Statistical Mechanics of Extreme Events

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- Extreme Events
- Gallavotti-Cohen Symmetry
- Classical Condensation Phenomena
- Breakdown of GCS
- Conclusions

UFF, Niteroi, 30/09/2009

1. Extreme Events

Various types:

• Rare events --> larger or smaller than some (big) threshold

• Extremal events --> largest or smallest in a given set

• Records --> larger or smaller than any previous

Interesting in stochastic dynamics (unpredictable):

- Fun (sports, Guiness book,…)
- Danger (weather, earthquakes, epileptic seizures,…)
- Money (lotto jackpot, insurance claims,…)
- Curiosity (how often, why, …)
- …

Difficult to handle mathematically:

- Described by tails of probability distribution --> poor statistics
- Normally interested in peak position (mean (LLN) and variance (CLT))
  --> machinery not so well-developed for tails

==> Statistical description by extreme value theory

Application to empirical data problematic:

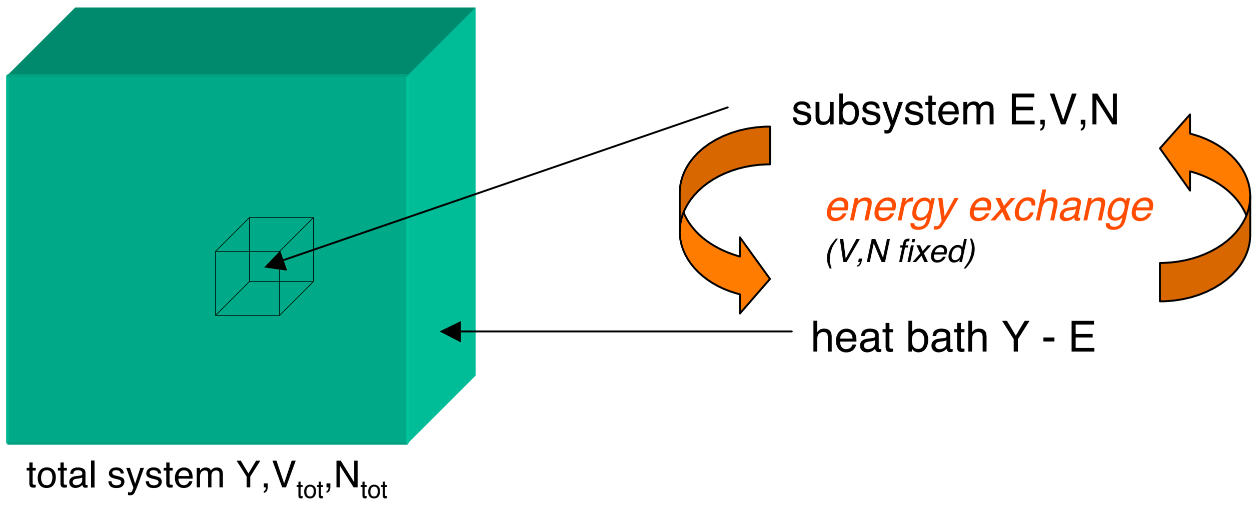
- approximations difficult because of poor convergence to limiting distributions
- no insight in mechanisms of origin
- no prediction and prevention

New: Interesting in Statistical Mechanics:

➢ Conceptual (Foundations of Stat Mech)
➢ Study causes and effects

Not so new: Extreme events in Equilibrium Stat Mech

Canonical ensemble = subsystem in heat bath



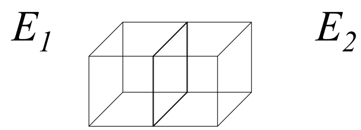
statistical weight of subsystem:

$$w(E) = \mathrm{e}^{-\beta E}$$

$\beta = S'(E)$: Inverse T of heat bath

Boltzmann distribution

- origin of exponential: statistical independence of subsystems



$$w_{12}(E_1 + E_2) = w_1(E_1)w_2(E_2)$$

- probability $p(T,V,N)$ to find microstate of subsystem with energy E: $p = w(E)/Z$

partition function

$$\begin{aligned} Z(T,V,N) &= \sum_{microstates} \mathrm{e}^{-\beta E} \\ &= \sum_E \Gamma(E,V,N)\mathrm{e}^{-\beta E} \\ &= \sum_E \mathrm{e}^{-\beta(E-TS)} \end{aligned}$$

- sharp peak at some U (mean energy of subsystem) → Helmholtz free energy

$$F(T,V,N) = -kT \ln Z = U - TS$$

- second equation: Legrende transformation $U(S,V,N) \leftarrow\rightarrow F(T,V,N)$

- extremal principle: F takes minimal value for given set of system parameters

- extensivity: $F = V f(T,\rho)$

Microscopic viewpoint (large deviation theory):

- Consider particle energies E_i in subsystem

- Large deviation theory: (i) $P(E) = \text{Prob}[\ \Sigma_i E_i = E] \sim e^{-A(E)}$

  (ii) $< e^{-\beta E} > \sim e^{-B(\beta)}$

- A,B extensive, satisfy extremal principle $A(E) = \max_\beta [\ B(\beta) - \beta E\ ]$

