Simulating rare events in dynamical processes

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Computation of transition trajectories and rare events in non-equilibrium systems

Outline

- Fluctuations of chaoticity in dynamical systems

- Large deviation functions in interacting particle systems

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Fluctuations in dynamical systems

Phase space is non uniform

- KAM Theorem, Arnol'd Web
- Laminar vs turbulent flows
- Solitons and Breathers in a non-linear crystals
- Regular orbits in planetary systems

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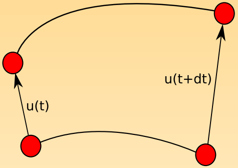
Fluctuations of chaoticity

- Sensitivity to initial conditions
- Fluct. of Lyapunov exponents [Ruelle 78, Benzi 84, Grassberger 88]
- Lots of theory, few applications in physics

Lyapunov exponents

- Divergence of nearby trajectories
- $|u(t)| \equiv |u(0)| \exp[\lambda(t) t]$
- $\lambda(t) \underset{t \to \infty}{\sim} \lambda$: Lyapunov exponent
- Fluctuations $\longrightarrow$ $P(\lambda, t)$

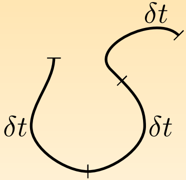


$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$$

$$\dot{\mathbf{u}} = \frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}} \mathbf{u}$$

A large deviation problem $P(\lambda, t) = \exp[S(\lambda, t)]$

- Total time $t \gg \delta t \gg$ correlation time τ;
- $\frac{|u(t)|}{|u(0)|} \equiv e^{\lambda t} = \prod_k \frac{|u(k\delta t)|}{|u((k-1)\delta t)|} = e^{(\lambda_1 + \cdots + \lambda_{t/\delta t})\delta t}$



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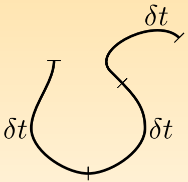

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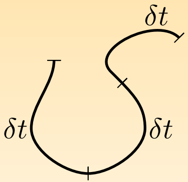

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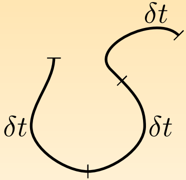

$$P(\lambda, t) \simeq \mathrm{e}^{ts(\lambda)}$$

- The larger the time, the more peaked $P(\lambda, t)$

Numerical methods

Sample $P(\lambda, t) \simeq \mathrm{e}^{ts(\lambda)}$

- Frequency map analysis (Laskar 93)
- Spectral analysis (Sepulveda, Badi, Pollak 95)
- Fast Lyapunov indicator (Lega 96)
- Correlation functions (Pollner, Vattay 96)
- Fast Lyapunov indicator (Froeschlé, Lega, Gongzi 97)
- SALI (Skokos 01)

Random sampling $\longrightarrow$ λ^* s.t. $s'(\lambda^*) = 0$

Grid $\longrightarrow$ Low dimension only

The thermodynamics of trajectories

- Give a weight $\exp(\alpha\lambda t)$ to each trajectory

$$P_\alpha(\lambda,t) = \frac{1}{Z_\alpha} P(\lambda,t) \mathrm{e}^{\alpha\lambda t} \qquad\qquad Z_\alpha(t) = \langle \mathrm{e}^{\alpha\lambda t} \rangle$$

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- Trajectories with $\lambda^*(\alpha)$ dominate

$s'(\lambda^*) = -\alpha$ differs from $s'(\lambda^*) = 0$

Temperature and entropy

$$P_\alpha(\lambda,t) \underset{t\to\infty}{\propto} \mathrm{e}^{t[s(\lambda)+\alpha\lambda]} \qquad Z_\alpha(t) = \langle \mathrm{e}^{\alpha\lambda t}\rangle$$

- $\lambda \leftrightarrow$ Macrostate

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- $\lambda \leftrightarrow$ Macrostate
- $\alpha \leftrightarrow$ Temperature
  - $\alpha > 0$ favors chaos
  - $\alpha < 0$ favors order
- Z_α is a dynamical partition function
- $\mu(\alpha) = \frac{1}{t}\log[Z_\alpha]$ is a dynamical free energy

Language of dynamical transitions (e.g. transition to turbulence)

Lyapunov Weighted Dynamics [Nat. Phys., 3, 203 (2007)]

