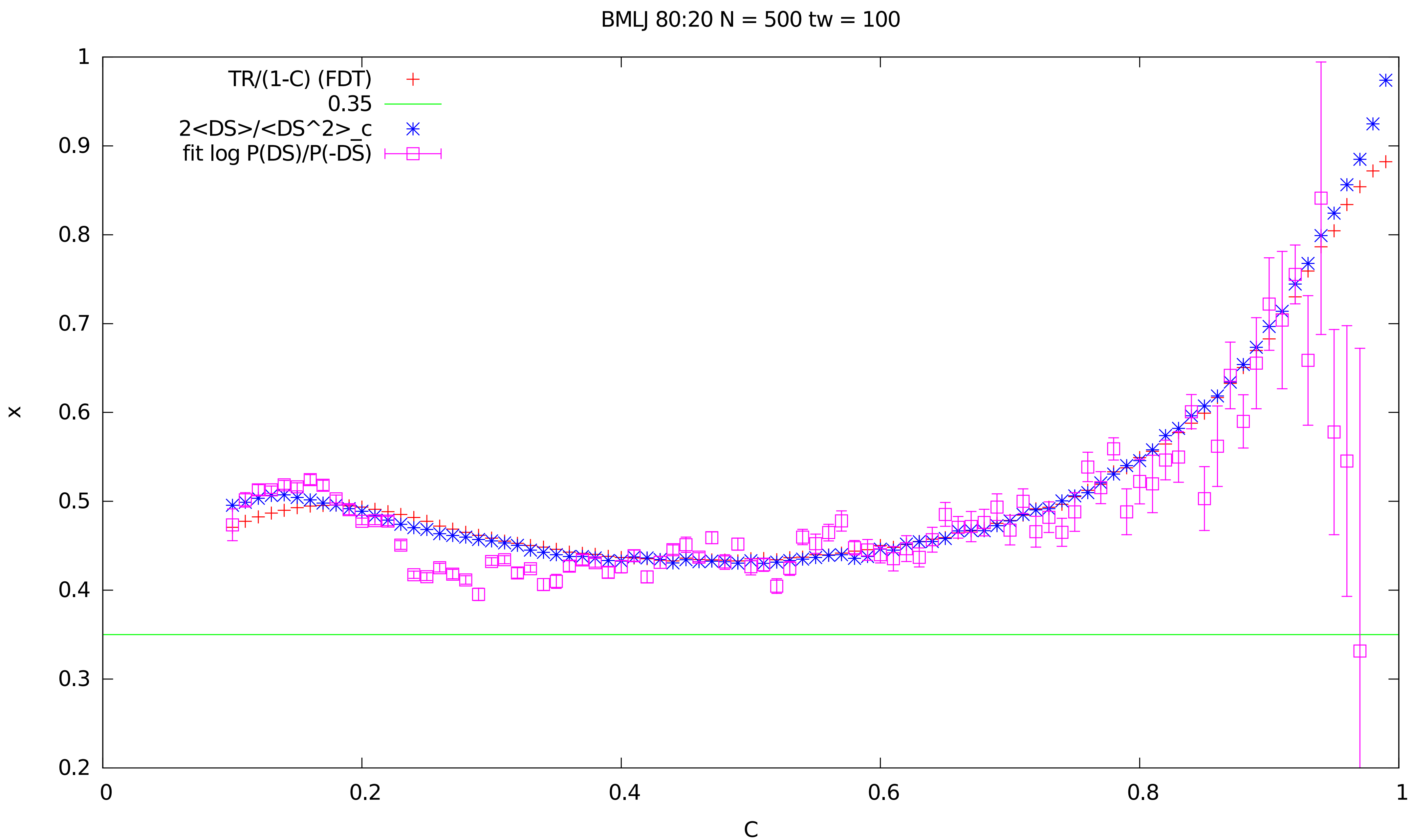
$$x = 2\, x_{\rm FDT} \frac{\langle \varphi_0^2 \rangle - \langle \varphi_t \varphi_0 \rangle}{\left\langle \varphi_t^2 \right\rangle + \left\langle \varphi_0^2 \right\rangle - 2 \left\langle \varphi_t\, \varphi_0 \right\rangle} + O(h)$$