- Microcanonical ensemble: $P(E) \sim \Gamma(E)$ ==> $A(E) = - S(E)$

- $B(\beta) = - \ln (Z) = \beta F(\beta)$

==> choosing β that maximizes S yields Legendre transformation $F = U - TS$

2. Gallavotti-Cohen Symmetry

Far from equilibrium:

- no generally applicable ensemble

- no large deviation theory (in general)

- but: generally valid Fluctuation Theorems

Gallavotti-Cohen
[Evans, Cohen, Morris ‘93,
Gallavotti, Cohen ‘95]

$$\frac{p(-\sigma,t)}{p(\sigma,t)} \sim e^{-\sigma t}$$

- mathematical asymptotic theorem for certain dynamical systems

- no specific information about entropy production σ

- allows (statistical) prediction of negative entropy production (extreme)

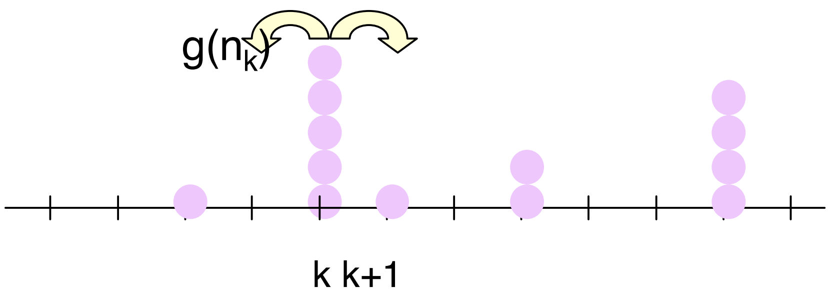
Stochastic dynamics: [Kurchan '98, Lebowitz, Spohn '99, Harris, G.M.S. '07]

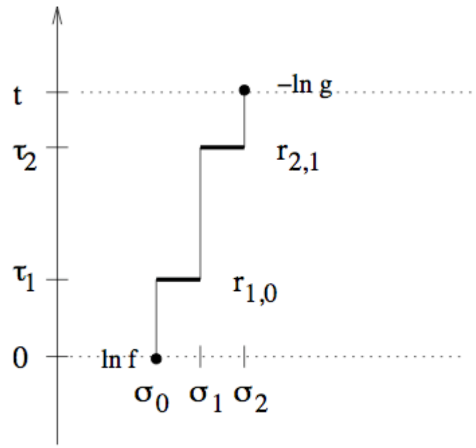
Consider stochastic process with set of configurations σ

- Trajectory (realization) $\{\sigma\} = \{\sigma_0, \sigma_1, \ldots \sigma_n\}$ with random jump times τ_i

- Measure some quantity r associated with each transition (energy transfer, mass transfer,…) --> (antisymmetric) $r_{\sigma',\sigma}$ for transition from σ --> σ'

- Example: Particles hopping on a lattice



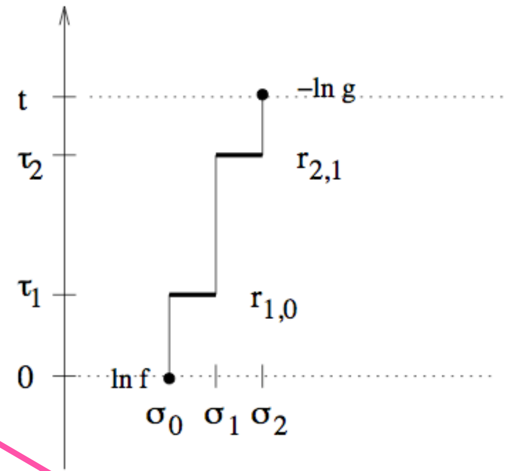


- r = +/- 1 for jump across k,k+1:

==> sum of all r along trajectory = integrated particle current

Associate some physical quantity with initial state (ln f) and final state (- ln g)
(Example for equilibrium: energy of initial and final configuration)

- Trajectory functional (measurement)



$$\mathcal{X}_F(t, \{\sigma\}, f, g) = \mathcal{J}_r(t, \{\sigma\}) + \mathcal{B}(f, g)$$

- Integrated current of trajectory (sum of all r) plus boundary parts

- boundary provide appropriate statistical weight in functional

- choice of f,g depends on experimental setting!

