Rare current events in non-equilibrium systems with long-range memory

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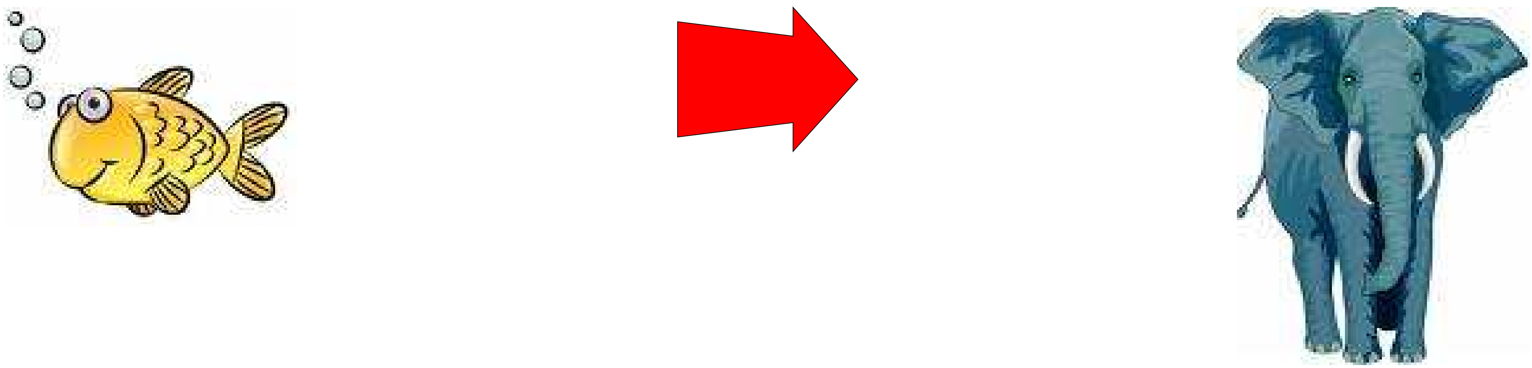
Computation of Transition Trajectories and Rare Events in
Non-Equilibrium Systems, Dresden, June 12th 2012

Current fluctuations

- Current large deviations quantify asymptotic probability of rare fluctuations
- Microscopic and macroscopic approaches to calculation
- Most previous work for Markov systems...

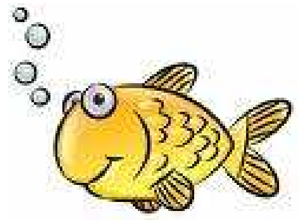
- **What happens if we add memory?**



Outline

- Introduction
- General approach for current-dependent rates
  - "Temporal additivity principle"
    [RJH and H. Touchette: J. Phys. A: Math. Theor. **42**, 342001 (2009)]
    * Toy example: random walk
  - Expansion about fixed-points
- Applications to many-particle systems
  - Example: Totally Asymmetric Simple Exclusion Process
    * Modified phase diagram, (super-)diffusive fluctuations, simulation
    * Comparison of approximation with exact numerics
  - Fluctuation symmetry for current-dependent processes?
  - Non-convex rate functions
- Summary and outlook

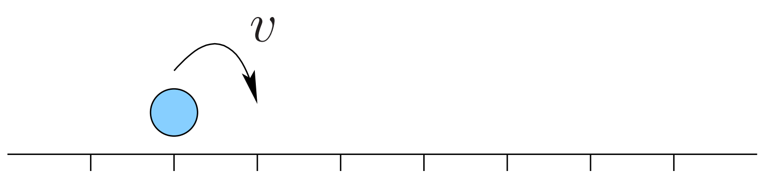
Introduction: Memoryless systems



- Discrete-space, continuous-time Markov process
  - Configurations $\sigma(t)$
  - Transition rates $w_{\sigma',\sigma}$
  - Non-equilibrium systems characterized by (time-integrated) currents $\mathcal{J}_t$
  - Typically have large deviation principle

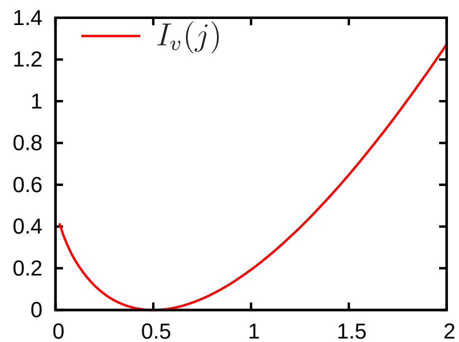
$$\text{Prob}(\mathcal{J}_t/t = j) \sim e^{-I_w(j)t}$$

- Toy example: Single particle hopping rightwards on an infinite lattice

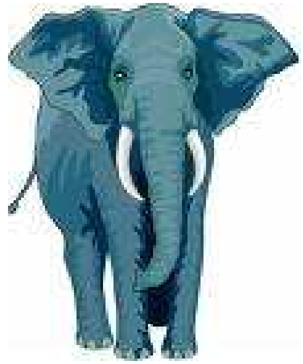


  - Let $\mathcal{J}_t$ count the number of jumps up to time t
  - Large deviation function given by