- If $\langle \varphi_t^2 \rangle \simeq \langle \varphi_0^2 \rangle$ → $x = x_{\rm FDT} + O(h)$

Back to Numerical
BMLJ 80:20



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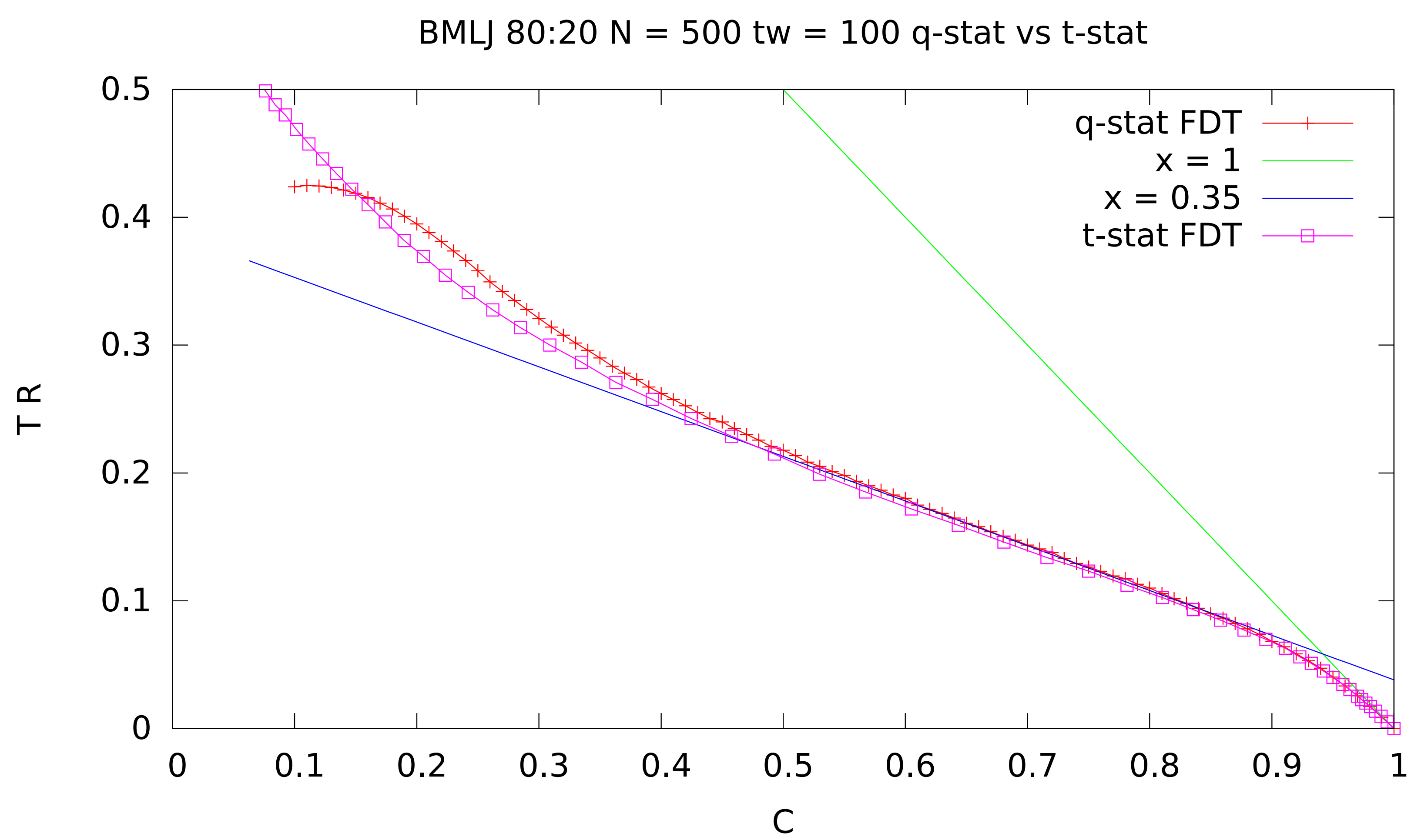

