Current fluctuations in stochastic systems with long-range memory

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Outline

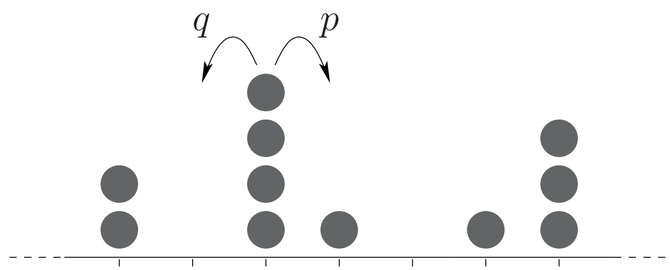
- Memoryless case
  - Stochastic Markovian dynamics
  - Current fluctuations, large deviations

- Memory-dependent case
  - Current-dependent rates
  - Temporal additivity principle
  - Random walk examples, fluctuation relations
  - *Open problems*
    - Many-particle models, phase transitions
    - Intrinsically non-Markovian systems

- Summary

Stochastic Markovian dynamics

- Interacting particles described by Markov process
- Configurations (microstates) $\sigma(t)$



- Stochastic approaches:
  - Langevin: Differential equation for $\sigma(t)$, deterministic + noisy forces
  - **Master equation:**
    - Transition rates $w_{\sigma',\sigma}$
    - Deterministic evolution for probability distribution $P(\sigma,t)$:

$$\frac{d}{dt}P(\sigma,t)=\sum_{\sigma'\neq\sigma}\left[w_{\sigma,\sigma'}P(\sigma',t)-w_{\sigma',\sigma}P(\sigma,t)\right]$$

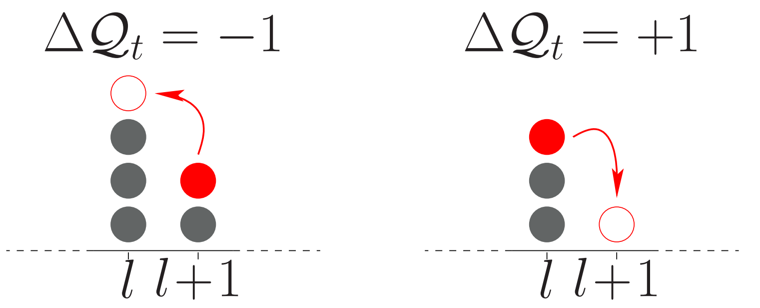
- *Non-equilibrium*
  - Broken detailed balance
  - Stationary state characterized by non-zero currents

Currents

- Counter $\mathcal{Q}_t$, value increases by $\Theta_{\sigma',\sigma}$ at each transition $\sigma \to \sigma'$
- Θ usually real and *antisymmetric* matrix
- $\mathcal{Q}_t$ is a functional of history $\{\sigma(\tau), 0 \le \tau \le t\}$.

$$\mathcal{Q}_t = \sum_{n=1}^{N-1} \Theta_{\sigma_{n+1},\sigma_n}$$

- Example: Integrated particle current across bond



- Probability distribution of $\mathcal{Q}_t$ characterized by generating function

$$\left\langle e^{-\lambda \mathcal{Q}_t} \right\rangle$$

Large deviations

- Particularly interested in long-time limiting behaviour

$$e_w(\lambda) := -\lim_{t\to\infty} \frac{1}{t} \ln \left\langle e^{-\lambda \mathcal{Q}_t} \right\rangle$$

- Now consider time-averaged current $\mathcal{Q}_t/t$
- Typically have large deviation principle:

$$\boxed{\text{Prob}(\mathcal{Q}_t/t = j) \sim e^{-\hat{e}_w(j)t}}$$

with "speed" t and rate function (analogous to entropy)

$$\hat{e}_w(j) := -\lim_{t\to\infty} \frac{1}{t} \ln \left[\text{Prob}(\mathcal{Q}_t/t = j)\right]$$

- $e_w(\lambda)$ and $\hat{e}_w(j)$ are related by Legendre transform[1]

$$\hat{e}_w(j) = \sup_\lambda \{e_w(\lambda) - \lambda j\}, \qquad e_w(\lambda) = \inf_j \{\hat{e}_w(j) + \lambda j\}$$

[1]Strictly true only when $e_w(\lambda)$ is differentiable

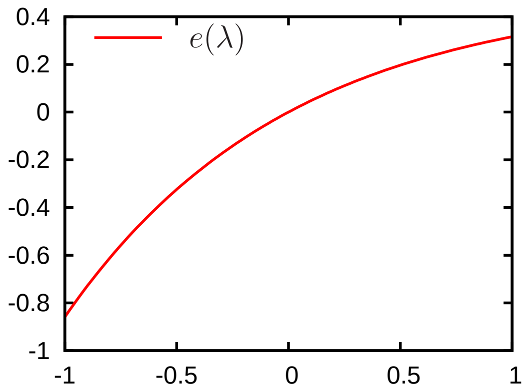
Single particle on an infinite lattice

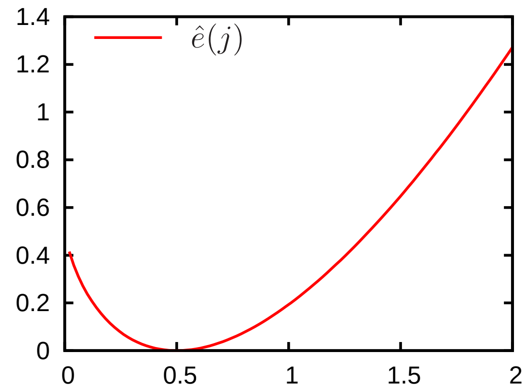
- Single particle hopping rightwards on an infinite lattice

