Fluctuation Theorems and the Zero-Range Process

Rosemary Harris

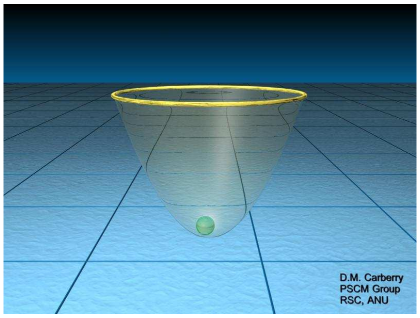
Forschungszentrum Jülich

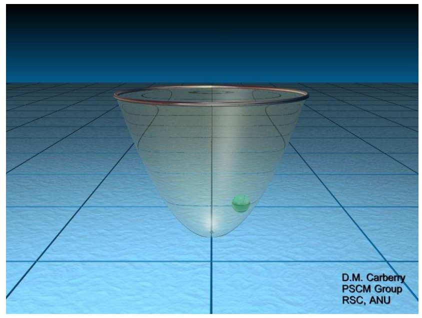
Isaac Newton Institute, 9th May 2006

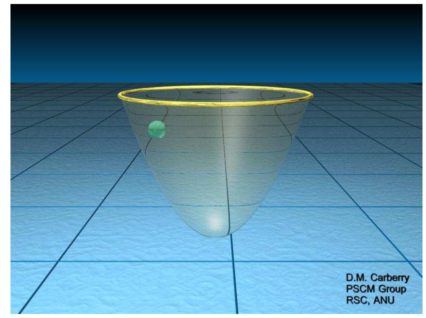
Based on joint work with A. Rákos & G. M. Schütz:

- J. Stat. Mech. (2005) P08003
- cond-mat/0512159

Experiment: colloidal particle in optical trap







"Experimental Demonstration of
Violations of the Second Law of Thermodynamics
for Small Systems and Short Time Scales"

G. Wang *et al.* Phys. Rev. Lett. **89** 050601 (2002)

Fluctuation theorems

What?

- "Relate the probability of observing a given rate of entropy increase to the probability of observing the same rate of entropy decrease"

Why?

- Theoretically interesting
  - Search for unifying principles in *non-equilibrium* statistical mechanics
- Experimentally relevant
  - Colloidal particle in optical trap [Wang *et al.* '02, '05]
  - Fluidized granular medium [Feitosa & Menon '04]
  - Electric circuits [Garnier & Ciliberto '05]
  - Nanoscale machines?

Gallavotti-Cohen Symmetry

$$\frac{p(-\sigma,t)}{p(\sigma,t)} \sim e^{-\sigma t} \tag{1}$$

- Computer simulations of sheared fluids [D.Evans *et al.* '93]
- Deterministic systems, steady state [Gallavotti & Cohen '95]
  - σ is rate of phase space contraction
- Stochastic systems. . . [Kurchan '98, Lebowitz & Spohn '99]
  - σ is usually identified with average particle current

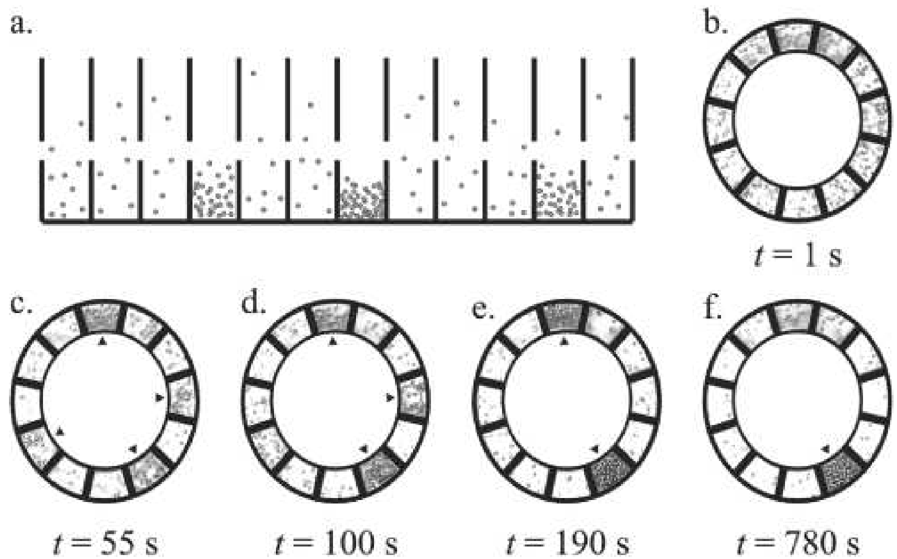
- For systems with unique stationary state, (1) is often assumed to hold for arbitrary initial states
  - General property of large deviation function
  - **"Gallavotti-Cohen symmetry property"**

What can we learn from the zero-range process?