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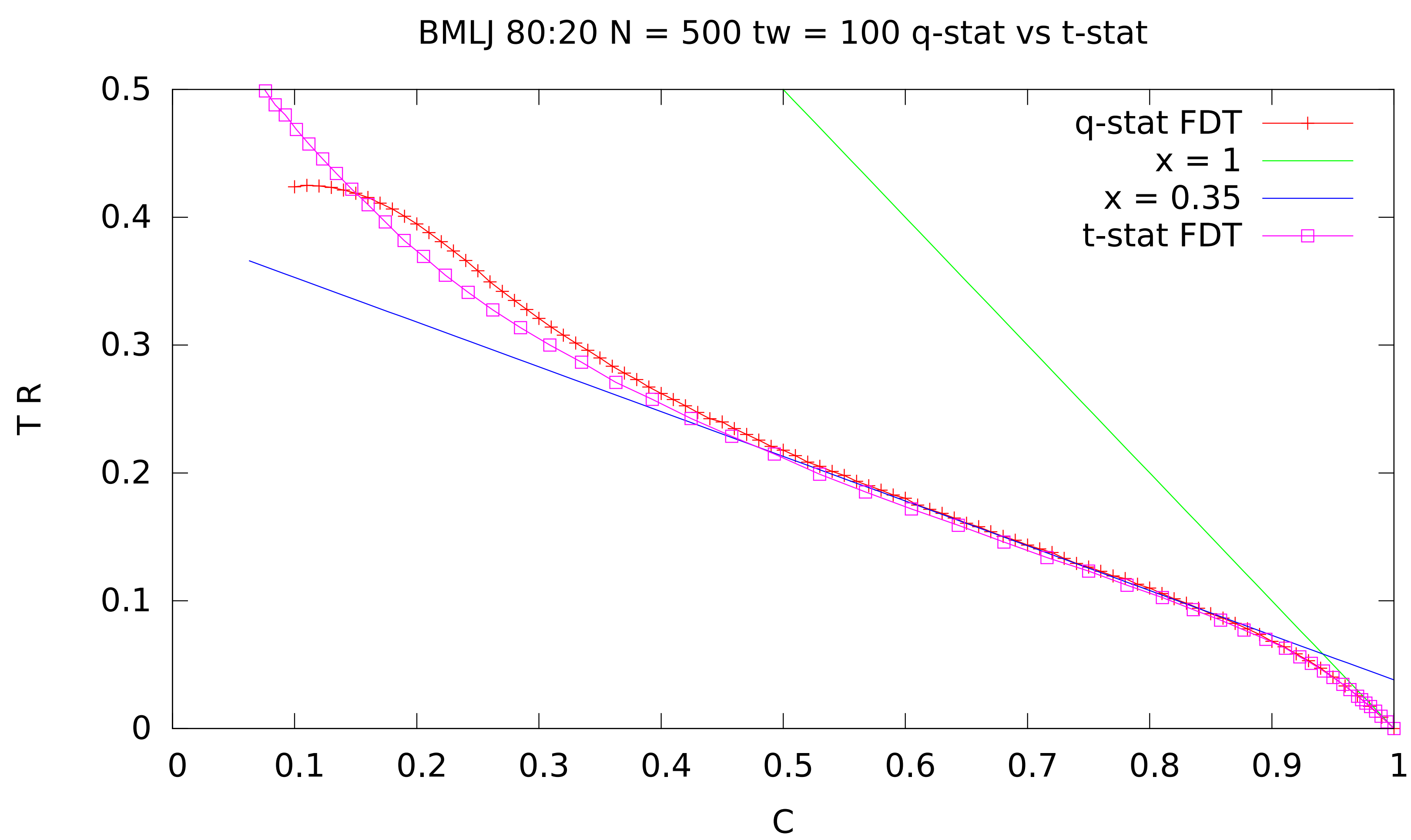