- Let $\mathcal{Q}_t$ count the number of jumps up to time t
- Large deviation function given by

$$e_v(\lambda) = v(1 - e^{-\lambda}) \qquad \Longleftrightarrow \qquad \hat{e}_v(j) = v - j + j \ln \frac{j}{v}$$

- For example, $v = 0.5$:





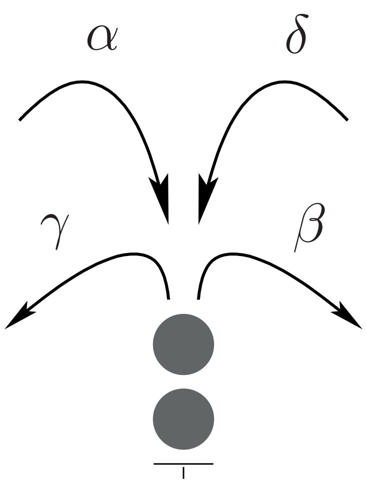
Driven many-particle systems: generic features

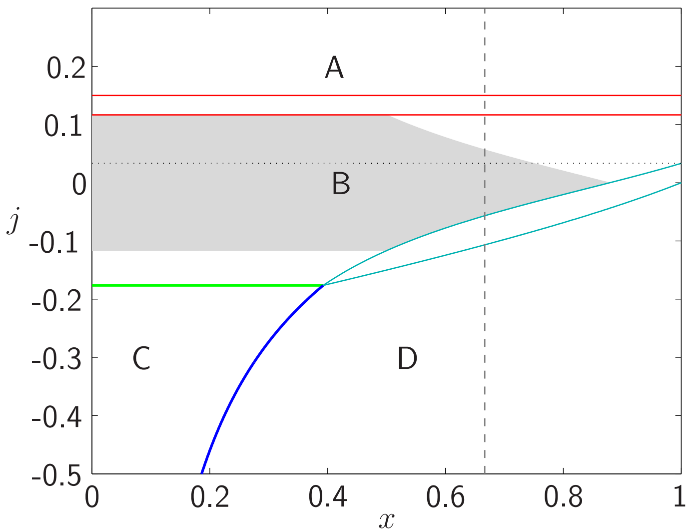
- Under general conditions, a fluctuation symmetry holds [Gallavotti & Cohen '95, Lebowitz & Spohn '99]

$$\frac{\text{Prob}(\mathcal{Q}_t/t = -j)}{\text{Prob}(\mathcal{Q}_t/t = +j)} \sim e^{-Ejt}$$

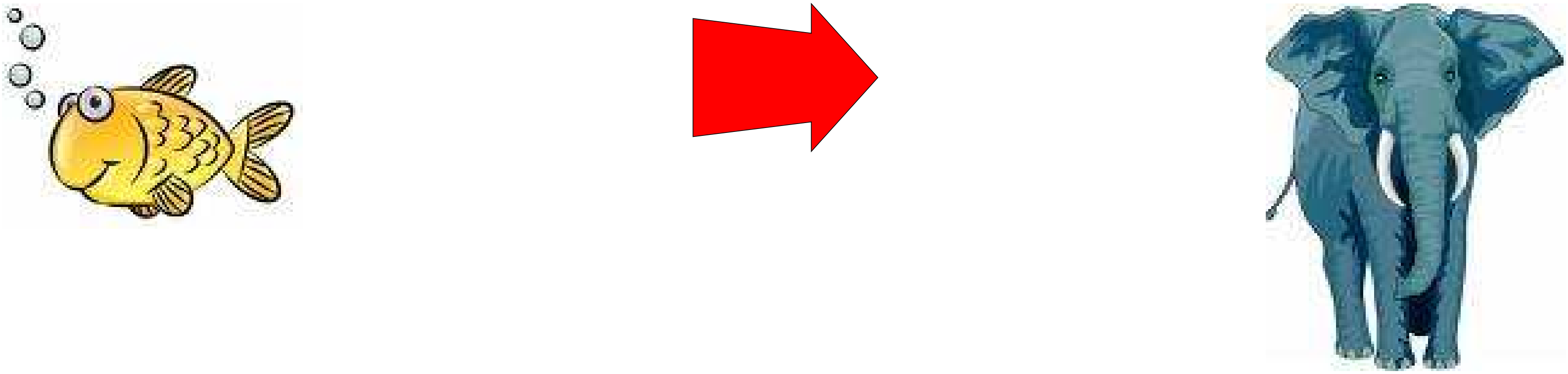
But can have breakdown in systems with unbounded state space

- Current large deviations can show complicated phase structure even in simple models
- Example: Single-site ZRP with open boundaries [RJH, Rákos & Schütz '06]





Current-dependent rates



- Many ways to introduce memory
- We consider class of process where rates $w_{\sigma',\sigma}$ depend explicitly on σ, σ' *and* $\mathcal{Q}_t/t$
  (To avoid singularities assume observations start at t_0, where $0 \ll t_0 \ll t$)
- Includes analogues of "elephant random walk" [Schütz and Trimper '04]
- Non-Markovian process but Markovian in joint current/configuration space

- *How does memory affect the current large deviation principle?*
  (i.e., do we still have form Prob$(\mathcal{Q}_t/t = j) \sim e^{-\hat{e}_w(j)t}$?)