- no restriction to any equilibrium condition

Consider instantaneous entropy production [Seifert '05]

$$r^{(1)}_{\sigma',\sigma}(\tau) = \ln\left[\frac{w_{\sigma',\sigma}(\tau)}{w_{\sigma,\sigma'}(\tau)}\right]$$

Then trajectory functional = entropy change in environment + boundary terms

- Detailed balance (equilibrium process): $r = \Delta E / (kT)$

==> Thermal systems: $\Delta S_{env} = Q/T$

- Otherwise still well-defined through transition rates

- Stochastic particle systems: proportional to particle current

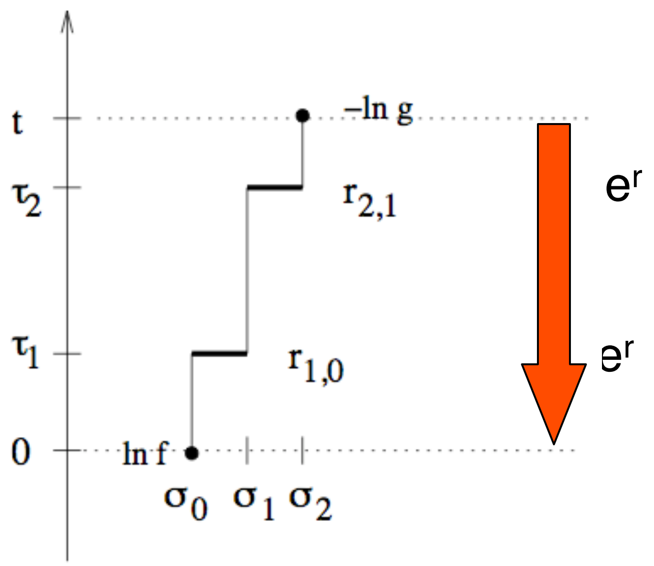
- Entropy production extensive in time (~t for each trajectory at large times)

Call corresponding trajectory functional R

- Consider generating function $< e^{-\lambda R} >$ ==> gives weight $e^{-\lambda r}$ to each transition

- TIME REVERSAL

transition rates of reversed process
= original rates x e^{r}



$$w(\sigma,\sigma') = w(\sigma',\sigma) \times \frac{w(\sigma,\sigma')}{w(\sigma',\sigma)}$$

$$= w(\sigma',\sigma)\, e^{r(\sigma',\sigma)}$$

==> weight $e^{(1-\lambda)r}$ to each transition

(reversal of entropy production in each elementary step of each trajectory)

- extra factor for as many transitions as in initial (forward) process

$$< e^{-\lambda R} >^F \; = < e^{-(1-\lambda)R} >^B$$

(includes interchange of boundary terms)

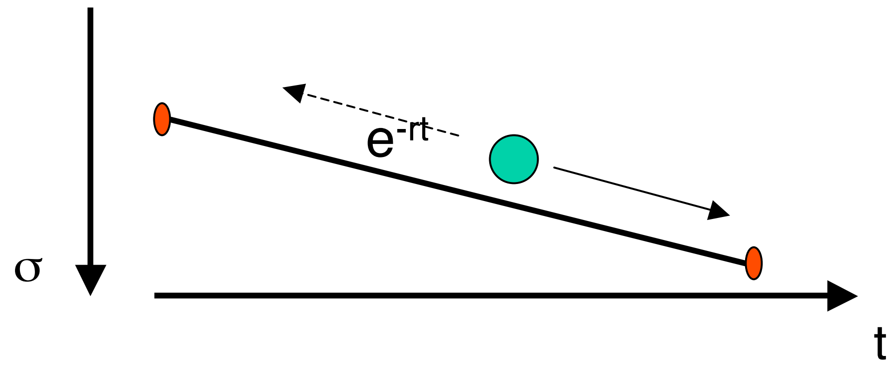
- Large deviation property (extensivity of R for t large)

$$< e^{-\lambda R} > \sim e^{-t g(\lambda)}$$

- or equivalently $g(\lambda) = g(1-\lambda)$ + ~~(boundary terms)/t~~

- Legrende transformation

==> Gallavotti-Cohen symmetry



Conceptually important

==> far-from-equilibrium generalization of Onsager relations
==> boosted the whole field of fluctuation theorems

• GC is asymptotic ==> one can use it to extrapolate

• Numerical tests can be performed in lattice gas models

What is the question?

Rigorous in lattice models with finite local state space (exclusion processes)

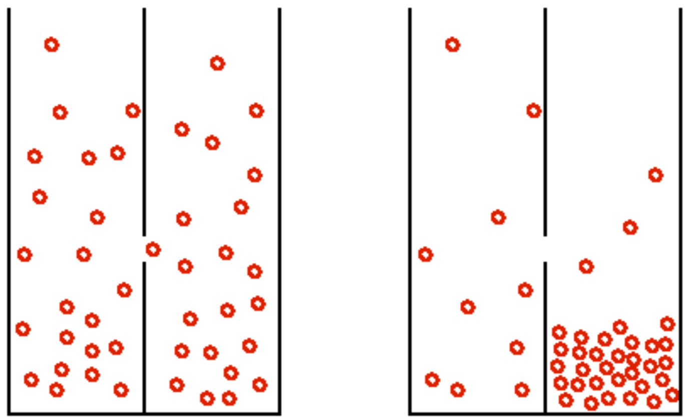
==> Is GCS valid, if we violate this condition?