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- For each copy, we compute $\left(\frac{|u(t+dt)|}{|u(t)|}\right)^{\alpha} \equiv \exp(\alpha\lambda \mathrm{d}t)$
- Each copy is replaced by [on average] $\exp(\alpha\lambda \mathrm{d}t)$ copies

At time t, 1 clone $\longrightarrow \exp(\alpha\lambda t)$ copies

$$\mathcal{N}(t)/\mathcal{N}(0) \simeq \langle \exp(\alpha\lambda t) \rangle \sim \exp[\mu(\alpha) t]$$

Two important 'tricks'

1. To prevent the number of clones to diverge or vanish

   $\longrightarrow$ overall cloning rate $R(t+dt) = \mathcal{N}(t)/\mathcal{N}(t+dt)$

   $\langle \exp(\alpha \lambda t) \rangle \sim \exp[\mu(\alpha) t] = \prod_t R(t)$

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2. To prevent degeneracy of clones

   $\longrightarrow$ small noise:

   - when we replicate the clones
   - to the dynamics

An integrable case : The double well potential

Localizing the separatrix

$$H(q,p) = \frac{p^2}{2} + (1-q^2)^2$$

LWD with $\alpha = 1$

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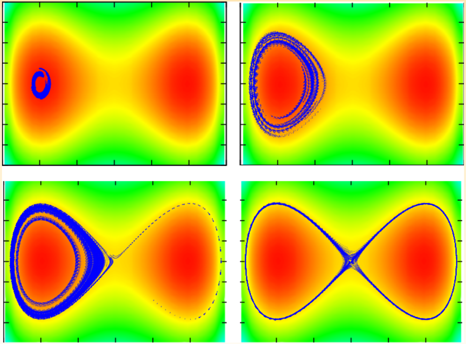

A toy model to study the transition to Chaos

The Standard Map

- $p_{n+1} = p_n - \frac{k\delta}{2\pi} \sin(2\pi q_n) \qquad q_{n+1} = q_n + \delta p_{n+1}$
- Chaoticity increases with k, δ

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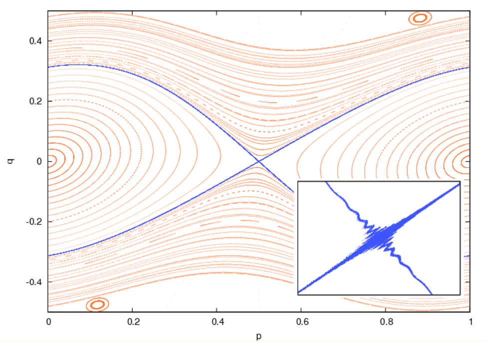
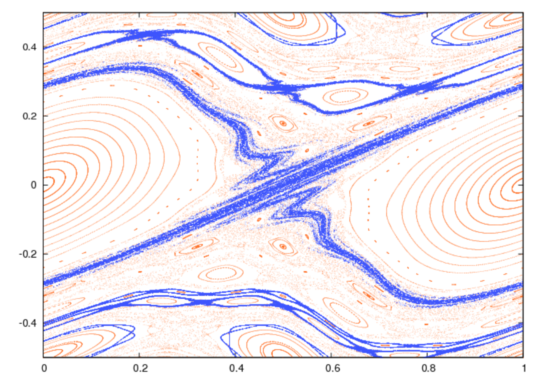
Almost Integrable Case ($\delta = 0.45,\ k = 1$); LWD with $\alpha = 1$