Temporal additivity principle

- Claim:

$$\mathsf{Prob}(\mathcal{Q}_t/t = j) \sim \exp\left[-\min_{q(\tau)} \int_{t_0}^{t} \hat{e}_{w(q)}(q + \tau q')\, d\tau\right]$$

where integral is minimized over all $q(\tau)$ with $q(t_0) = j_0$ and $q(t) = j$

- General idea: Look for most probable path $q(\tau)$ satisfying boundary conditions
- Temporal analogue of additivity principle of [Bodineau and Derrida '04]

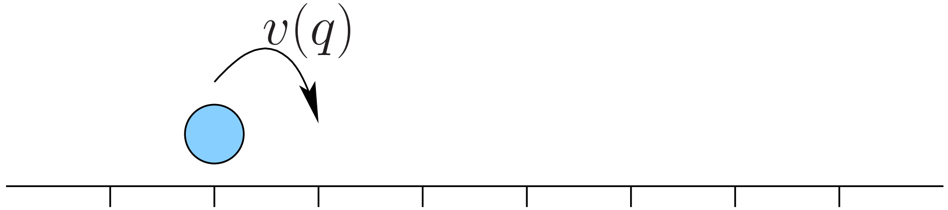
- *If Markovian rate function is known, can find large deviation principle for system with current-dependent rates by minimizing relevant integral...*
  - Analytically (Euler-Lagrange, Gaussian approximation)
  - Numerically

Example 1: Uni-directional random walk

- Recall Markovian case of single particle hopping rightwards on an infinite lattice

$$\hat{e}_v(j) = v - j + j \ln \frac{j}{v}$$

- Now modify picture so that rate for hopping at time t depends on average current $q(t)$ up to t



- Predict that distribution of number of jumps $\mathcal{Q}_t$ has asymptotic form

$$\text{Prob}(\mathcal{Q}_t/t = j) \sim \exp\left[-\min_{q(\tau)} \int_{t_0}^{t} \hat{e}_{v(q)}(q + \tau q')\, d\tau\right]$$

- Minimizing integral gives Euler-Lagrange equation

$$\frac{dv}{dq} - q\frac{dv/dq}{v_R} - \frac{2\tau q'}{q + \tau q'} - \frac{\tau^2 q''}{q + \tau q'} = 0$$

Example 1: Uni-directional random walk

- Exactly solvable cases include $v(q) = aq$, i.e., rate for particle to move at given time is directly proportional to average velocity up to that time
- In this case, solving E-L equation and carrying out integration gives

$$\min_{q(\tau)} \int_{t_0}^{t} \hat{e}_{v(q)}(q + \tau q')\, d\tau \approx j t_0^a t^{1-a} + (a-1) j_0 t_0 \ln t$$

- Crossover at $a = 1$:
  - $a > 1$, escape regime: no large deviation principle
  - $a < 1$, localized regime:
    * System approaches state where particle has zero velocity
    * Large deviation principle with "speed" $t^{1-\alpha}$:

$$\text{Prob}(\mathcal{Q}_t/t = j) \sim e^{-j t_0^a t^{1-a}}, \qquad \text{for } j > 0.$$

    * Can show

$$\text{Var}[\mathcal{Q}_t] \sim (t/t_0)^{2a}$$

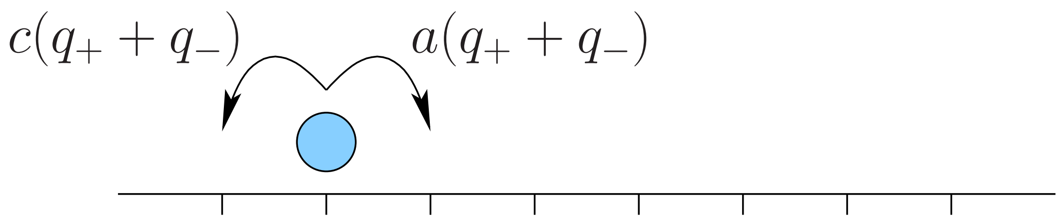
so transition from subdiffusive regime to superdiffusive regime at $a = 1/2$

Example 2: Bi-directional random walk with activity dependent rates

- Bi-directional random walk, count separately jumps to right and left so that

$$\mathcal{Q}_t = \mathcal{Q}_{+,t} - \mathcal{Q}_{-,t}$$

- Consider rates proportional to "activity"