3. Classical condensation phenomena

Granular shaking

N=100 plastic particles in box with two compartments separated by wall with slit [Schlichting and Nordmeier '96, Eggers '99, Lohse '02]

Gaseous state



Condensed state

$T > T_c$ $T < T_c$

i) Strong shaking (fixed amplitude, 50 Hz frequency): ➔ Equal gaseous distribution

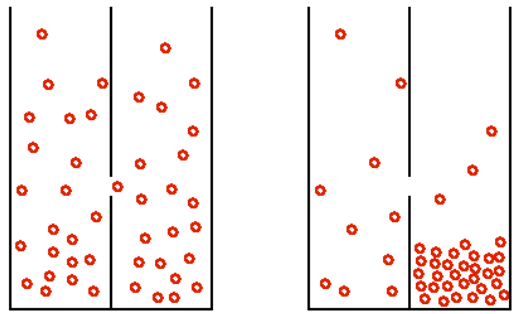
ii) Moderate shaking (same amplitude, 30 Hz): ➔ Condensation (with SSB)

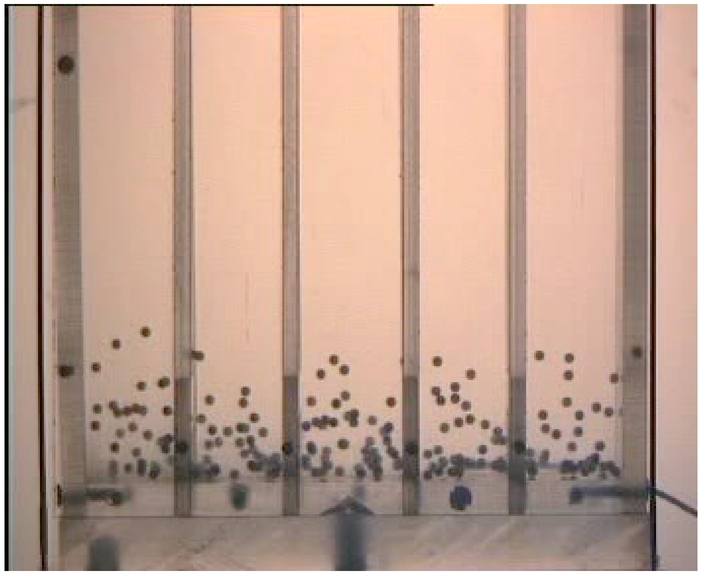
Effective, frequency-dependent temperature leads to phase transition

Granular Clustering: L=5

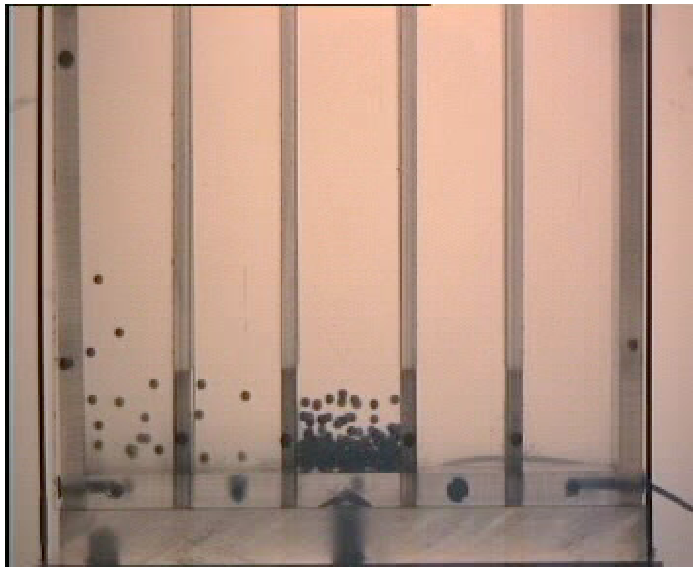
http://stilton.tnw.utwente.nl/people/rene/clustering.html

Detlef Lohse, Devaraj van der Meer, Michel Versluis,
Ko van der Weele, René Mikkelsen





Time t = 0…12 sec

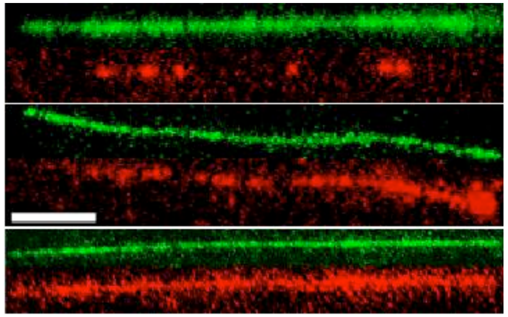


t approx. 1 min

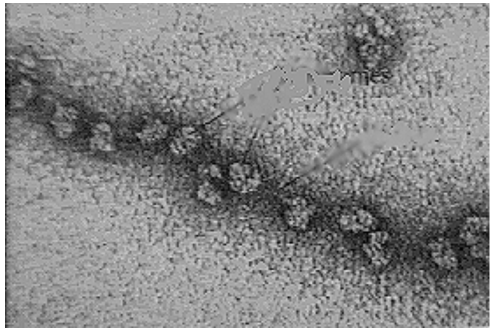
Single File Diffusion:

SFD: Quasi <u>one-dimensional diffusion</u> without passing

- molecular diffusion in zeolites
- colloidal particles in narrow channels
- transport in carbon nanotubes
- molecular motors and ribosomes
- gel electrophoresis
- automobile traffic flow



Three phases of kinesin transport (Chodhury et al.)