Current fluctuations in the open boundary ZRP

- Zero-range model
  - What?
  - Why?
- Quantum Hamiltonian formalism
- Current fluctuations, large deviations
- Subtleties due to unbounded state space
- Illuminating examples
  - TAZRP
  - Single-site PAZRP
- Validity of Gallavotti-Cohen symmetry
- General implications for systems with unbounded state space
- Conclusions, extensions

Condensation and the ZRP

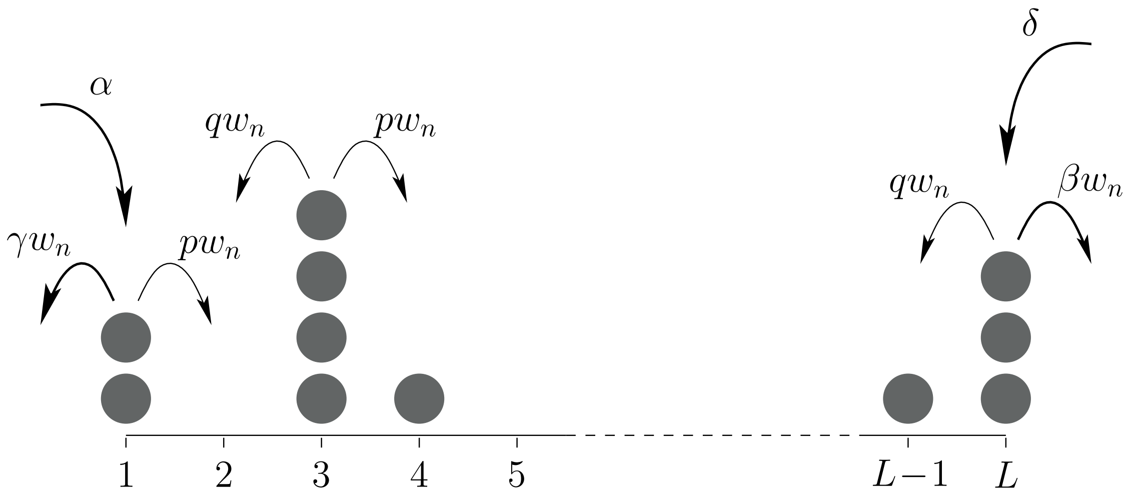


[from van der Meer et al, J. Stat. Mech. (2004) P04004]

- Examples: granular systems, socio-economics, biology, traffic, networks . . . [M.Evans and Hanney '05]
- Phenomenon analogous to Bose-Einstein condensation
- ZRP is simple lattice model with such a phase transition [Spitzer '70, M.Evans '00]
- ZRP can also be mapped to well-studied exclusion processes
- Simple enough for analytical progress but offers both
  - Relevance for real applications
  - Insight into properties of non-equilibrium systems

Open boundary ZRP

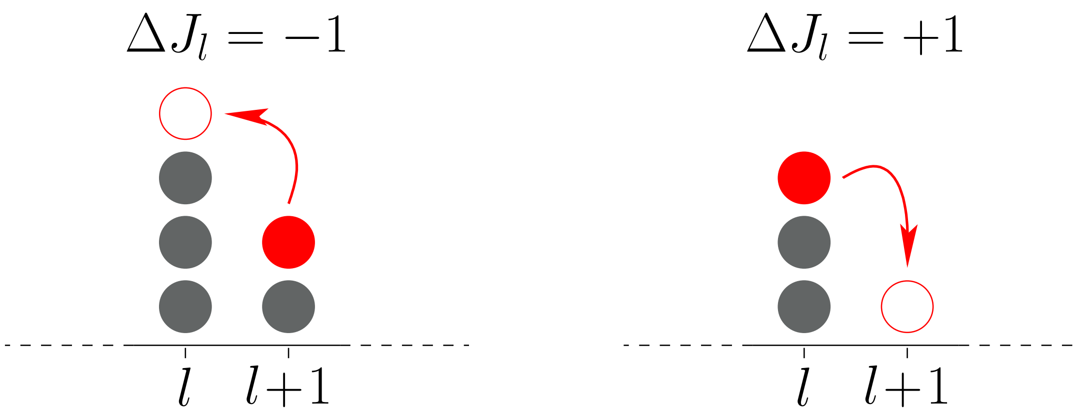
- We study current fluctuations in 1d open-boundary ZRP [Levine et al. '05]:



- Hopping rates w_n depend only on departure site

- Stationary state is still product state
- Strong boundary driving can lead to boundary condensation
- For example, for $w_n = 1$ get growing boundary condensate if $\alpha - \gamma > p - q$ or $\alpha - \gamma > \beta - \delta$
- We consider case where there is no condensation, i.e., steady state is well-defined