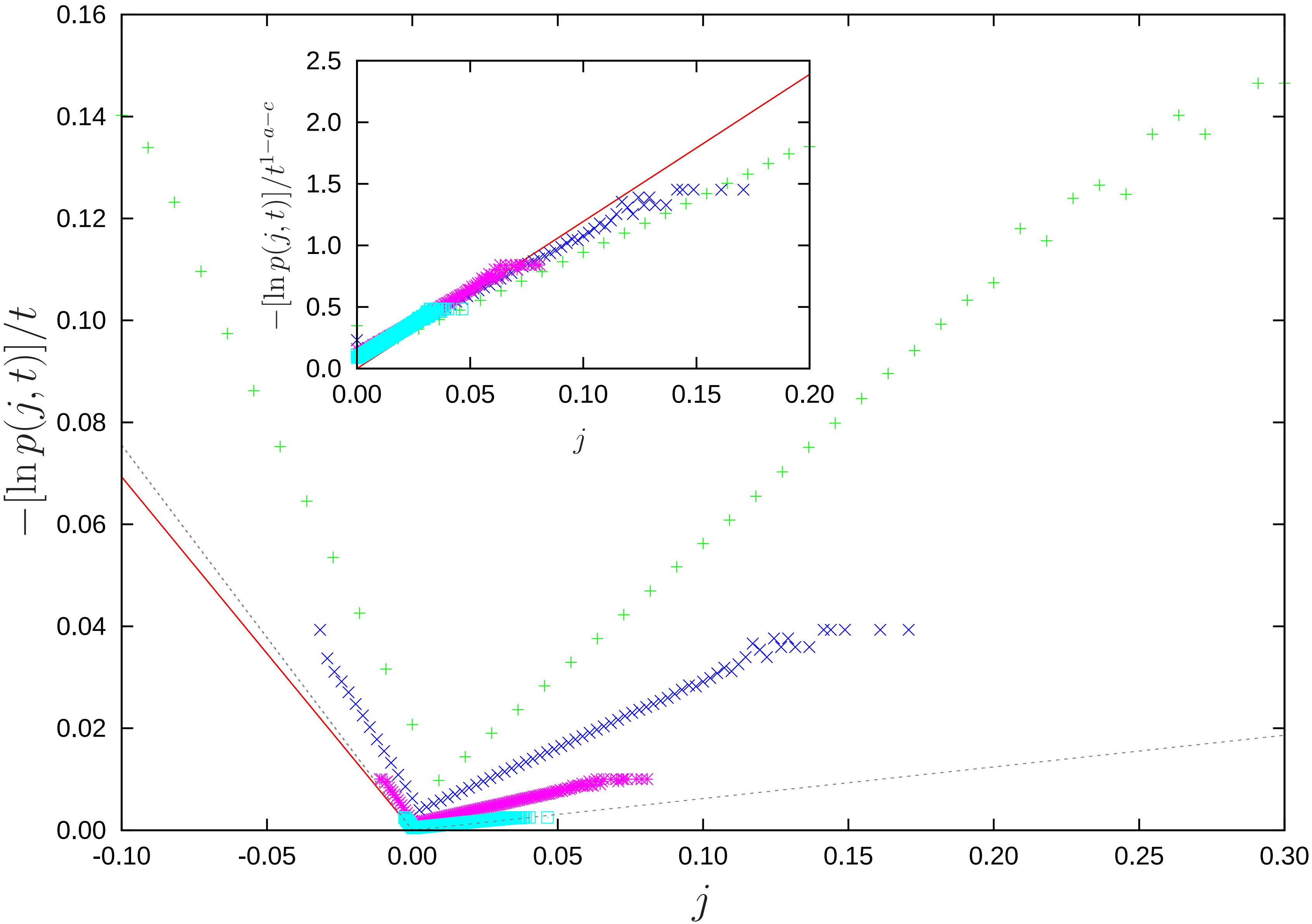
- Without loss of generality take $a > c$, i.e., drive to right
- For $a + c < 1$, we find

$$\text{Prob}(\mathcal{Q}_t/t = j) \sim \begin{cases} \exp[-j t_0^{a+c} \left(\frac{a+c}{a-c}\right) t^{1-a-c}] & \text{for } j \geq 0 \\ \exp[j(\ln \frac{a}{c})t + j t_0^{a+c} \left(\frac{a+c}{a-c}\right) t^{1-a-c}] & \text{for } j < 0. \end{cases}$$

- *Leading term in exponent is different for currents in forward and backward directions*

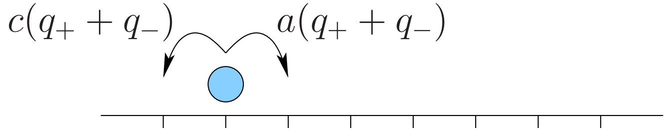
Example 2: Bi-directional random walk with activity dependent rates

Comparison with simulation:



Fluctuation theorems

- For activity-dependent random walk

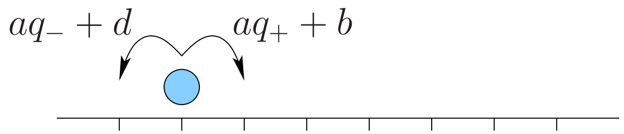


$$\frac{\text{Prob}(\mathcal{Q}_t/t = -j)}{\text{Prob}(\mathcal{Q}_t/t = +j)} \sim \exp\left[-j\left(\ln\frac{a}{c}\right)t\right]$$

i.e., fluctuation theorem still holds

- Expected here since relative bias is constant $v_R/v_L = a/c$
  (also holds for $a + c > 1$ when there is no stationary state)

- But for "generalized elephant" random walk

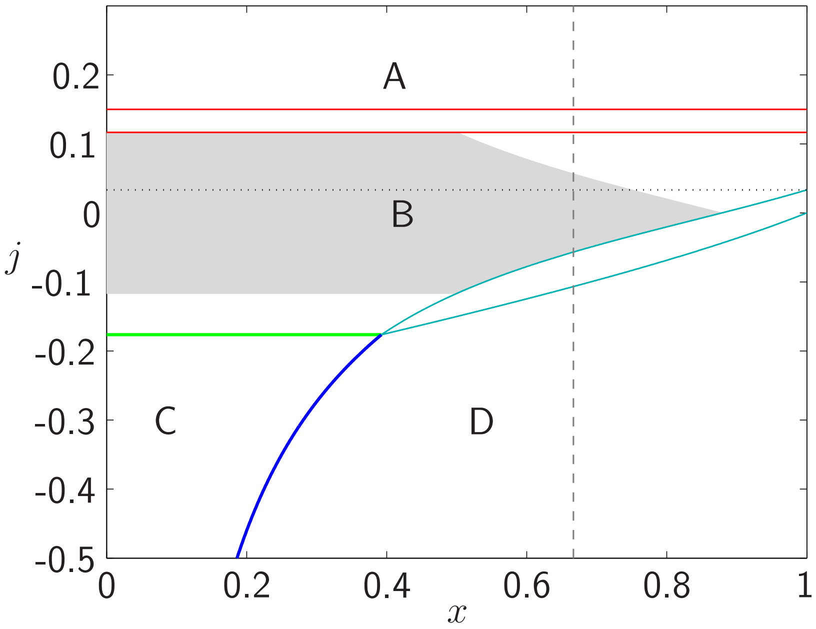


$$\frac{\text{Prob}(\mathcal{Q}_t/t = -j)}{\text{Prob}(\mathcal{Q}_t/t = +j)} \sim \begin{cases} \exp\left[-j\frac{2(b-d)(1-2a)}{1-a}t\right] & \text{for } 0 < a < 1/2 \\ \exp\left[-j\frac{2(b-d)(1-2a)}{1-a}t_0^{2a-1}t^{2-2a}\right] & \text{for } 1/2 < a < 1. \end{cases}$$