Polyribosome:
[http://omega.dawsoncollege.qc.ca/ray/protein/protein.htm

Condensation = traffic jam = phase separation

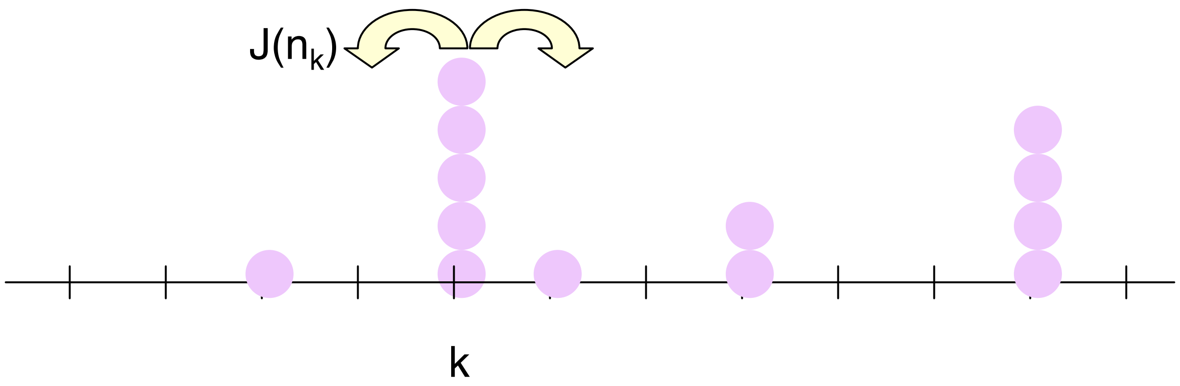
Other Complex Systems

- Network rewiring
- Accumulation of wealth

Condensation transition in the zero-range process

Zero-range process (ZRP) with symmetric nearest-neighbour hopping [Spitzer (1970)]

- Stochastic particle hopping model
- Cluster of size n (or length of domain) ⇔ occupation number in ZRP
- particle flux $J(n_k)$ between compartments (domains) ⇔ hopping rate in ZRP



Exact grand canonical stationary distribution [Spitzer, (1970)]

➔ Product measure with marginals P(n) and local partition function Z

$$P(\vec{n}) = \prod_{i \in \Lambda} P(n_i)$$

$$P(n) = \frac{1}{Z} z^n \prod_{k=1}^{n} J^{-1}(k), \qquad Z = \sum_{n=0}^{\infty} \tilde{P}(n)$$

- Fugacity z determines (fluctuating) density $\rho(z)$
- Well-defined for fugacities within radius of convergence z* (that depends on J)
- Canonical ensembles for any N by projection on fixed N
- Grand canonical ensemble: What happens if $\rho(z^*)$ is finite?

Spatially homogeneous systems

1) Asymptotically vanishing flux J(n) → 0: ➔ $z^*=0$ and hence $\rho_c = 0$

2) Consider generic case where for large n

$$J(n) = A\,(1 + b/n^{\sigma})$$

➔ radius of convergence of partition function: $z < z^* = A$

➔ at z^* one has finite density ρ_c for $\sigma < 1$

→ For $\sigma = 1$: ➔ $P(n) \sim 1/n^b$

$$\rho(z^*) = \begin{cases} \infty & \text{for } b \leq 2 \\ \rho_c = 1/(b-2) & \text{for } b > 2 \end{cases}$$

Interpretation of critical density for b>2 or $\sigma < 1$ for canonical ensemble:

- Above critical density all sites except one (background) are at critical density
- One randomly selected site carries remaining O(L) particles

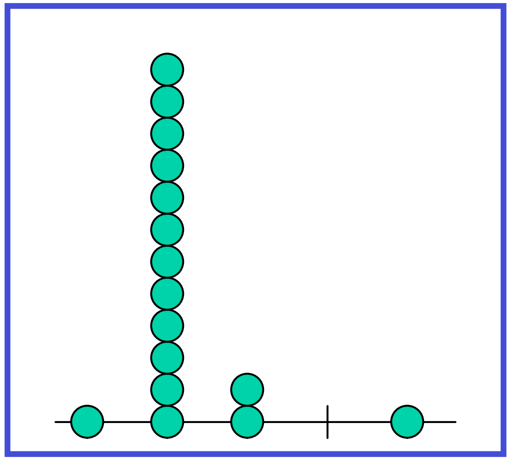
➔ Classical analogue of Bose-Einstein condensation
[Evans '96, Ferrari, Krug '96, O'Loan, Evans, Cates, '98, Jeon, March '00]

➔ Single random condensation site
[Grosskinsky, GMS, Spohn, '05, Ferrari, Landim, Sisko '07, Loulakis, Armendariz '08, Evans, Majumdar '08]]

➔ Continuous condensation transition ($\rho_{bg} = \rho_c$)

➔ Coarsening as precursor of condensation
[Grosskinsky, GMS, Spohn, '05; Godreche '05]

Generic model for classical condensation phenomena



4. Breakdown of GCS

Validity of Gallavotti-Cohen symmetry:

- It's a mathematical theorem (Good-bye, experimental physics?!)
- Related fluctuation theorems (Jarzinsky, Crooks, …) also rigorous…
- … but then, in which experimental system can you check the hypotheses of the theorem?