Current distribution, large deviations



- Aim to determine the distribution of integrated current $J_l(t)$
- Consider the generating function of $J_l(t)$ and define

$$e_l(\lambda) = \lim_{t\to\infty} -\frac{1}{t} \ln \langle e^{-\lambda J_l(t)} \rangle \tag{2}$$

- From (2) get large deviation property for $j_l = J_l/t$

$$p_l(j,t) \sim e^{-t\hat{e}_l(j)}$$

  where $\hat{e}_l(j)$ is the Legendre transformation of $e_l(\lambda)$

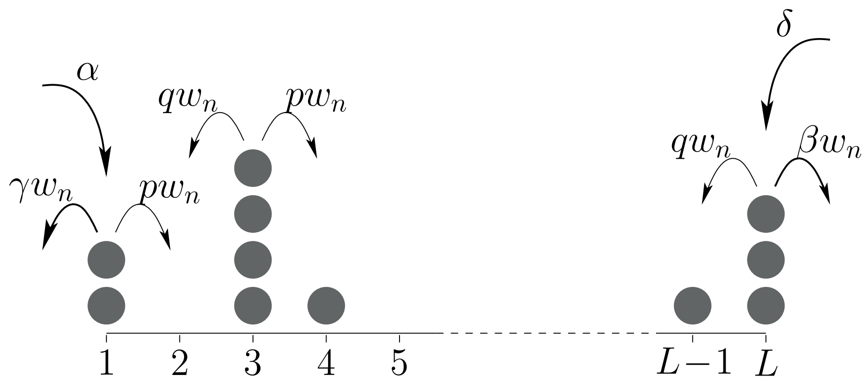
- Large deviation functional is a quantity analogous to free energy of an equilibrium system
- *Insight into properties of non-equilibrium steady states*

Quantum Hamiltonian formalism

- Master equation

$$\frac{d}{dt}|P_t\rangle = -H|P_t\rangle$$

- For PAZRP...



$$H = -\Bigg\{ \sum_{l=1}^{L-1} \left[p(a_l^- a_{l+1}^+ - d_l) + q(a_l^+ a_{l+1}^- - d_{l+1}) \right]$$

$$+ \alpha(a_1^+ - 1) + \gamma(a_1^- - d_1) + \delta(a_L^+ - 1) + \beta(a_L^- - d_L) \Bigg\}$$

- Current generating function involves modified Hamiltonian $\tilde{H}_l$ which counts jumps across bond l

$$\langle e^{-\lambda J_l(t)} \rangle = \langle s| e^{-\tilde{H}_l t} |P_0\rangle$$

- Interested in long-time properties of this object...

Gallavotti-Cohen symmetry?

- Long-time limit?

$$\langle e^{-\lambda J_l(t)} \rangle \sim \langle s|\tilde{0}\rangle\langle\tilde{0}|P_0\rangle e^{-\tilde{e}_l(\lambda)t}$$

where $\tilde{e}_l(\lambda)$ is lowest eigenvalue of $\tilde{H}_l$

$$\tilde{e}_l(\lambda) = \frac{(p-q)(e^{\lambda}-1)\left[\alpha\beta\left(\frac{p}{q}\right)^{L-1} e^{-\lambda} - \gamma\delta\right]}{\gamma(p-q-\beta) + \beta(p-q+\gamma)\left(\frac{p}{q}\right)^{L-1}} \qquad (3)$$

- GC symmetry:

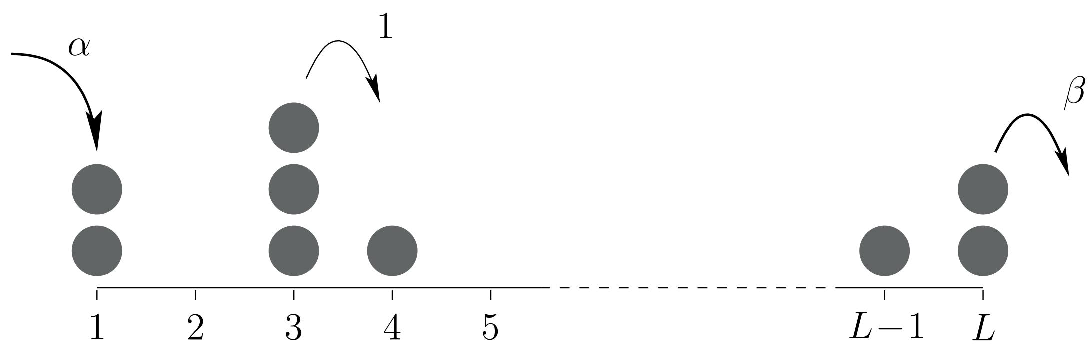
$$\tilde{e}_l(\lambda) = \tilde{e}_l(2E-\lambda)$$
$$\frac{p_l(-j,t)}{p_l(j,t)} \sim e^{-2Ejt}$$