- For $1/2 < a < 1$ current symmetry apparently modified by superdiffusive spreading
  (may still hold for appropriately defined entropy)

Many-particle systems

- In general would need to minimize integral numerically to find large deviations for memory-dependent case
- For example, Markovian 1-site open-boundary ZRP [RJH, Rákos & Schütz '06]



A: $\hat{e}_w(j) = f_j(\alpha, \gamma)$

B: $\hat{e}_w(j) = f_j\left(\frac{\alpha\beta}{\beta+\gamma}, \frac{\gamma\delta}{\beta+\gamma}\right)$

C: $\hat{e}_w(j) = f_j(\alpha, \gamma) + f_j(\beta, \delta)$

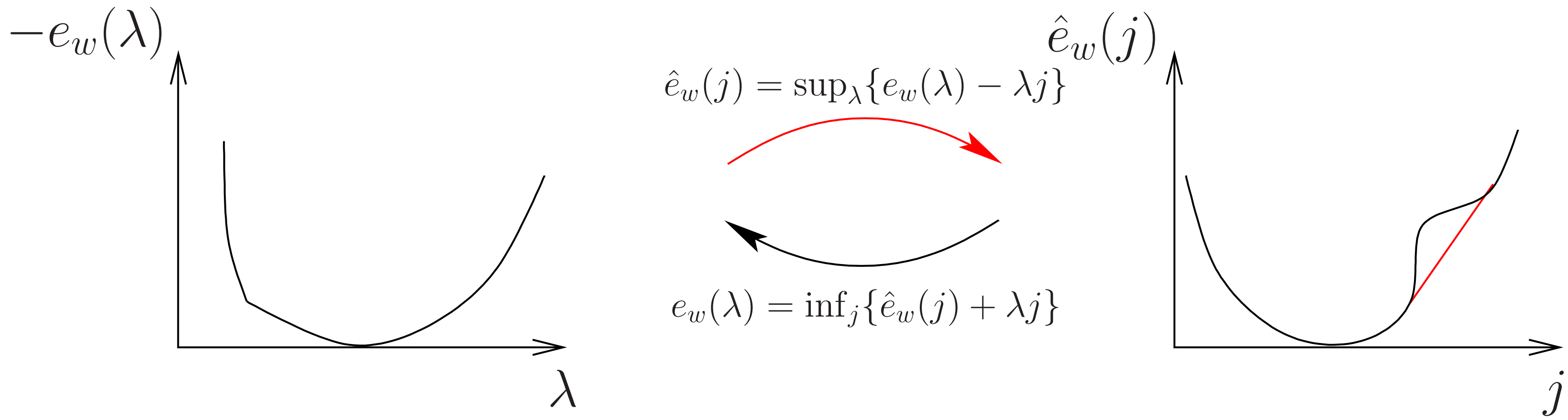
D: $\hat{e}_w(j) = f_j(\alpha, \gamma) + \beta(1-x) + \delta\left(1 - x^{-1}\right) + j \ln x$

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

- Particularly interested in effect of memory on dynamical phase transitions...

Non-convex rate functions

- For $e_w(\lambda)$ non-differentiable, Legendre transform *only* yields convex envelope of $\hat{e}_w(j)$



- For short-range temporal correlations then system can phase separate in time...
  – Gives straight-line section of rate function
- ...But not necessarily so for systems with memory/long-range temporal correlations
  – Non-convex rate functions are possible
- Analogy: long-range spatial correlations in equilibrium give non-concave entropies
- Can we demonstrate this explicitly in ZRP with appropriate current-dependent rates?

Harder problem

- Suppose rates at time t depend not on $q(t)$ but on full history, i.e., $q(\tau)$ for $0 \leq \tau \leq t$.
- Now have an intrinsically non-Markovian problem
- For example, take rates at time t which depend on $q(t/2)$
  - cf. "Alzheimer random walk" [Cressoni *et al.* '07, Kenkre '07]
- In principle, can still use additivity-type approach but have to minimize non-local integral...

Summary

- Have proposed a general approach to calculate current fluctuations in systems with memory-dependent rates

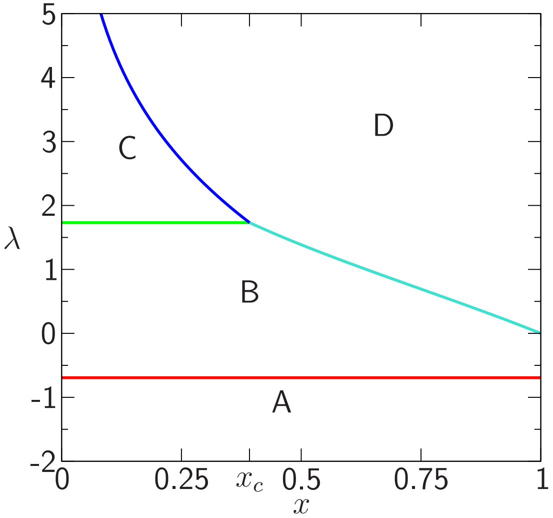
- Long-range temporal correlations in non-equilibrium systems seem to have analogous effects to long-range spatial correlations in equilibrium
  - Modified speed (power of t) in current large deviation principle
  - Possibility of non-convex rate function

