

# Statistical Mechanics of Extreme Events

Gunter M. Schütz

*Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany  
and  
Interdisziplinäres Zentrum für Komplexe Systeme, Universität Bonn*

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

IIT Kanpur, 30/01/2010

# 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, Guinness 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:

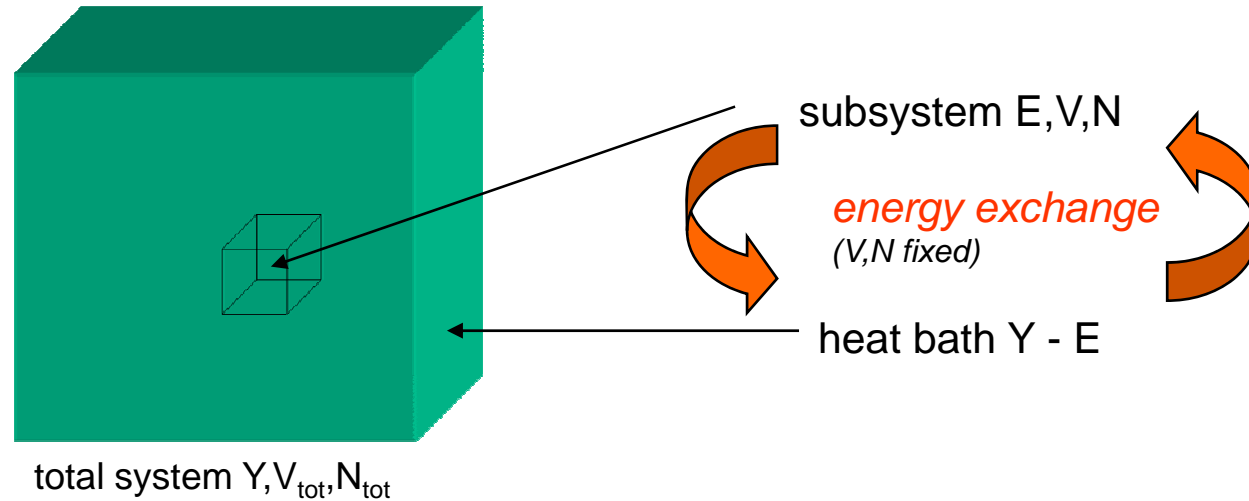
- approximations difficult because of poor convergence to limiting distributions
- **no insight in mechanisms of origin**
- no prediction and prevention

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



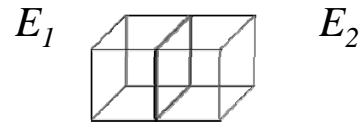
statistical weight of subsystem:

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

$\beta = S'(E)$ : 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

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

- sharp peak at some  $U$  (mean energy of subsystem)  $\rightarrow$  Helmholtz free energy

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

- second equation: Legendre transformation  $U(S, V, N) \leftrightarrow F(T, V, N)$
- 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)  $P(E) = \text{Prob}[\sum_i E_i = E] \sim e^{-A(E)}$   
(ii)  $\langle e^{-\beta E} \rangle \sim e^{-B(\beta)}$
- $A, B$  extensive, satisfy extremal principle  $A(E) = \max_{\beta} [ B(\beta) - \beta E ]$
- Microcanonical ensemble:  $P(E) \sim \Gamma(E) \implies A(E) = -S(E)$
- $$B(\beta) = -\ln(Z) = \beta F(\beta)$$
- $\implies$  choosing  $\beta$  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]

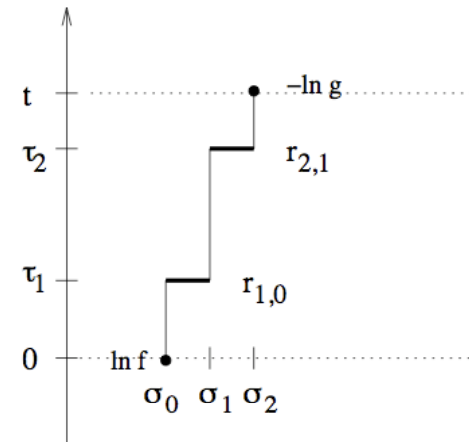
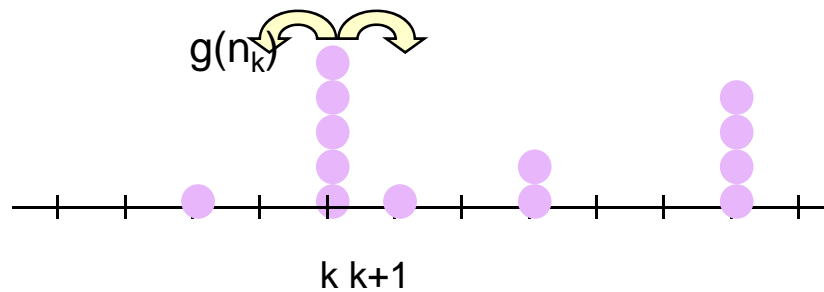
$$\frac{p(-\sigma, t)}{p(\sigma, t)} \sim e^{-\sigma t}$$