with effective field E

$$e^{2E} = \frac{\alpha\beta}{\gamma\delta}\left(\frac{p}{q}\right)^{L-1}$$

- (3) is independent of w_n *but* for w_n bounded...
  - $\langle\tilde{0}|\tilde{0}\rangle$ diverges for some $\lambda \longrightarrow$ spectrum becomes gapless
  - $\langle s|\tilde{0}\rangle$ or $\langle\tilde{0}|P_0\rangle$ can diverge $\longrightarrow$ *GC symmetry?*
- What does this mean physically?
  - TAZRP
  - Single-site PAZRP

L-site TAZRP



1. Large deviations can be bond dependent

2. Large deviations depend on initial condition

- Fixed initial particle configuration [$\alpha < \beta < 1$]:

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

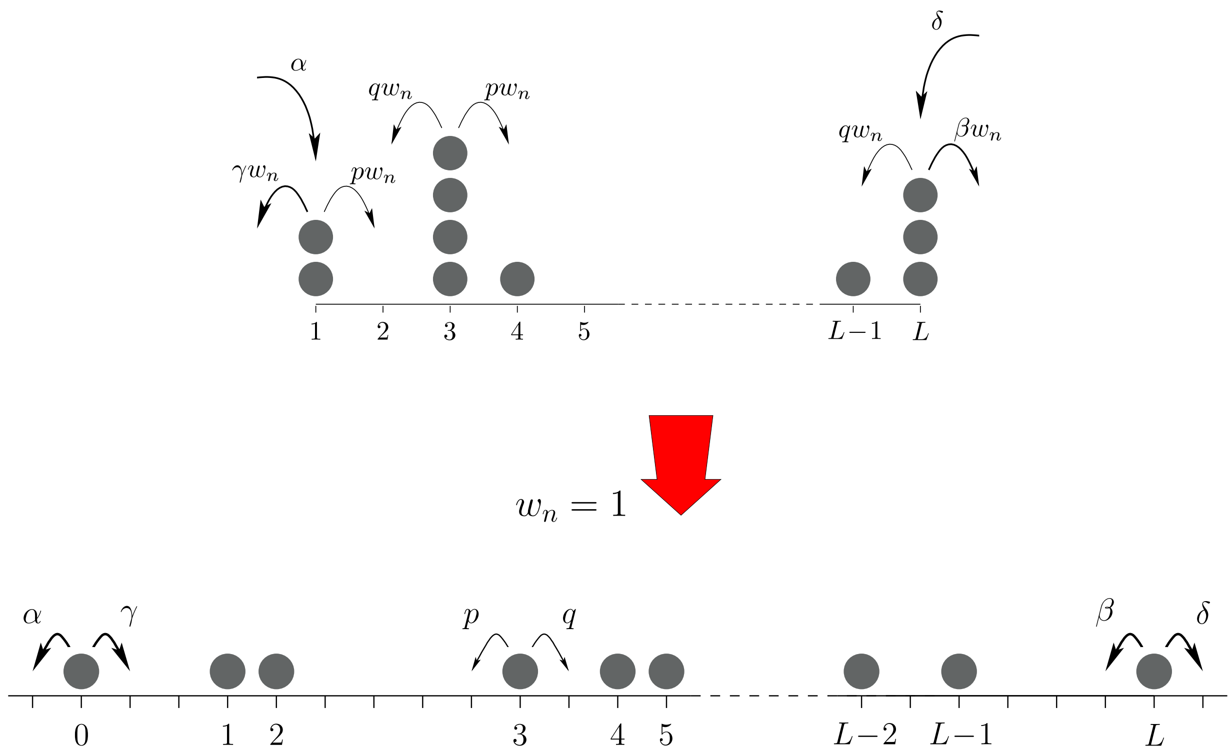
$$p_{l\neq 0,L}(j,t) \sim \begin{cases} e^{-t(\alpha-j+j\ln\frac{j}{\alpha})} & j<1 \\ e^{-t(\alpha-j+j\ln\frac{j}{\alpha})} \times e^{-t(1-j+j\ln j)l} & j\geq 1 \end{cases}$$