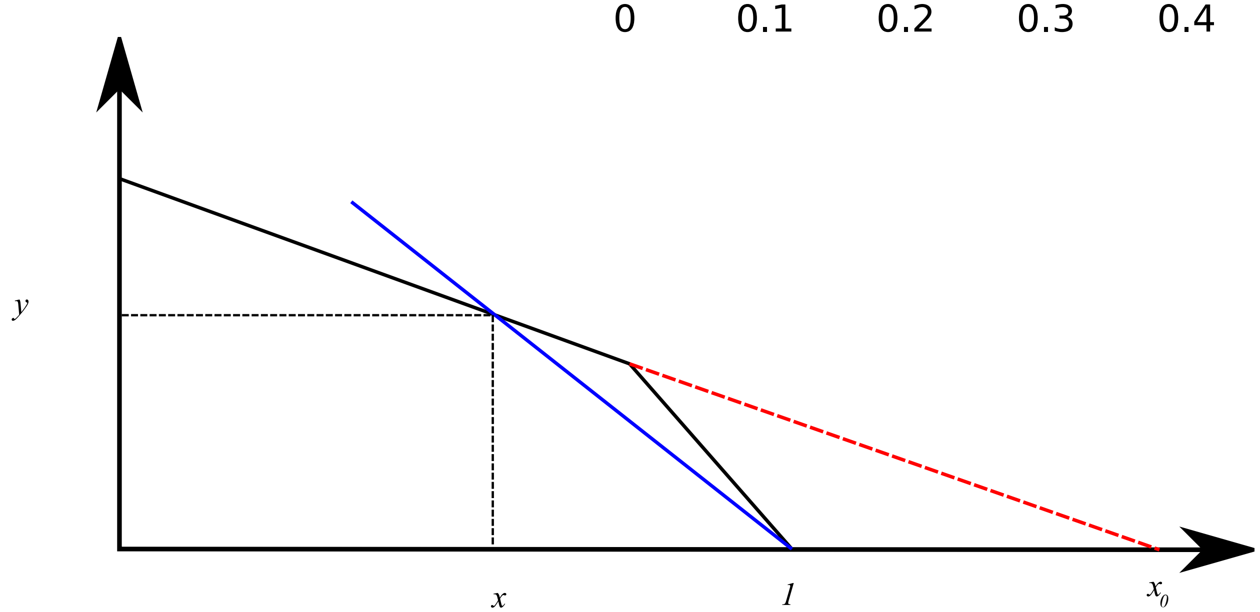

$$\frac{y}{1-x} > \frac{y}{x_0 - x}$$

Back to Numerical