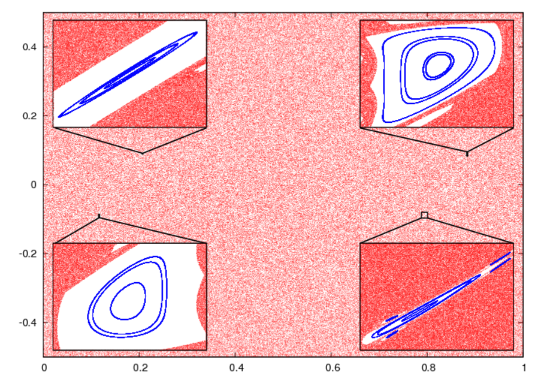


A mixed case



$k = 1,\ \delta = 1,\ \alpha = 1$ LWD $\alpha = 1$

Integrable islands in a chaotic sea

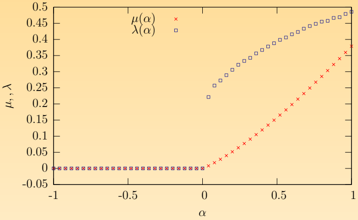


$k = 7.8,\ \delta = 1,\ \alpha = -1$ LWD $\alpha = -1$

Dynamical free energy

$\mu(\alpha) = \frac{1}{t}\log(Z_\alpha)$

$\lambda(\alpha) = \mu'(\alpha) = Z_\alpha^{-1}\int \mathrm{d}\lambda\,\lambda\,P(\lambda)\,\mathrm{e}^{\alpha\lambda t}$



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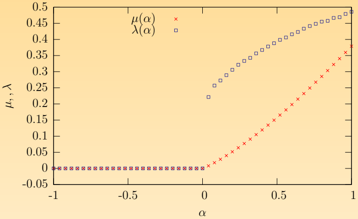

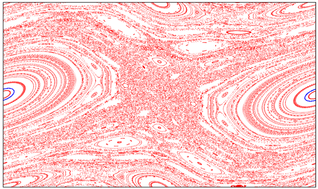

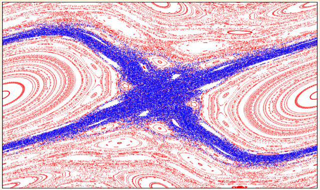

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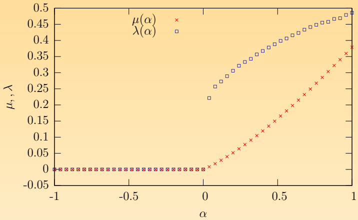
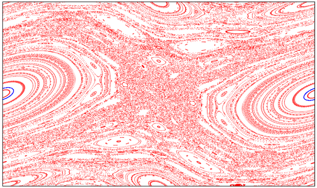
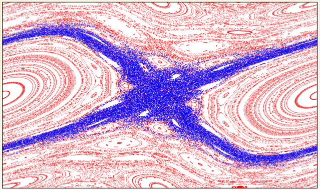






First order transition point

The Fermi Pasta Tsingou Ulam chain

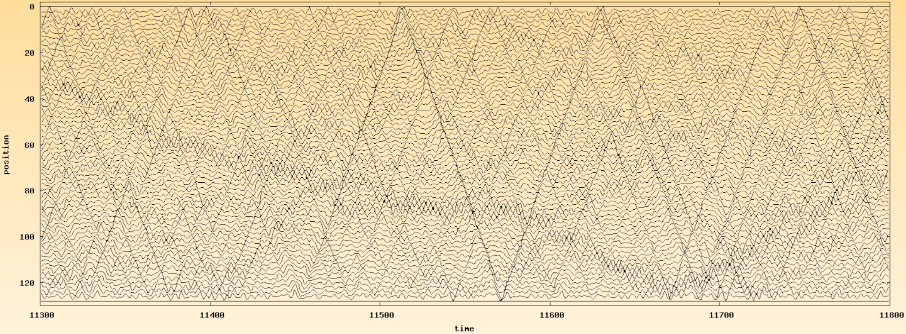
- Chain of non-linear oscillators

$$H = \sum_{i=1}^{N} \left(\frac{1}{2} p_i^2 + \frac{1}{2} (x_i - x_{i+1})^2 + \frac{\beta}{4} (x_i - x_{i+1})^4 \right)$$

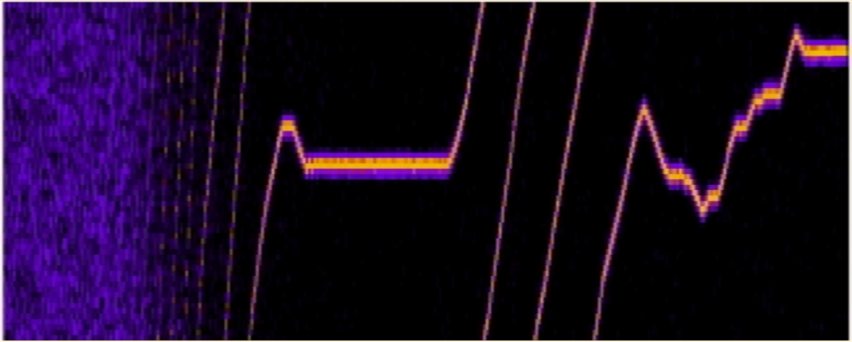
- $\beta = 0 \leftrightarrow$ uncoupled fourier modes