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

- Cf. steady state [Prähofer & Spohn '02]:

$$p_l(j,t) \sim e^{-t(\alpha-j+j\ln\frac{j}{\alpha})}$$

Mapping to exclusion process, Bethe ansatz

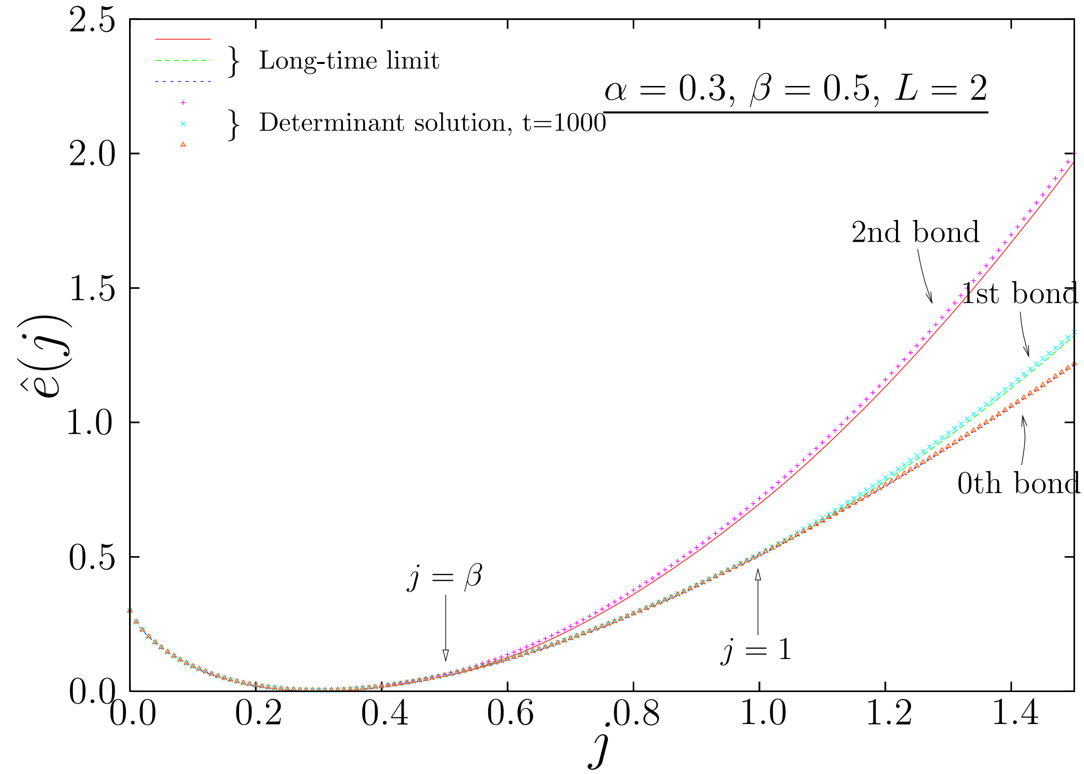


TASEP: Bethe ansatz solution with particle-dependent rates [Rákos & Schütz '05]

$$p_l(j,t) = \prod_{i=0}^{l} e^{-t(v_i - j \ln v_i)} \times \begin{vmatrix} F_0(jt,t) & F_l(jt+1,t) & F_l(jt+2,t) & \dots & F_l(jt+l,t) \\ F_0(jt-1,t) & F_l(jt,t) & F_l(jt+1,t) & \dots & F_l(jt+l-1,t) \\ \dots & \dots & \dots & \dots & \dots \\ F_0(jt-l,t) & F_l(jt-l+1,t) & F_l(jt-l+2,t) & \dots & F_l(jt,t) \end{vmatrix}$$

$$F_l(x,t) = \frac{1}{2\pi i} \oint e^{\frac{t}{z}} z^{x-1} \prod_{i=0}^{l} (1 - v_i z)^{-1} \, dz$$

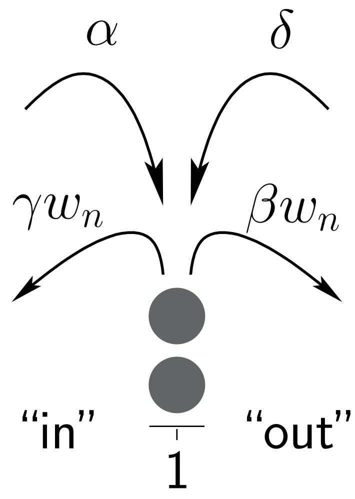
Example: 2-site TAZRP with empty initial condition



Current fluctuations are bond-dependent for high currents

- Physically due to temporary build-up of particles
  – "instantaneous condensates"
- Precursor to condensation transition

Single-site PAZRP



- Take $w_n = 1$, qualitatively same results for any bounded w_n
- $\alpha - \gamma < \beta - \delta$ for well-defined steady state
- $$|P_0\rangle = (1-x)\sum_{n=0}^{\infty} x^n |n\rangle$$

  where $|n\rangle$ is state with site occupation n, x is fugacity

- Integral representation of input current generating function

$$\langle s|e^{-\tilde{H}_0 t}|P_0\rangle = \frac{x-1}{2\pi i}\Bigg\{\oint_{C_1} e^{-\varepsilon(z)t}\frac{1}{(z-1)(z-x)}\,dz + \oint_{C_2} e^{-\varepsilon(z)t}\frac{x^{-1}[u_\lambda/v_\lambda - z u_\lambda/(\beta+\gamma)]}{(z-1)[z-x^{-1}u_\lambda/v_\lambda][z-u_\lambda/(\beta+\gamma)]}\,dz\Bigg\}$$

- Saddle-point analysis gives $e_0(\lambda)$...