- mathematical asymptotic theorem for certain dynamical systems
- no specific information about entropy production  $\sigma$
- 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  $\sigma$

- Trajectory (realization)  $\{\sigma\} = \{\sigma_0, \sigma_1, \dots, \sigma_n\}$  with random jump times  $\tau_i$
- Measure some quantity  $r$  associated with each transition (energy transfer, mass transfer,...) --> (antisymmetric)  $r_{\sigma',\sigma}$  for transition from  $\sigma \rightarrow \sigma'$
- Example: Particles hopping on a lattice



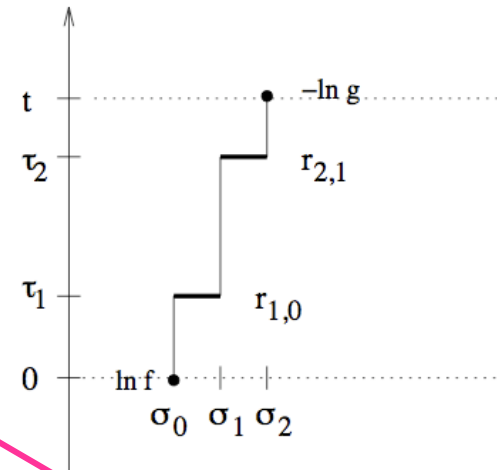
- $r = +/- 1$  for jump across  $k, k+1$ :  
 ==> sum of all  $r$  along trajectory = **integrated particle current**



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]

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

Then trajectory functional = entropy change in environment + boundary terms

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

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

- Otherwise still well-defined through transition rates

- Stochastic particle systems: proportional to particle current

- Entropy production extensive in time ( $\sim t$  for each trajectory at large times)

Call corresponding trajectory functional R

- Consider generating function  $\langle e^{-\lambda R} \rangle \implies$  gives weight  $e^{-\lambda r}$  to each transition

- **TIME REVERSAL**

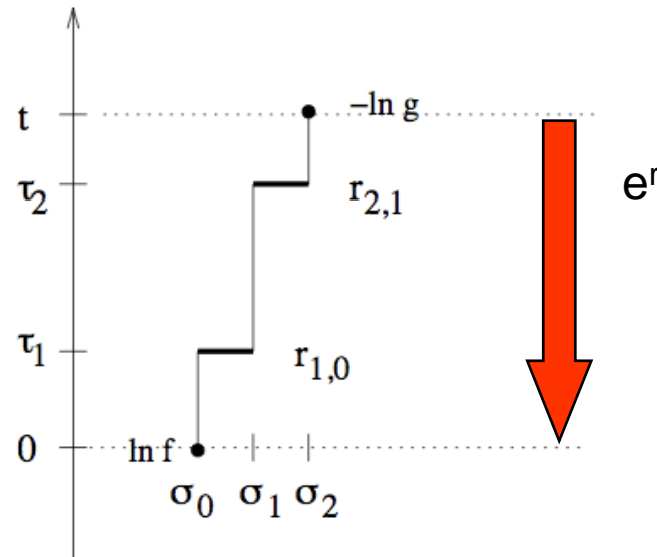
transition rates of reversed process  
= original rates  $\times e^r$

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

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

$\implies$  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

$$\langle e^{-\lambda R} \rangle^F = \langle e^{-(1-\lambda)R} \rangle^B$$

(includes interchange of boundary terms)