➔ In other words, how robust is GC symmetry? (Experimentalists, please return!)

Related fluctuation theorems experimentally well-confirmed in systems with

- relatively small number of degrees of freedom
- boundary terms matter for experimental time scales

Test of GCS for zero-range process

Exactly solvable for b=0

➔ large time regime accessible

➔ many degrees of freedom

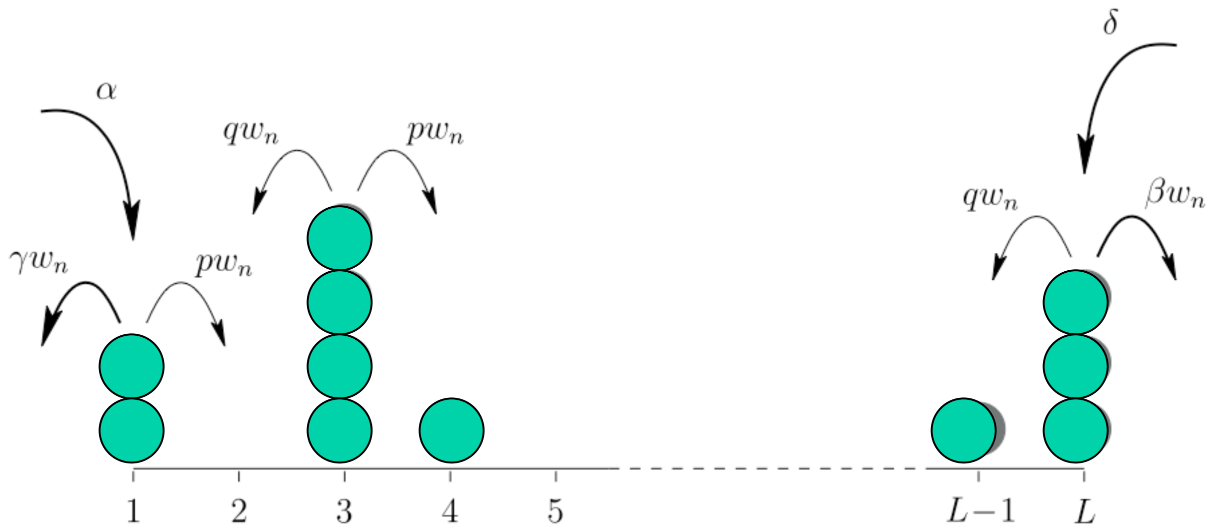
➔ unbounded state space

BUT:

- no condensation
- exponentially small probability for large occupation

} ??

Zero-range process with open boundaries [R.J.Harris, A. Rakos, G.M.S., '05-'07]



General case w_n arbitrary

Consider integrated current J_l across bond l,l+1, starting from some initial distribution

Take t large, study mean current $j_l = J_l / t$

➔ Compute large deviation function $e_l(\lambda)$ from generation function $\langle e^{-\lambda J_l}\rangle$

➔ Compute Legendre transform (probability to observe specific j_l

Exact result:

- write master equation in Quantum Hamiltonian form
- make product ansatz for groundstate to obtain lowest eigenvalue (LDF)

Large deviation function

$$e_0(\lambda) = \frac{(p-q)(\mathrm{e}^{\lambda}-1)\left[\alpha\beta\,(p/q)^{L-1}\,\mathrm{e}^{-\lambda}-\gamma\delta\right]}{\gamma(p-q-\beta)+\beta(p-q+\gamma)\,(p/q)^{L-1}}$$

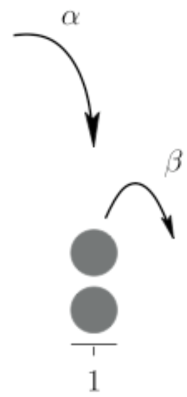
Legrende transform

$$\begin{aligned}\hat{e}_0(j) = {} & \frac{(p-q)[\alpha\beta(p/q)^{L-1}+\gamma\delta]}{\gamma(p-q-\beta)+\beta(p-q+\gamma)(p/q)^{L-1}} \\ & - \sqrt{j^2+\frac{4\alpha\beta\gamma\delta(p/q)^{L-1}(p-q)^2}{[\gamma(p-q-\beta)+\beta(p-q+\gamma)(p/q)^{L-1}]^2}} \\ & - j\ln\left[\frac{2\alpha\beta(p/q)^{L-1}(p-q)}{\gamma(p-q-\beta)+\beta(p-q+\gamma)(p/q)^{L-1}}\right] \\ & + j\ln\left[j+\sqrt{j^2+\frac{4\alpha\beta\gamma\delta(p/q)^{L-1}(p-q)^2}{[\gamma(p-q-\beta)+\beta(p-q+\gamma)(p/q)^{L-1}]^2}}\right]\end{aligned}$$