Single-site PAZRP: $e(\lambda)$

For

$$x < x_c \equiv \frac{-\eta + (\beta+\gamma)^2 - \alpha\gamma + \beta\delta}{2\beta(\beta+\gamma)}$$

we find

$$e_0(\lambda) = \begin{cases} \alpha(1-e^{-\lambda}) + \gamma(1-e^{\lambda}) & \lambda < \lambda_1 \\ \alpha + \delta - \frac{u_\lambda v_\lambda}{\beta+\gamma} & \lambda_1 < \lambda < \lambda_2 \\ \alpha+\beta+\gamma+\delta - 2\sqrt{u_\lambda v_\lambda} & \lambda_2 < \lambda < \lambda_3 \\ \alpha+\beta+\gamma+\delta - v_\lambda x - u_\lambda x^{-1} & \lambda_3 < \lambda \end{cases}$$

whereas for $x > x_c$

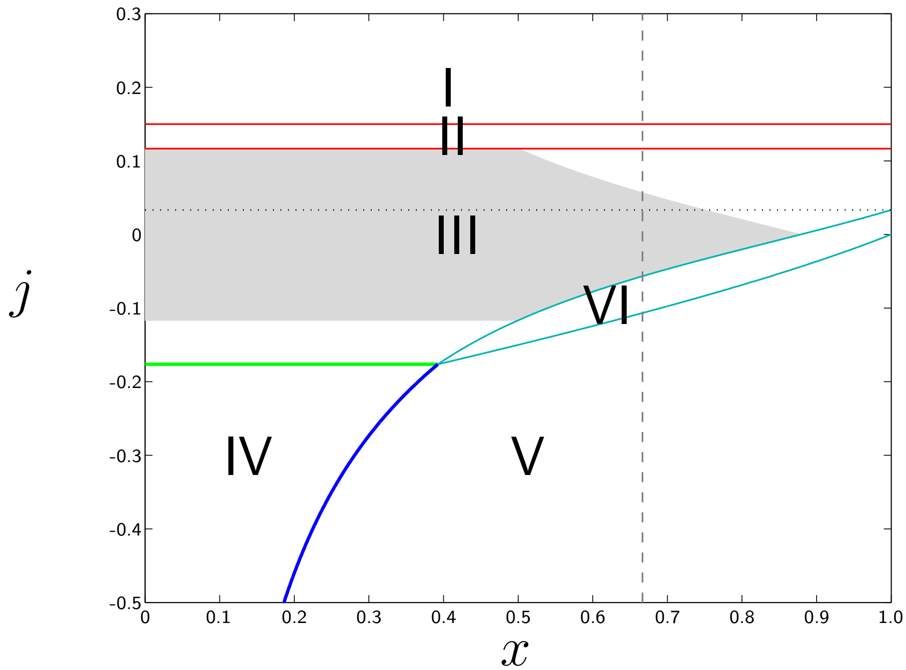
$$e_0(\lambda) = \begin{cases} \alpha(1-e^{-\lambda}) + \gamma(1-e^{\lambda}) & \lambda < \lambda_1 \\ \alpha + \delta - \frac{u_\lambda v_\lambda}{\beta+\gamma} & \lambda_1 < \lambda < \lambda_4 \\ \alpha+\beta+\gamma+\delta - v_\lambda x - u_\lambda x^{-1} & \lambda_4 < \lambda \end{cases}$$

where

$$\begin{aligned} \varepsilon(z) &= \alpha+\beta+\gamma+\delta - v_\lambda z - u_\lambda z^{-1} \\ u_\lambda &= \alpha e^{-\lambda} + \delta \\ v_\lambda &= \beta + \gamma e^{\lambda} \\ \eta &= \sqrt{[(\beta+\gamma)^2 - \beta\delta - \alpha\gamma]^2 - 4\alpha\beta\gamma\delta} \end{aligned}$$