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

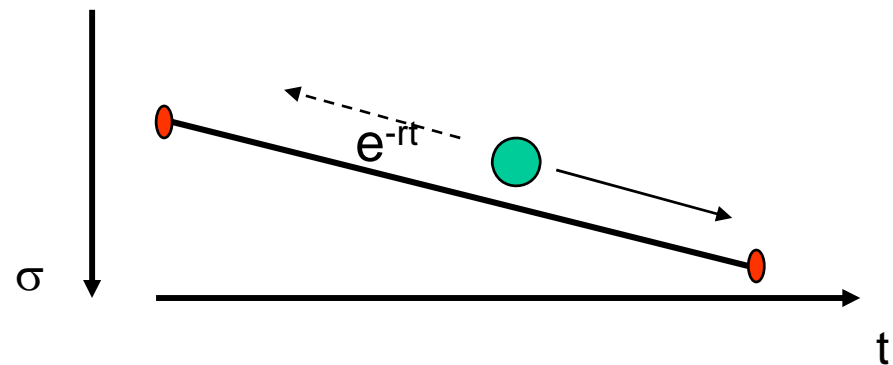
$$\langle e^{-\lambda R} \rangle \sim e^{-tg(\lambda)}$$

- or equivalently

$$g(\lambda) = g(1-\lambda) + \cancel{\text{(boundary terms)}/t}$$

- Legendre 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?

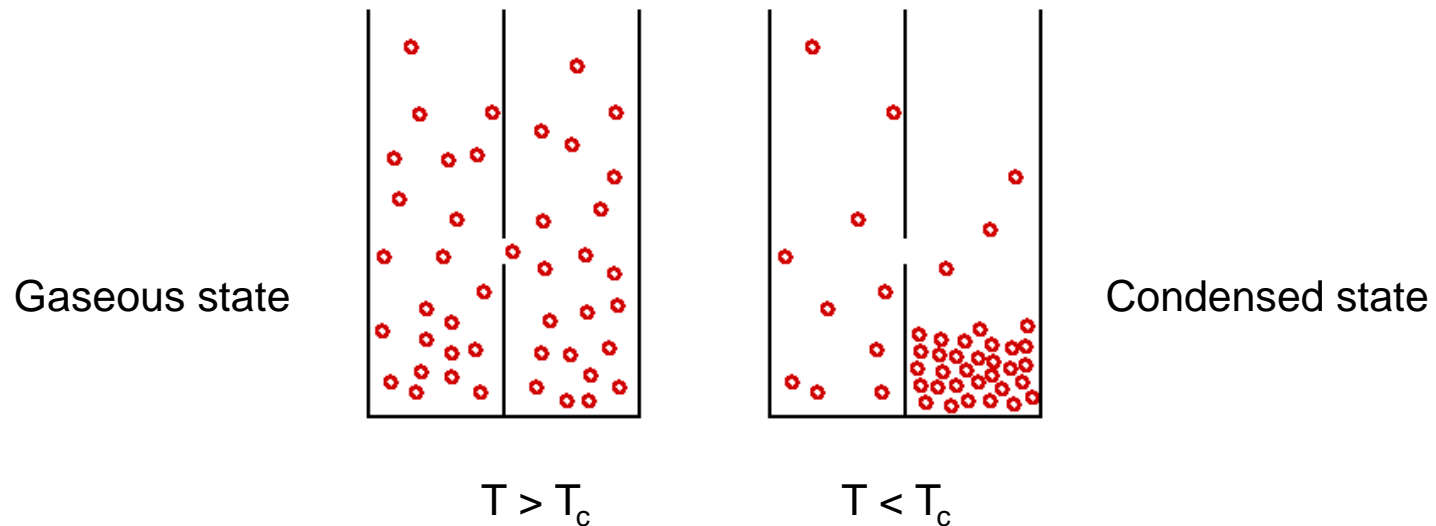
Rigorous in lattice models with finite local state space (exclusion processes)

==> 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]



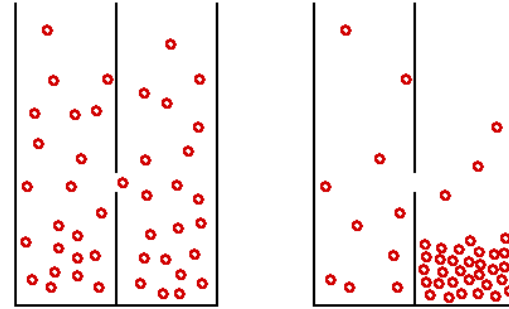
- i) Strong shaking (fixed amplitude, 50 Hz frequency): → Equal gaseous distribution
- ii) Moderate shaking (same amplitude, 30 Hz): → **Condensation (with SSB)**

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



QuickTime™ and a  
decompressor  
are needed to see this picture.