- satisfies GCS, independent of l, but boundary terms ignored

For boundary terms consider totally asymmetric ZRP, $w_n = 1$

- direct computation of complete LDF (no diagonalization --> inclusion of boundary terms)
- mapping to totally asymmetric simple exclusion process
- Bethe ansatz --> determinantal transition probabilities
- summation of determinants yields exact expression



current distribution
input bond

$$p_0(j,t) \sim \mathrm{e}^{-t[\alpha - j + j\ln(j/\alpha)]}$$

Poisson, by definition of process

output bond

$$p_1(j,t) \sim \begin{cases} \mathrm{e}^{-t[\alpha - j + j\ln(j/\alpha)]} & j < \beta \\ \mathrm{e}^{-t[\alpha - j + j\ln(j/\alpha)]} \times \mathrm{e}^{-t[\beta - j + j\ln(j/\beta)]} & j \geq \beta \end{cases}$$

- different from bond 0

- non-analytic behaviour at $j = \beta$

How can a mean current larger than exit rate be realized?

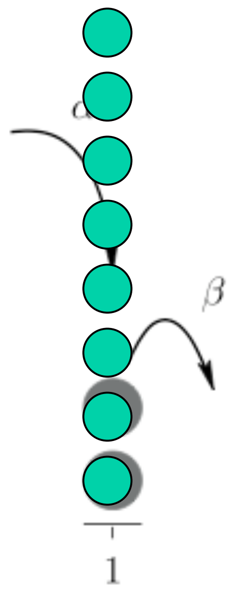
- requires previous build-up of large number of particles at site 1 (~t) followed by rapid extraction

- implies input/output are independent Poisson processes --> product form

- transient condensate through (rare) fluctuation

- causes non-analytic behaviour in tale of probability distribution (extreme events)

- mathematical: divergence of boundary term, possible because of unbounded local state



Conjecture for full lattice:

- Input bond

$$p_0(j,t) \sim \mathrm{e}^{-t[\alpha - j + j\ln(j/\alpha)]}.$$

- Bulk bonds, $l \neq 0, L$

$$p_l(j,t) \sim \begin{cases} \mathrm{e}^{-t[\alpha - j + j\ln(j/\alpha)]} & j < 1 \\ \mathrm{e}^{-t[\alpha - j + j\ln(j/\alpha)]} \times \mathrm{e}^{-t(1 - j + j\ln j)l} & j \geq 1. \end{cases}$$

- Output bond

$$p_L(j,t) \sim \begin{cases} \mathrm{e}^{-t[\alpha - j + j\ln(j/\alpha)]} & j < \beta \\ \mathrm{e}^{-t[\alpha - j + j\ln(j/\alpha)]} \times \mathrm{e}^{-t[(\beta - j + j\ln(j/\beta)]} & \beta \leq j < 1 \\ \mathrm{e}^{-t[\alpha - j + j\ln(j/\alpha)]} \times \mathrm{e}^{-t(1 - j + j\ln j)(L-1)} \times \mathrm{e}^{-t[\beta - j + j\ln(j/\beta)]} & j \geq 1. \end{cases}$$

- proof for small L by determinant formula obtained from Bethe ansatz

Exact expression for current distribution:

$$p_l(j,t) = \prod_{i=1}^{l+1} \mathrm{e}^{-t(v_i - j\ln v_i)}$$

$$\times \begin{vmatrix} D_0(jt,t) & D_0(jt-1,t) & \dots & D_0(jt-l+1,t) & D_{l+1}(jt-l,t) \\ D_0(jt+1,t) & D_0(jt,t) & \dots & D_0(jt-l+2,t) & D_{l+1}(jt-l+1,t) \\ \dots & \dots & \dots & \dots & \dots \\ D_0(jt+l,t) & D_0(jt+l-1,t) & \dots & D_0(jt+1,t) & D_{l+1}(jt,t) \end{vmatrix}$$

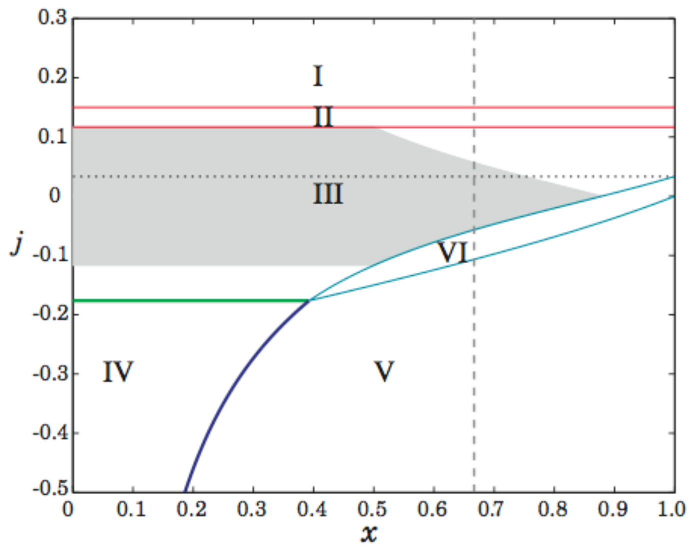
with elements

$$D_s(x,t) = \frac{1}{2\pi\mathrm{i}} \oint \mathrm{e}^{t/z} z^{x-1} \prod_{i=s+1}^{l+1} (1 - v_i z)^{-1}\, \mathrm{d}z.$$