$$\omega_k = 2 \sin \left(\frac{\pi k}{N} \right)$$

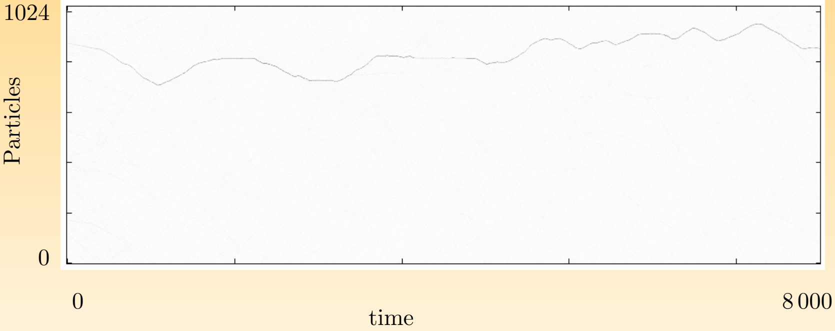
Equilibrium



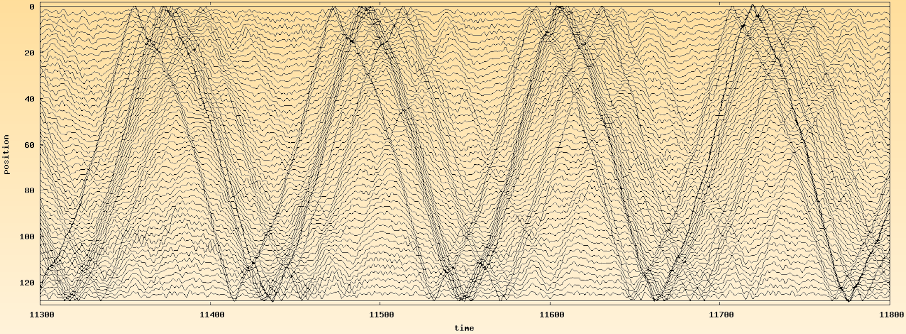
LWD with $\alpha = 5N$ (N=128)



LWD with $\alpha = 5N$ (N=1024)



LWD with $\alpha \ll -1$



Phase transition? Scaling with N...

- How do the fluctuations of λ scale with N?

$$P(\lambda,t) \simeq \mathrm{e}^{tN^{\xi}s(\lambda,t,N)}; \qquad s(\lambda,t,N) \underset{N,t\to\infty}{\sim} \mathcal{O}(1)$$

$$Z_\alpha = \int \mathrm{d}\lambda \mathrm{e}^{\alpha\lambda t + tN^{\xi}s(\lambda)}$$

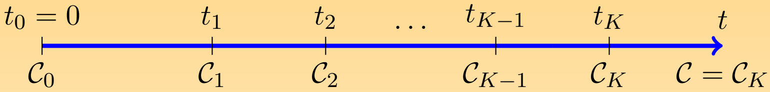
- Select λ^*: $s'(\lambda^*) = -\frac{\alpha}{N^{\xi}} \underset{N\to\infty}{\to} 0$

- Need to find the good scaling (hard !)
  see [Kuptsov& Politi PRL 2011]

Conclusion Part I

- Numerical method to sample the fluctuations of λ
- Detect atypical trajectories
- Study dynamical phase transition (turbulence !)
- [J. Tailleur, J. Kurchan, Nature Physics, 3, p. 203-207, (2007)]

Dynamical free energies



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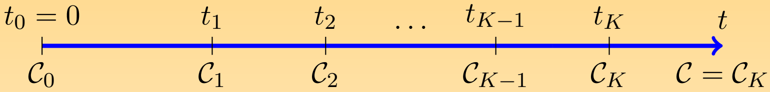

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- Observable $Q = \sum_k Q_{\mathcal{C}_k,\mathcal{C}_{k+1}} \equiv q \cdot t$