Time  $t = 0 \dots 12$  sec

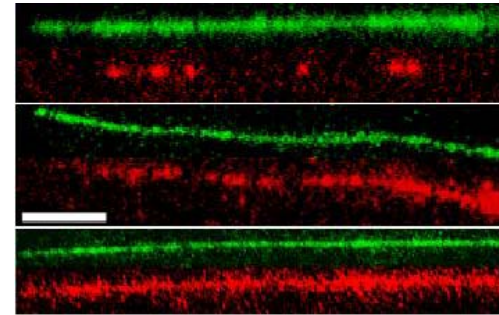
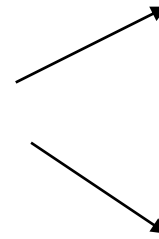
QuickTime™ and a  
decompressor  
are needed to see this picture.

$t$  approx. 1 min

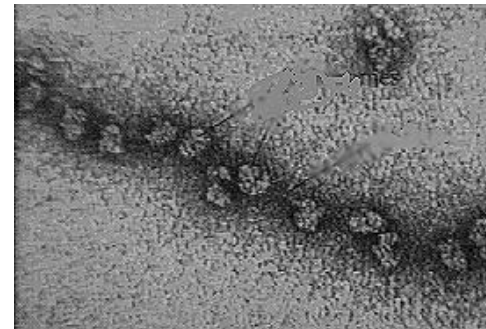
## Single File Diffusion:

SFD: Quasi one-dimensional diffusion 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

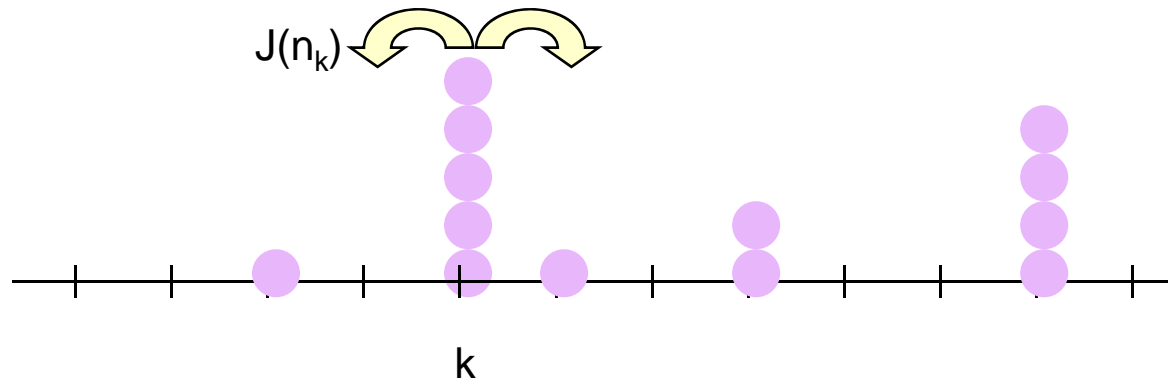
- Network rewiring
- Accumulation of wealth



## 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)  $\Leftrightarrow$  occupation number in ZRP
- particle flux  $J(n_k)$  between compartments (domains)  $\Leftrightarrow$  hopping rate in ZRP



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

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

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

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

- 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  $J(n) \rightarrow 0$ :  $\rightarrow z^*=0$  and hence  $\rho_c = 0$

2) Consider generic case where for large  $n$

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

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

$\rightarrow$  at  $z^*$  one has finite density  $\rho_c$  for  $\sigma < 1$

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

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

## 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

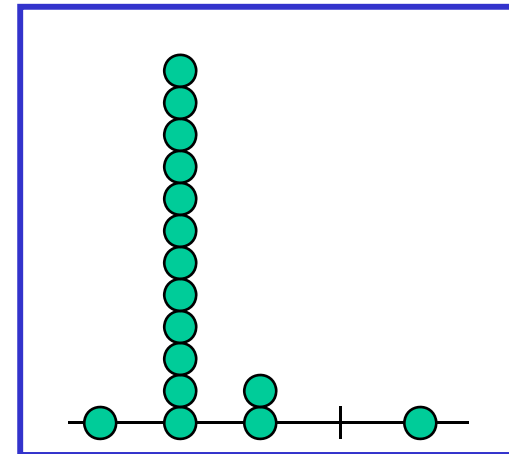
[Grosskinsky, GMS, Spohn, '05, Ferrari, Landim, Sisko '07, Loulakis, Armendariz '08, Evans, Majumdar '08]]