Single-site PAZRP: $\hat{e}(j)$

- ...Legendre transformation gives large deviations of j_0:



$$\hat{e}_0(j) = \begin{cases} f_j(\alpha,\gamma) & \text{I} \\ g_j\left(\frac{(\alpha-\beta-\gamma+\delta)(\beta-\delta)}{\beta+\gamma-\delta}, \frac{\beta+\gamma-\delta}{\alpha}\right) & \text{II} \\ f_j\left(\frac{\alpha\beta}{\beta+\gamma}, \frac{\gamma\delta}{\beta+\gamma}\right) & \text{III} \\ f_j(\alpha,\gamma) + f_j(\beta,\delta) & \text{IV} \\ f_j(\alpha,\gamma) + g_j(\beta(1-x)+\delta(1-x^{-1}), x) & \text{V} \\ g_j\left(\frac{(1-x)\{\alpha\beta x-\delta[\beta(1-x)+\gamma]\}}{x[\beta(1-x)+\gamma]}, \frac{\gamma x}{\beta(1-x)+\gamma}\right) & \text{VI} \end{cases}$$

$$f_j(a,b) = a + b - \sqrt{j^2+4ab} + j\ln\frac{j+\sqrt{j^2+4ab}}{2a}$$

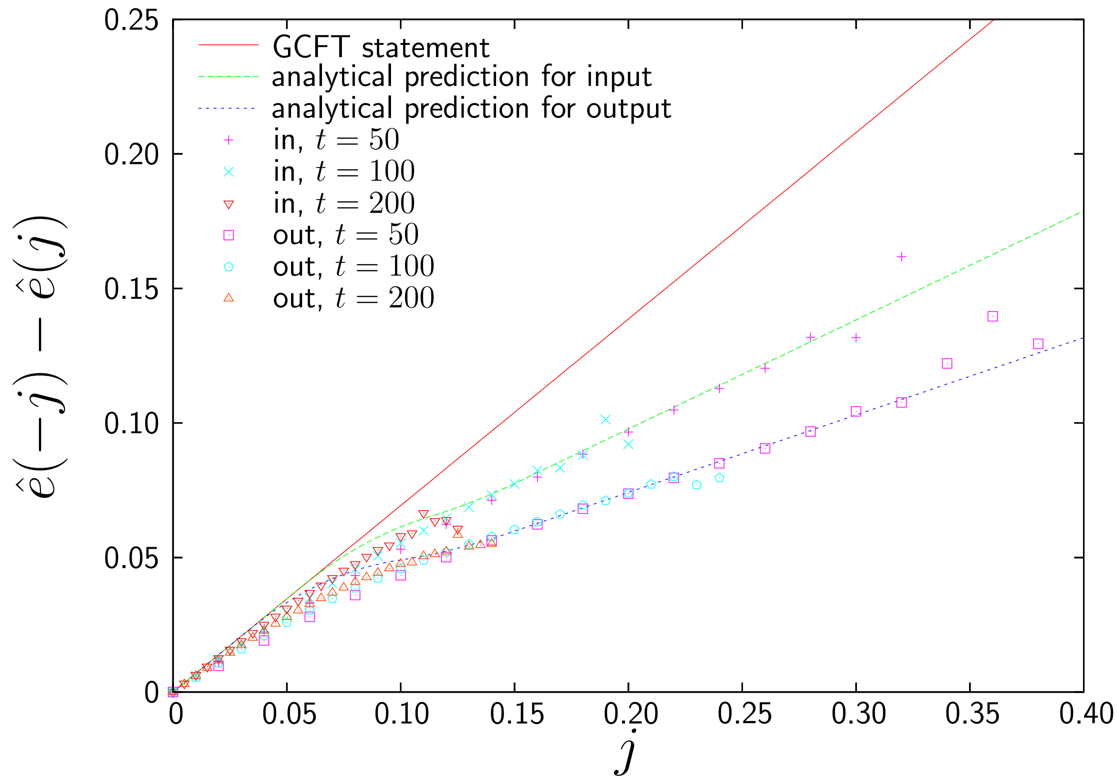
$$g_j(a,b) = a + j\ln b.$$

3. GC symmetry only observed in shaded region!

Comparison with simulation

- Compare probabilities of observing forward and backward currents, GC symmetry predicts