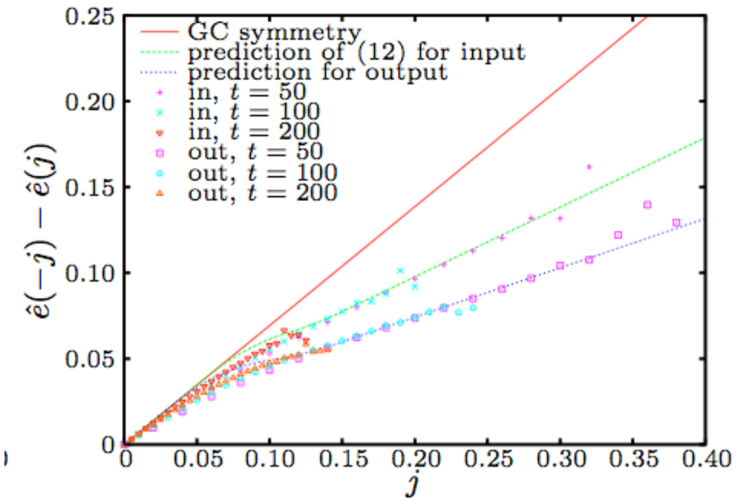
- evaluation by steepest descent for finite L

Back to partially asymmetric ZRP

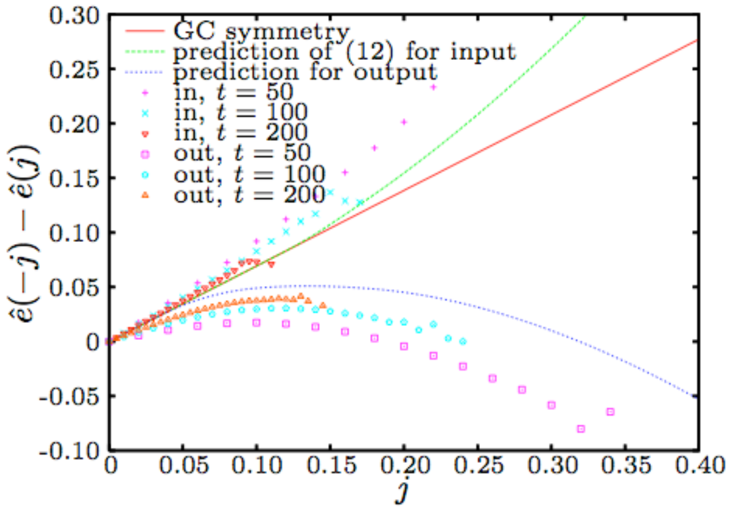
- take one site, b=0 for analytic calulation
- generate equilibrium with fugacity x
- change boundary parameters to non-equilibrium situation
- obtain different non-analyticities, depending both on j and x
- large deviation phase diagram
- validity of GCS only in restriced region, depending on preparation of system
- origin transient condensates



Simulation results for larger lattice:



steady state



empty lattice

- breaking of GCS persists
- measurable in Monte- Carlo simulations

5. Conclusions

Statistical Mechanics of extreme events yields:

- Fluctuation theorems through time reversal

- Gallavotti-Cohen symmetry may break down in “natural” setting

- Violation caused by transient condensation

==> dynamical mechanism underlying non-analytic change of extreme event identified

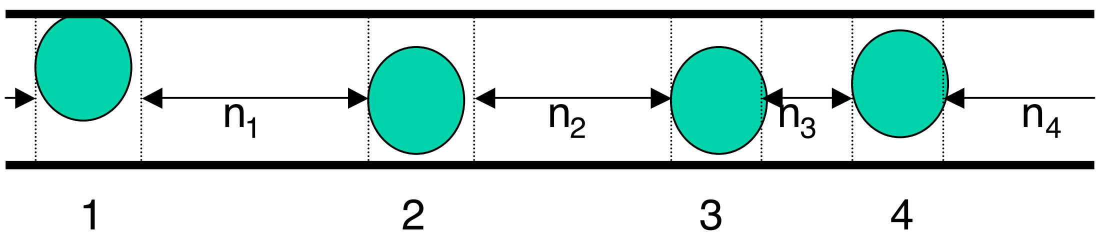
- Large deviation phase diagram

==> Large deviations, fluctuation theorems, extremal events should be studied together

==> Study of critical phenomena in extreme events

Mapping of single-file diffusion to zero range process:

- Label particles consecutively



- Map particle label to lattice site

- Map discretized interparticle distance to particle number