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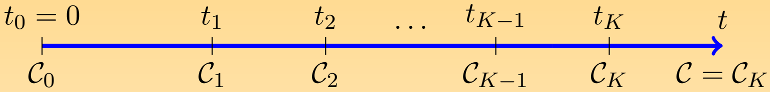

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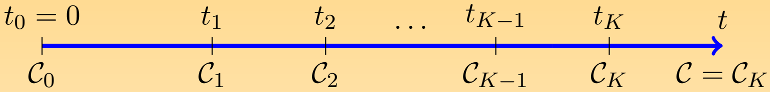

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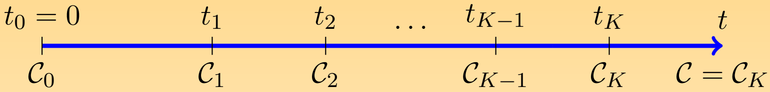

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$\psi(\beta)$ is a dynamical free energy

How can one compute it ?

Computation of $Z(\beta) = \langle e^{-\beta Q} \rangle$

- Transition rates $W(\mathcal{C} \to \mathcal{C}')$

$$\partial_t P(\mathcal{C}) = \sum_{\mathcal{C}' \neq \mathcal{C}} W(\mathcal{C}' \to \mathcal{C}) P(\mathcal{C}') - r(\mathcal{C}) P(\mathcal{C})$$

- Escape rate $r(\mathcal{C}) = \sum_{\mathcal{C}' \neq \mathcal{C}} W(\mathcal{C} \to C')$

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- $(r_\beta(\mathcal{C}) - r(\mathcal{C})) \hat{P}_\beta(\mathcal{C}) \longrightarrow \sum_{\mathcal{C}} \hat{P}_\beta$ not conserved
- $Z(\beta) = \sum_{\mathcal{C}} \hat{P}_\beta(\mathcal{C}, t)$

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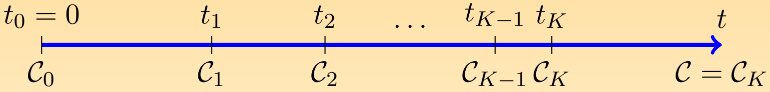
- Population dynamics: $Z(\beta, t) = \sum_{\mathcal{C}} \hat{P}_\beta(\mathcal{C}, t) = N(t)/N(0)$

Population dynamics

- N copies of the system evolve with rates W_β



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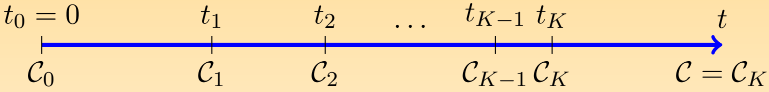

- Cloning term $\propto e^{(t_{k+1}-t_k)[r_\beta(\mathcal{C}_k)-r(\mathcal{C}_k)]}$

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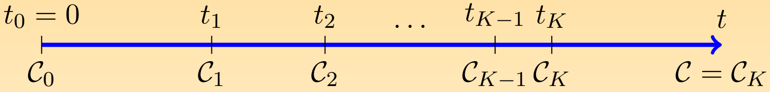

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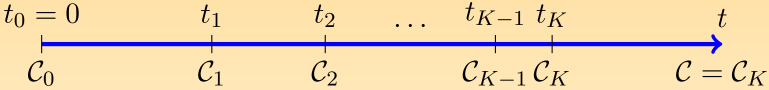

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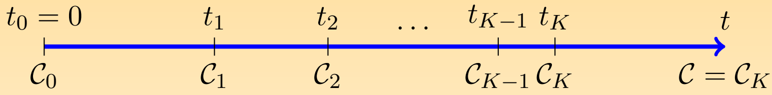

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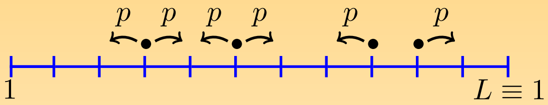
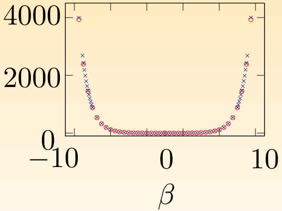
$$\mathbf{Z}(\beta) = \prod_{\mathbf{k}} \mathbf{R_k} \qquad \psi(\beta) = \lim_{\mathbf{t}\to\infty} \frac{\mathbf{1}}{\mathbf{t}} \sum_{\mathbf{k}} \log \mathbf{R_k}$$