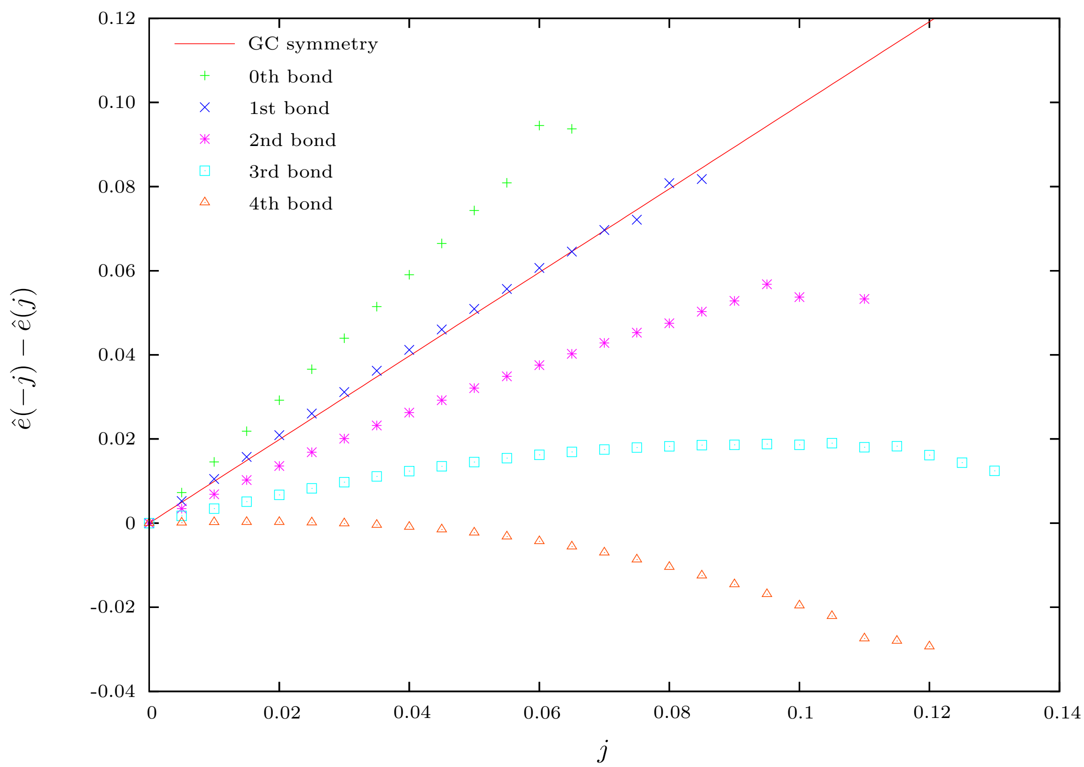
$$\frac{p_l(-j,t)}{p_l(j,t)} \sim e^{-2Ejt}$$



- Simulation results converge towards analytical predictions:
  - *GC symmetry only seen for small fluctuations*
  - Form of breakdown depends on initial state of system

Discussion: Breakdown of GC symmetry

- Physically, breakdown of GC symmetry due to temporary build-up of particles – "instantaneous condensates"
- Mathematically, due to divergence of $\langle s|\tilde{0}\rangle$ and $\langle\tilde{0}|P_0\rangle$
- Violation of symmetry expected for any ZRP with bounded w_n, e.g., 4-site system



- More generally, possibility of similar effects for any system with unbounded state space

Discussion: Restoring symmetry

- Consider "action functional" $W(t)$ [for $w_n = 1$]

$$W(t) = 2\sum_{l=0}^{L} E_l J_l(t) - \ln \frac{P_0(\{n\}(t))}{P_0(\{n\}(0))}$$

- Distribution of $w(t) = W(t)/t$ obeys

$$\frac{p(-w,t)}{p(w,t)} = e^{-wt}$$

$\longrightarrow$ transient fluctuation theorem [D.Evans & Searles '94]

- *For bounded state space*, in the long-time limit one can replace $W(t)$ by $2(\sum_{i=0}^{L} E_i)J_l$
- **For unbounded state space, boundary terms are non-vanishing and GC symmetry can be violated**
- Analogous effects due to unbounded potentials:
  - Deterministic forces
    [Bonetto *et al.* '05, van Zon & Cohen '03]
  - Single-particle Langevin dynamics
    [Farago '02, Baiesi *et al.* '06]
  - Physical models: granular gases, Brownian transducers...
    [Visco '06, Gomez-Marin '06]

Conclusion

- ***Fluctuations in non-equilibrium systems have a rich structure***

- ***Zero-range process is a simple test model allowing exact calculations***

- Distribution of large current fluctuations does not satisfy Gallavotti-Cohen symmetry
- Generic effect for systems with unbounded state space
- First(?) discussion for a stochastic many-particle system
- Much scope for future work...

Extensions

Work in progress:

- Direct numerical evaluation of $e(\lambda)$ using algorithm with modified dynamics [Giardinà, Kurchan & Peliti '05]

Future directions:

- Time-dependent, periodic driving [Jarzynski]
- Two-species [M.Evans, Hanney, Großkinsky]
- Higher dimensions?
- Generalized mass-transfer model [M.Evans, Majumdar]
- Models without product state [M.Evans, Hanney, Majumdar]
- ...??