### → 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

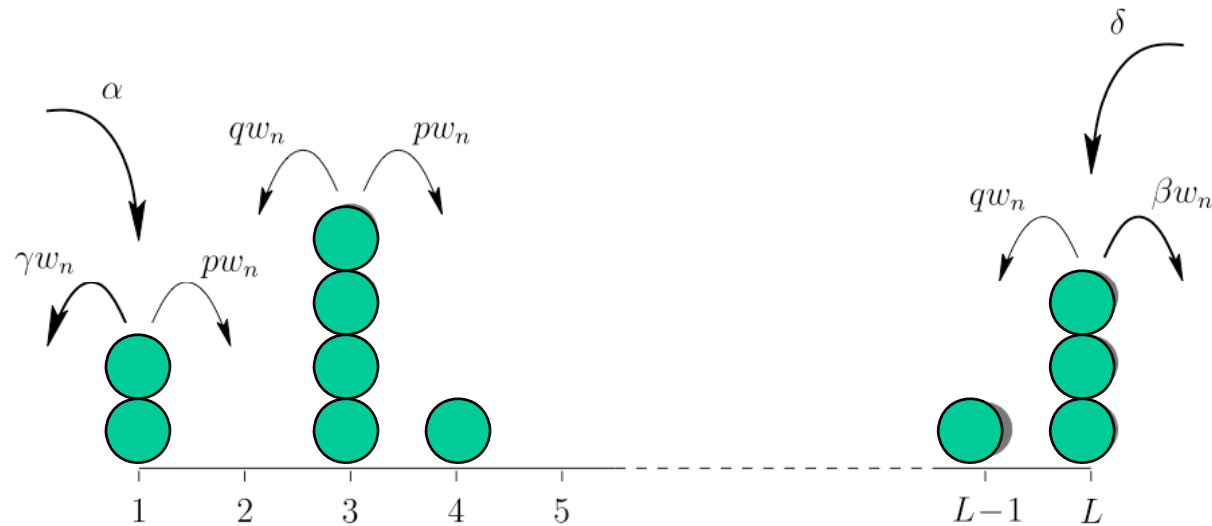
→ unbounded state space

BUT:

- no condensation
- exponentially small probability for large occupation

} ??

## Zero-range process with open boundaries [R.J.Harris, A. Rakoš, 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

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

Legendre  
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

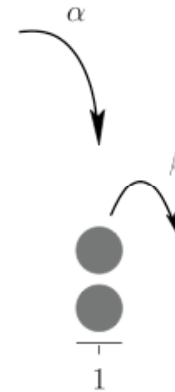


For boundary terms consider totally asymmetric ZRP,  $w_n = 1$

- 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

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



Poisson, by definition of process

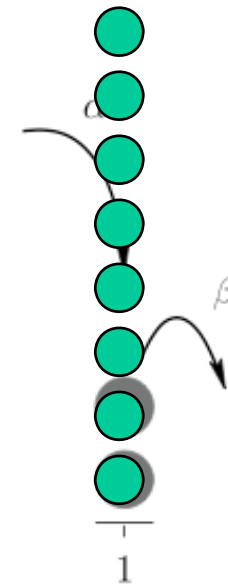
output bond

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

- 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 ( $\sim t$ ) 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

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

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

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

- Output bond

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

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

Exact expression for current distribution:

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

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

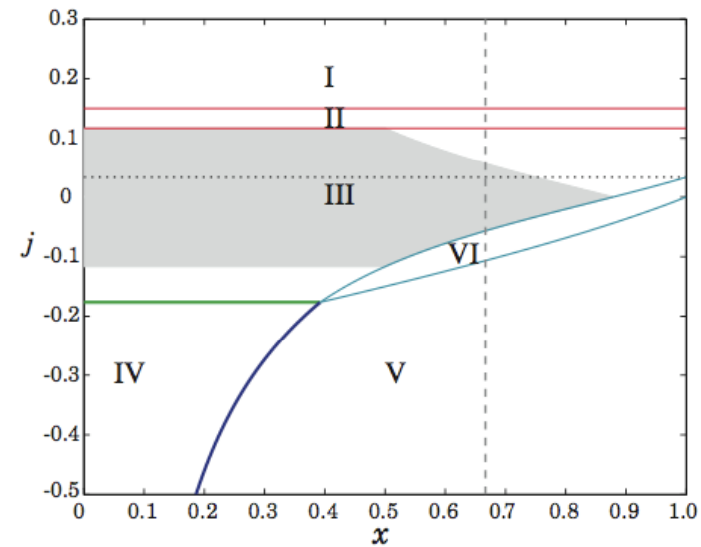
with elements

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

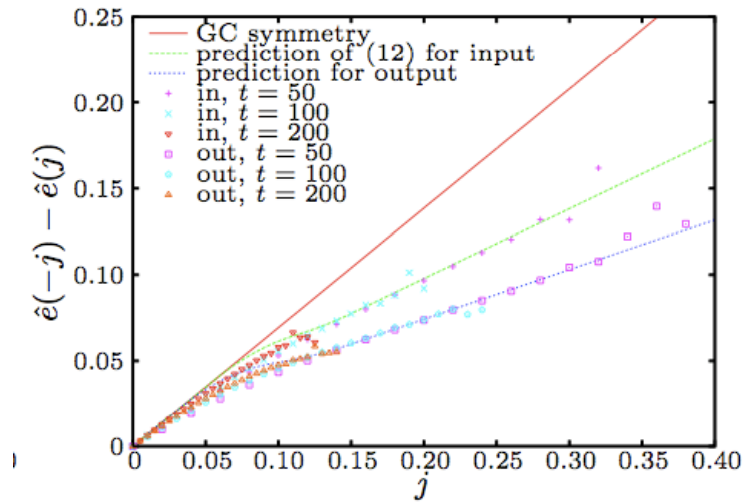
- evaluation by steepest descent for finite L

## Back to partially asymmetric ZRP

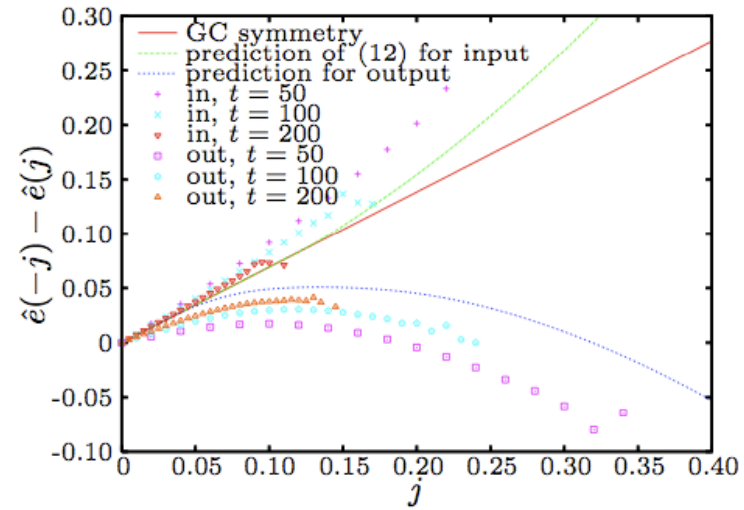
- take one site,  $b=0$  for analytic calculation
- generate equilibrium with fugacity  $x$
- change boundary parameters to non-equilibrium situation
- obtain different non-analyticities, depending both on  $j$  and  $x$
- **large deviation phase diagram**
- validity of GCS only in restricted region, 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

# Acknowledgments

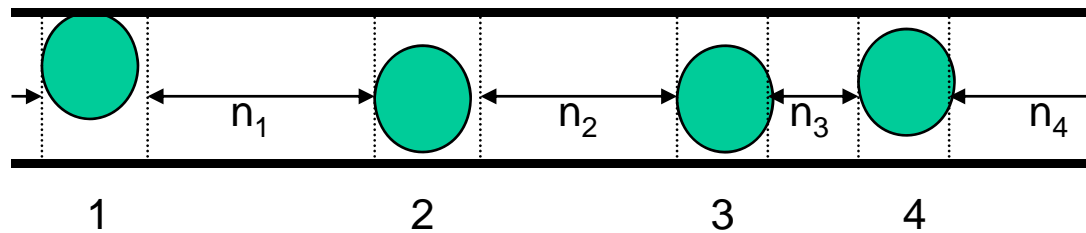
Thanks to:

- Weizmann Institute of Science



## 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