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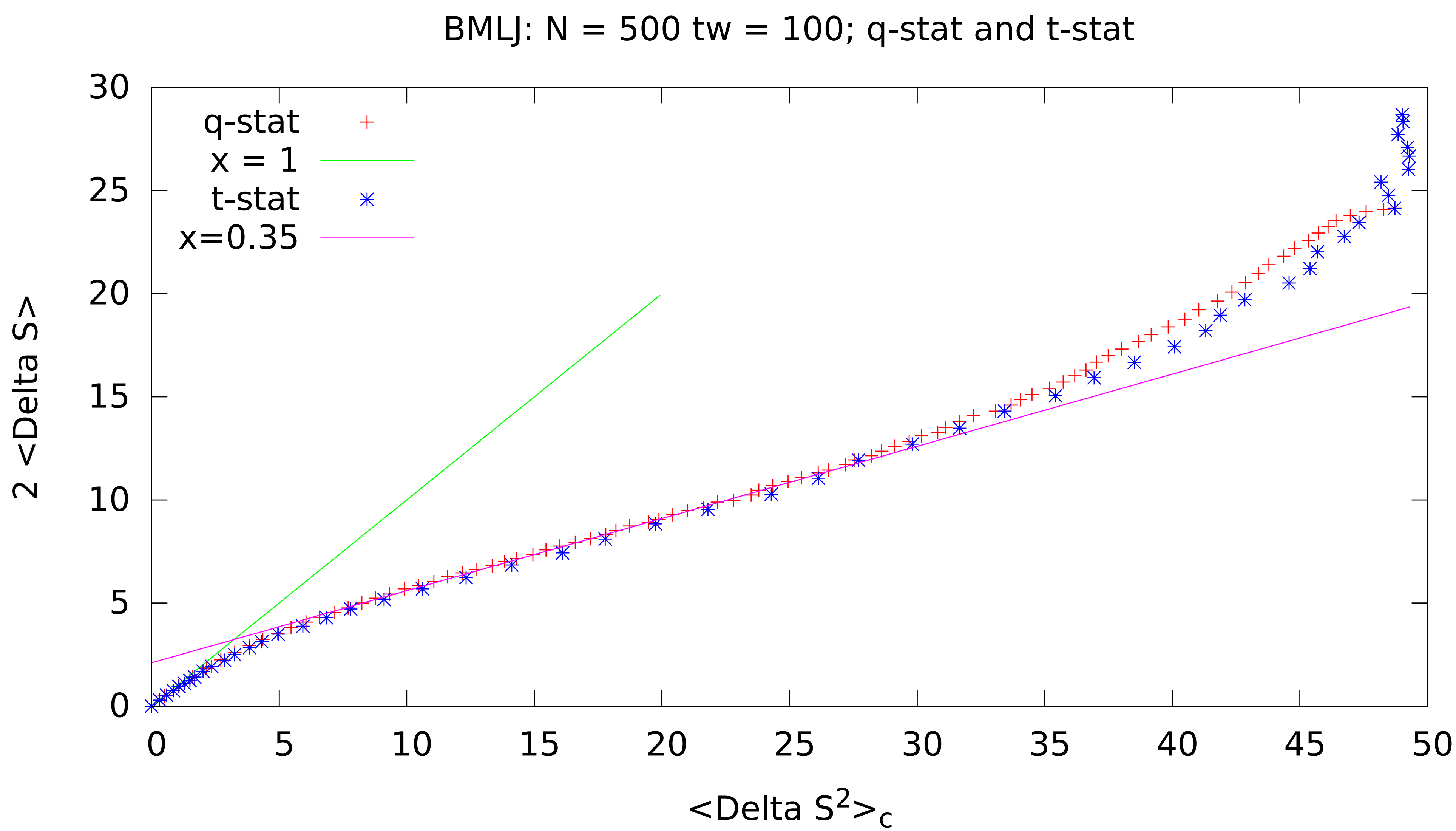