SSEP



- LDF of the particle current J: $\frac{\psi_J(\beta)}{L}$ $(N = 200\ L = 400)$



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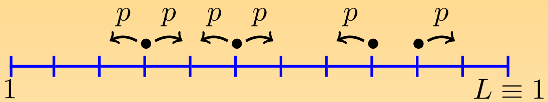

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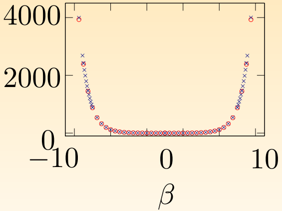

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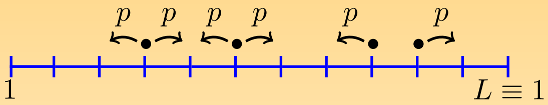
SSEP



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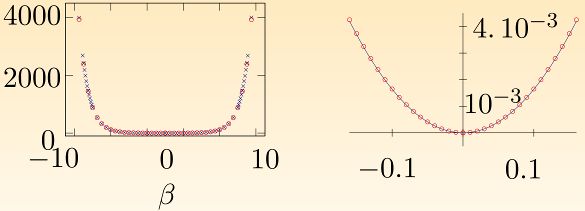

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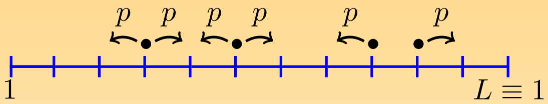

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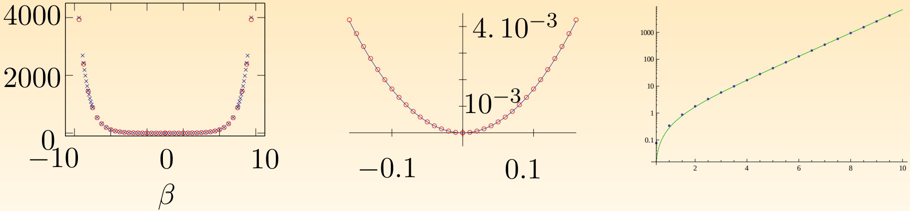

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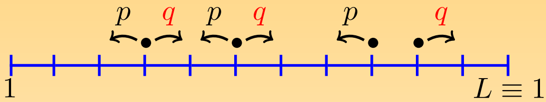

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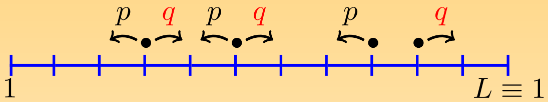

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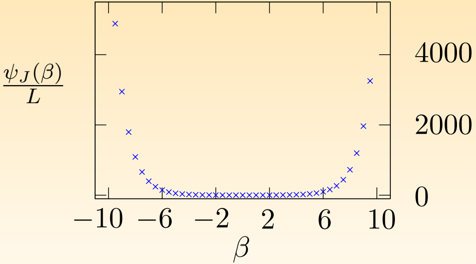

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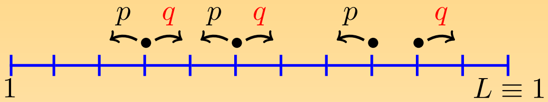

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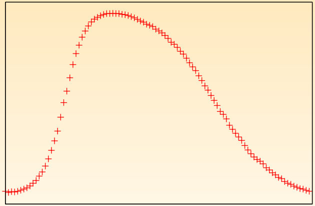
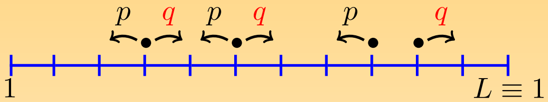


Small current

ASEP



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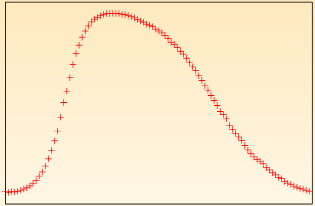

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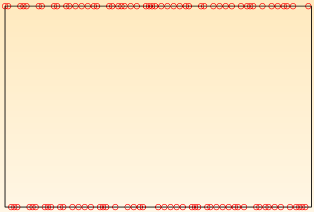

Large current

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