- Simple examples offer insight into applicability of fluctuation theorems for non-Markovian systems

References

- Current fluctuations in the zero-range process with open boundaries, R. J. Harris, A. Rákos and G. M. Schütz, J. Stat. Mech., P08003 (2005)
- Breakdown of Gallavotti-Cohen symmetry for stochastic dynamics, R. J. Harris, A. Rákos and G. M. Schütz, Europhys. Lett. **75**, 227 (2006)
- On the range of validity of the fluctuation theorem for stochastic Markovian dynamics, A. Rákos and R. J. Harris, J. Stat. Mech., P05005 (2008)
- Current fluctuations in stochastic systems with long-range memory, R. J. Harris and H. Touchette, J. Phys. A: Math. Theor. **42**, 342001 (2009)

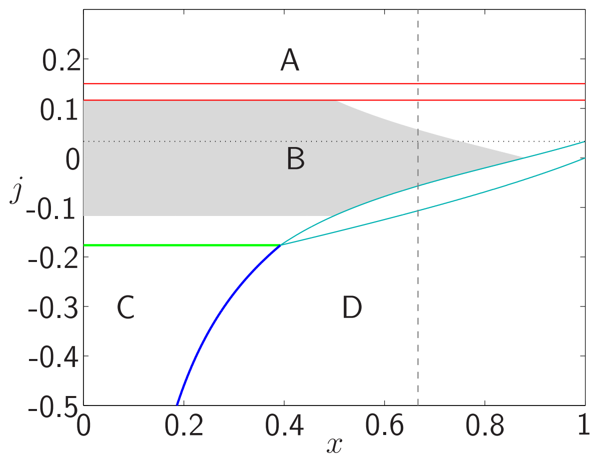
Dynamical phase transitions in 1-site ZRP



$$\longleftrightarrow$$

$$\hat{e}(j) = \sup_{\lambda}\{e(\lambda) - \lambda j\}$$

$$e(\lambda) = \inf_{j}\{\hat{e}(j) + \lambda j\}$$



- Analogy to equilibrium:

$$j \longrightarrow \text{(specific) volume}$$

$$\lambda \longrightarrow \text{pressure}$$

$$\hat{e}(j) \longrightarrow \text{Helmholtz free energy (density)}$$

$$e(\lambda) \longrightarrow \text{Gibbs free energy (density)}$$

$$t \longrightarrow \text{system size}$$

Sketch of argument for temporal additivity principle

1. Divide interval $[t_0, t]$ into N subintervals of length $\Delta\tau$.

2. Chapman-Kolmogorov equation for joint probabilities of being found in configuration σ_i with average current q_i:

$$p(q_N, \sigma_N, t | q_0, \sigma_0, t_0)$$
$$= \sum_{\substack{q_1,\dots,q_{N-1} \\ \sigma_1,\dots,\sigma_{N-1}}} p(q_N, \sigma_N, t | q_{N-1}, \sigma_{N-1}, t_{N-1}) \cdots p(q_2, \sigma_2, t_2 | q_1, \sigma_1, t_1) p(q_1, \sigma_1, t_1 | q_0, \sigma_0, t_0)$$

3. If $\Delta\tau \gg 0$, then assume $p(q_{n+1}, \sigma_{n+1}, t_{n+1} | q_n, \sigma_n, t_n)$ independent of σ_n (true for an ergodic system with finite state space)

$$p(q_N, t | q_0, t_0) = \sum_{q_1,\dots,q_{N-1}} p(q_N, t | q_{N-1}, t_{N-1}) \cdots p(q_2, t_2 | q_1, t_1) p(q_1, t_1 | q_0, t_0)$$

Sketch of argument for temporal additivity principle

4. Now take t and N large whilst preserving their ratio (so $t \gg \Delta\tau \gg 0$); $q(\tau)$ almost constant in each timeslice (adiabatic approx.)

5. Observed average current in timeslice $(t_n, t_{n+1}]$ is

$$q_{\Delta\tau}^{(n)} = \frac{q_{n+1}t_{n+1} - q_n t_n}{\Delta\tau}$$

6. So using *Markovian* large deviation principle have

$$p(q_{n+1}, t_{n+1}|q_n, t_n) \approx A_n e^{-\Delta\tau \hat{e}_{w(q_n)}(q_{\Delta\tau}^{(n)})}$$

7. Putting all the slices together gives

$$p(q_N, t|q_0, t_0) \approx A \sum_{q_1,\dots,q_{N-1}} e^{-\sum_{n=0}^{N-1} \Delta\tau I_{w(q_n)}(q_{\Delta\tau}^{(n)})}.$$

8. Then pass to continuum limit $N, t, \Delta\tau \to \infty$, $q_n \to q(\tau)$

$$p(j, t|j_0, t_0) \sim \int_{q(t_0)=j_0}^{q(t)=j} \mathcal{D}[q]\, e^{-\int_{t_0}^{t} \hat{e}_{w(q)}(q+\tau q')\, d\tau}$$

Sketch of argument for temporal additivity principle

9. In $t \to \infty$ limit, path integral dominated by most probable path in q-space, so

$$\text{Prob}(\mathcal{Q}_t/t = j) \sim \exp\left[-\min_{q(\tau)} \int_{t_0}^{t} \hat{e}_{w(q)}(q + \tau q')\, d\tau\right]$$

   where integral is minimized over all $q(\tau)$ with $q(t_0) = j_0$ and $q(t) = j$

10. To make t-dependence more explicit write

$$\text{Prob}(\mathcal{Q}_t/t = q) \sim e^{-t^\alpha F(j)},$$

   If $F(j)$ exists and is not everywhere zero then have large deviation principle.

$$F(j) = \lim_{t\to\infty} \min_{q(\tau)} \frac{1}{t^\alpha} \int_{t_0}^{t} \hat{e}_{w(q)}(q + \tau q')\, d\tau.$$

If Markovian rate function is known, can find large deviation principle for system with current-dependent rates by minimizing relevant integral...