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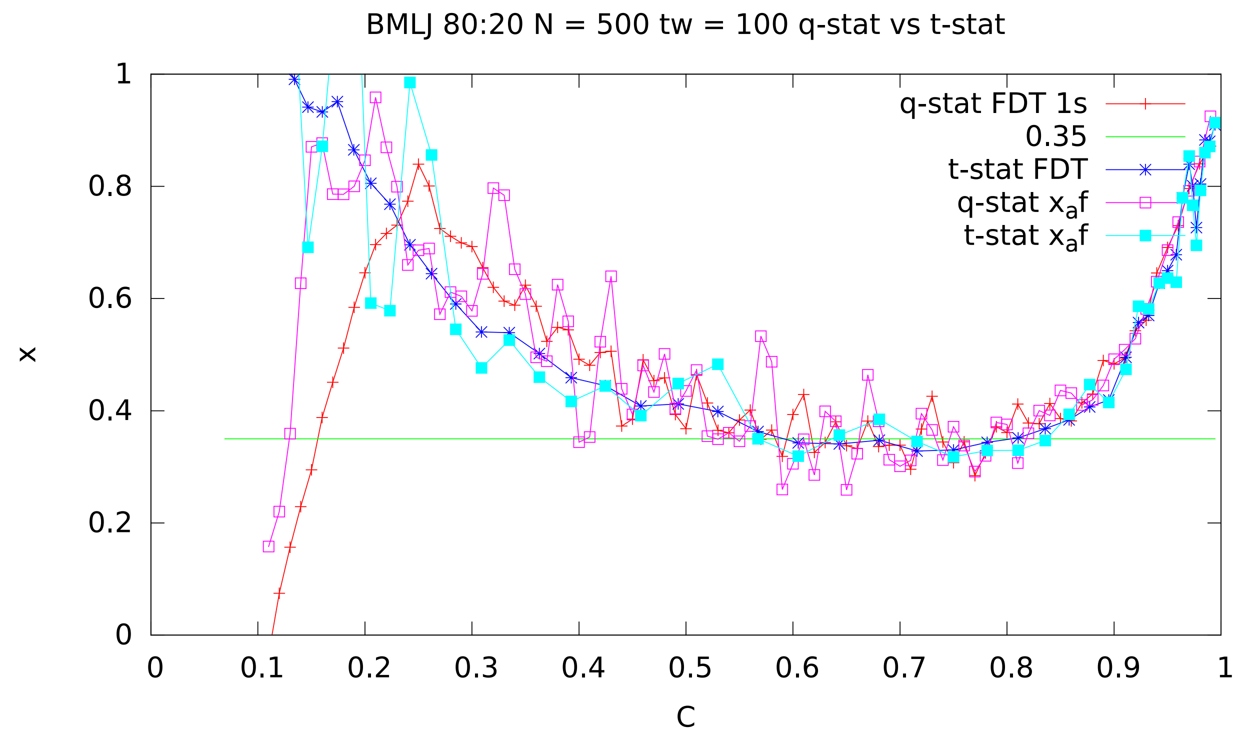
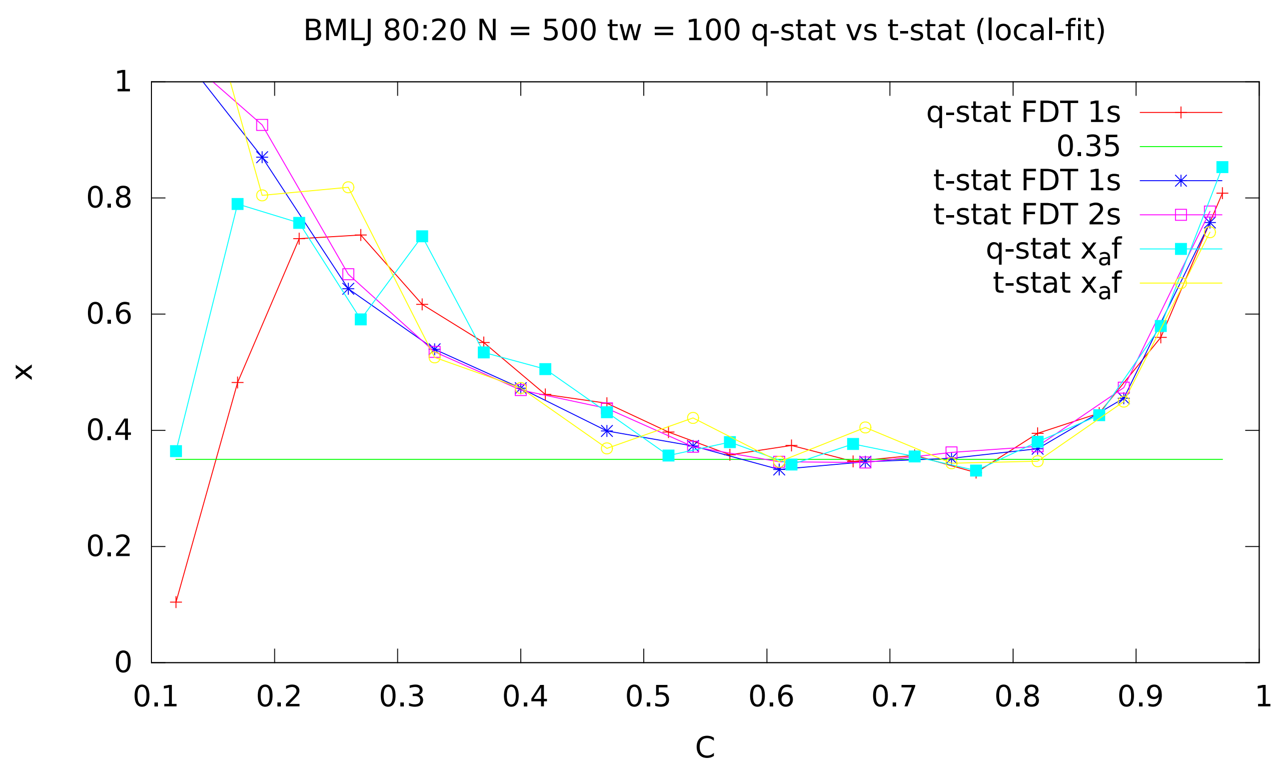
<u>Local slopes</u>





Conclusions

Conclusions

Auguri

Grande Capo!

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