- Analytically (Euler-Lagrange, Gaussian approximation)
- Numerically

Example 2: Bi-directional random walk with activity dependent rates

- What about fluctuation symmetry?
- Since

$$\text{Prob}(\mathcal{Q}_t/t = j) \sim \begin{cases} \exp[-j t_0^{a+c} \left(\frac{a+c}{a-c}\right) t^{1-a-c}] & \text{for } j \geq 0 \\ \exp[j(\ln \frac{a}{c})t + j t_0^{a+c} \left(\frac{a+c}{a-c}\right) t^{1-a-c}] & \text{for } j < 0. \end{cases}$$

then

$$\frac{\text{Prob}(\mathcal{Q}_t/t = -j)}{\text{Prob}(\mathcal{Q}_t/t = +j)} \sim \exp\left[-j\left(\ln\frac{a}{c}\right)t\right]$$

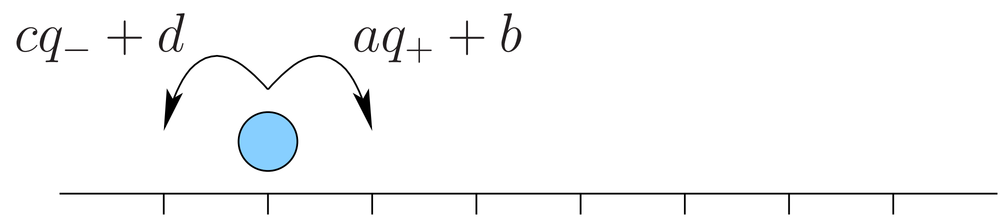
i.e., fluctuation theorem still holds

- Expected here since relative bias is constant $v_R/v_L = a/c$

(also holds for $a + c > 1$ when there is obviously no stationary state)

Example 3: Generalized elephant

- Again consider bi-directional random walk but with rates



- For $a, c < 1$ have mean currents

$$\bar{q}_+ = \frac{b}{1-a}, \qquad \bar{q}_- = \frac{d}{1-c} \qquad \text{and} \qquad \bar{q} = \bar{q}_+ - \bar{q}_-$$

- Gaussian expansion (about means) and minimization of integral gives, for $a = c$:

  – $0 < a < 1/2$, diffusive behaviour:

$$\text{Prob}(\mathcal{Q}_t/t = j) \sim \exp\left\{ -\left[\frac{1}{2} \frac{\left(j - \frac{b-d}{1-a}\right)^2}{\frac{b+d}{(1-a)(1-2a)}} \right] t \right\}$$

  – $1/2 < a < 1$, superdiffusive behaviour:

$$\text{Prob}(\mathcal{Q}_t/t = j) \sim \exp\left\{ -\left[\frac{1}{2} \frac{\left(j - \frac{b-d}{1-a}\right)^2}{\frac{b+d}{(1-a)(2a-1)}} \right] t_0^{2a-1} t^{2-2a} \right\}$$

(generalization of results for original symmetric discrete-time elephant)

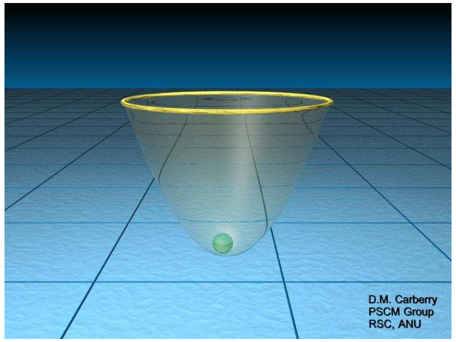
Example 3: Generalized elephant

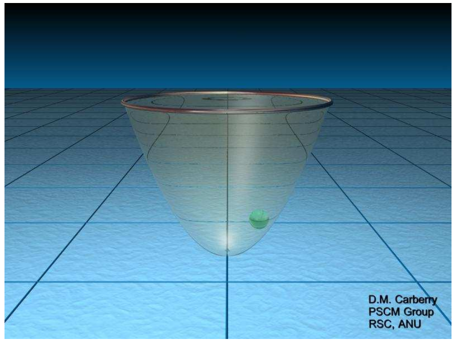
- Within this Gaussian approximation

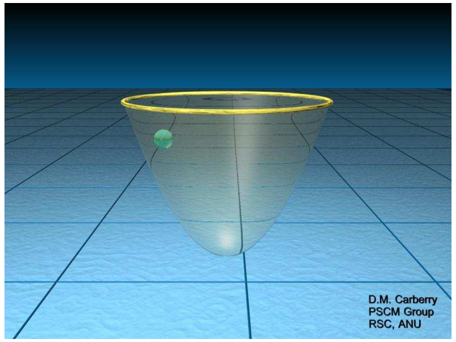
$$\frac{\text{Prob}(\mathcal{Q}_t/t=-j)}{\text{Prob}(\mathcal{Q}_t/t=+j)} \sim \begin{cases} \exp\left[-j\frac{2(b-d)(1-2a)}{1-a}t\right] & \text{for } 0<a<1/2 \\ \exp\left[-j\frac{2(b-d)(1-2a)}{1-a}t_0^{2a-1}t^{2-2a}\right] & \text{for } 1/2<a<1. \end{cases}$$

- Both cases have well-defined mean stationary current...
- ...but only have usual fluctuation symmetry for $0<a<1/2$
- For $1/2<a<1$ symmetry is apparently modified by superdiffusive spreading about the mean
  - Logarithm of probabilities for forward and backward currents still asymptotically proportional to j but sublinear in t
- Scenario merits closer investigation

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)

Non-equilibrium fluctuation theorems

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

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

1. Computer simulations of sheared fluids [D.Evans *et al.* '93]
2. Steady state of deterministic systems [Gallavotti & Cohen '95]:

- $\mathcal{X}$ is rate of phase space contraction

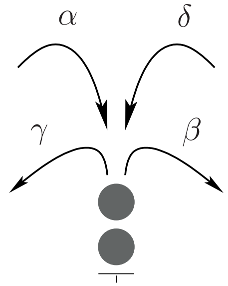
3. Stochastic systems (with bounded state space) [Lebowitz & Spohn '99]

- $\mathcal{X}$ can often be identified with average particle current
- Symmetry $\tilde{H}(\lambda)^T = P_{\mathrm{eq}}^{-1}\tilde{H}(E-\lambda)P_{\mathrm{eq}} \quad \Rightarrow \quad e(\lambda) = e(E-\lambda)$
- *But the zero-range process has unbounded state space!*

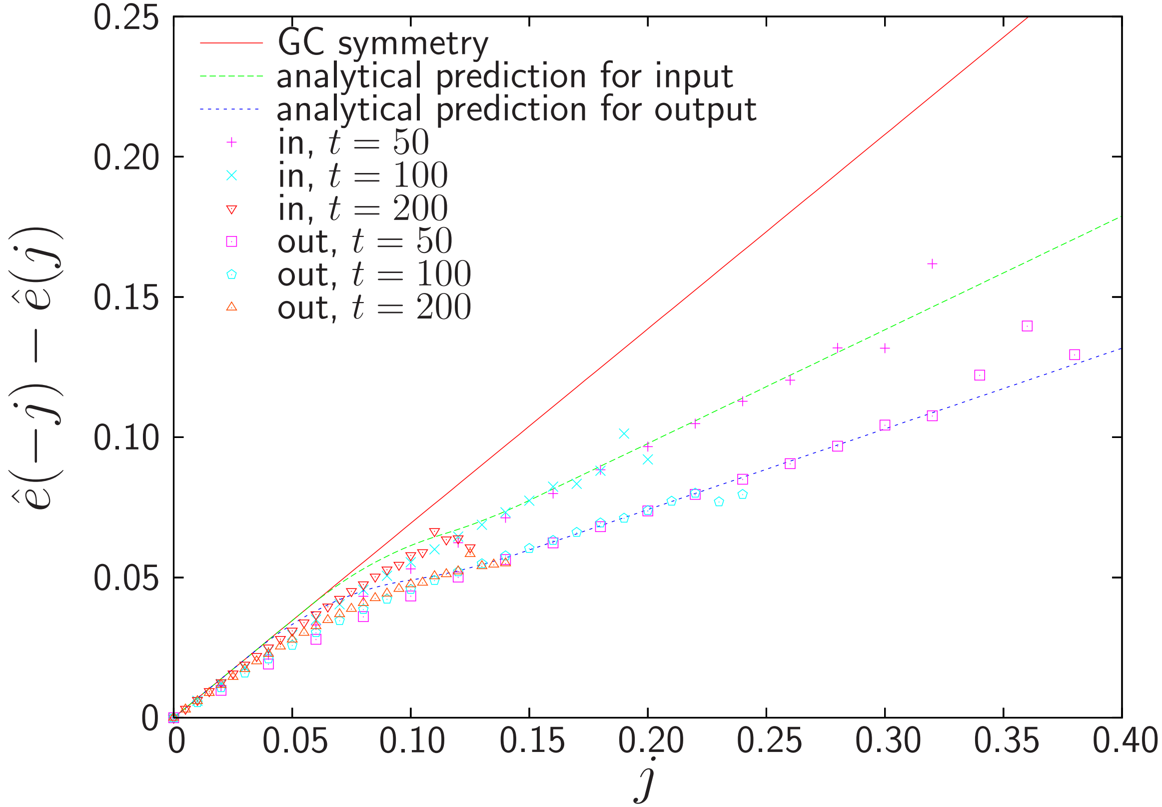
Back to single-site ZRP

- Prediction:

$$\frac{p(-j,t)}{p(j,t)} \sim e^{-Ejt} \quad \text{with } E \text{ an effective field}$$



- e.g., 1 site ZRP with steady-state initial condition:



- *Breakdown of Gallavotti-Cohen symmetry*

  — Physically due to "instantaneous condensates"

Fluctuation Theorems: General perspective

- Consider "dissipation function" $W(t)$ [for $w_n = 1$]

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

- 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 $(\sum_{i=0}^{L} E_i) J_l$
- **For unbounded state space, boundary terms are non-vanishing and GC symmetry can be violated**
- Analogous effects due to unbounded potentials:
  - Deterministic forces, single-particle Langevin dynamics
    [Bonetto *et al.* '05, van Zon & Cohen '03, Farago '02, Baiesi *et al.* '06]

[Experimentally relevant, e.g., trapped colloids, granular media, electric circuits, ...]