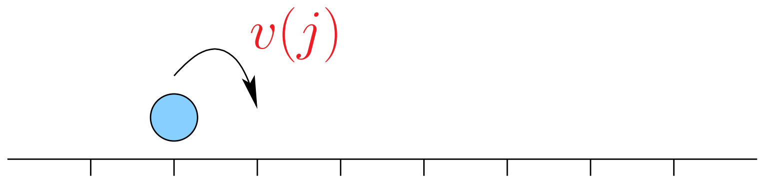
$$I_v(j) = v - j + j \ln \frac{j}{v}$$



Introduction: Adding memory



- Many ways to introduce memory
- We consider *current-dependent* rates
- Class of processes where $w_{\sigma',\sigma}$ depend explicitly on σ, σ' *and* $\mathcal{J}_t/t$
  (To avoid singularities, assume initial time 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
- Back to toy example:



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

Temporal additivity principle

- Claim: [RJH and Touchette '09]

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

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

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

Temporal additivity principle

- To make t-dependence more explicit write

$$\text{Prob}(\mathcal{J}_t/t = j) \sim e^{-t^\alpha \tilde{I}(j)},$$

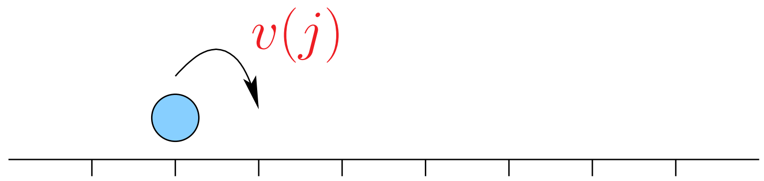
  If $\tilde{I}(j)$ exists and is not everywhere zero then have large deviation principle with

$$\tilde{I}(j) = \lim_{t\to\infty} \min_{j(\tau)} \frac{1}{t^\alpha} \int_{t_0}^{t} I_{w(j)}(j + \tau j')\, d\tau.$$

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

- But very few analytically solvable cases so...
  - Toy example (random walk)
  - Approximation (TASEP)
  - Exact numerics (TASEP)

Toy example: Uni-directional random walk



- Euler-Lagrange equation:

$$\frac{dv}{dj} - j\frac{dv/dj}{v} - \frac{2\tau j'}{j+\tau j'} - \frac{\tau^2 j''}{j+\tau j'} = 0$$

- Consider case $v(j) = aj$ (rate proportional to average velocity so far)
- *Results depend on a:*
  - $a > 1$, 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-a}

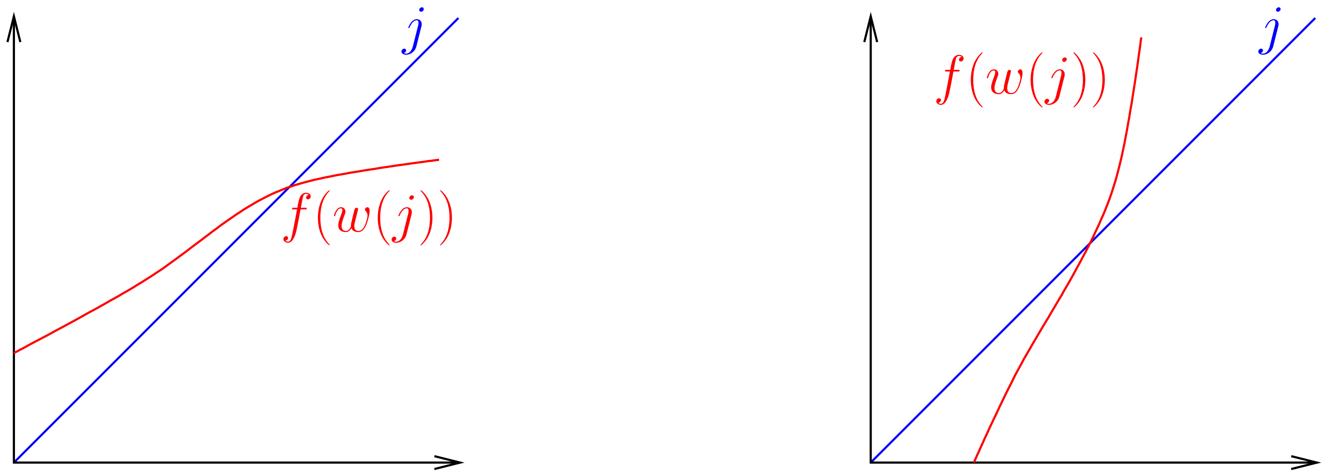
$$\text{Prob}(\mathcal{J}_t/t = j) \sim e^{-jt_0^a t^{1-a}}, \qquad \text{for } j > 0$$

    - ∗ Transition from subdiffusive regime to superdiffusive regime at $a = 1/2$

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

Fixed points, stability

- Mean current in memoryless case, given by $\bar{j} = f(w)$
- Fixed-point in current-dependent case at $j^* = f(w(j^*))$
- Two possible scenarios:



- Stability determined by slope

$$A^* = \left.\frac{\partial f}{\partial j}\right|_{j=j^*}$$

$A^* < 1 \implies$ stable $\qquad A^* > 1 \implies$ unstable

Expansion about fixed point

- Assume only one stable fixed point j^*
- Expanding to second order about this fixed point, E-L equations have solution

$$j(\tau) = j^* + K_1 \tau^{-A^*} + K_2 \tau^{A^*-1}$$

- ...fixing boundary conditions and integrating gives

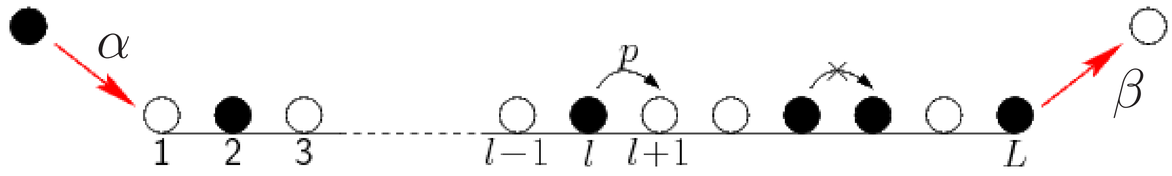
$$\text{Prob}(\mathcal{J}_t/t = j) \sim \begin{cases} \exp\left[\frac{(1-2A^*)(j-j^*)^2}{2D^*} t\right] & \text{for } A^* < \frac{1}{2} \\ \exp\left[\frac{(2A^*-1)(j-j^*)^2}{2D^*} t_0^{2A^*-1} t^{2-2A^*}\right] & \text{for } A^* > \frac{1}{2} \end{cases}$$

with

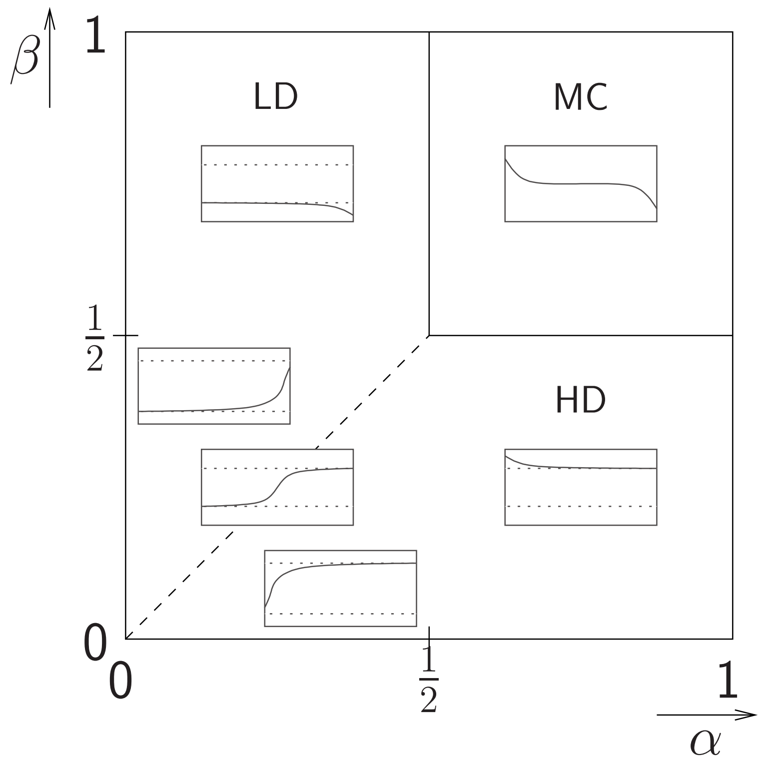
$$D^* = \left(I''_{w(j)}(j) \Big|_{j=j^*} \right)^{-1}$$

- Transition at $A^* = \frac{1}{2}$
  - For $A^* < \frac{1}{2}$ have diffusive behaviour with modified diffusion coefficient
  - For $A^* > \frac{1}{2}$ have superdiffusive behaviour

Example 1: Totally Asymmetric Exclusion Process



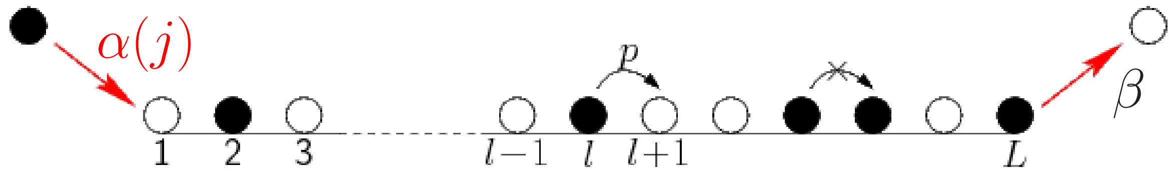
- Well-known phase diagram ($p = 1$):



- Current large deviations known in all phases [Lazarescu & Mallick '11]...

  ...but can already get some information by expanding about fixed points

Current-dependent TASEP



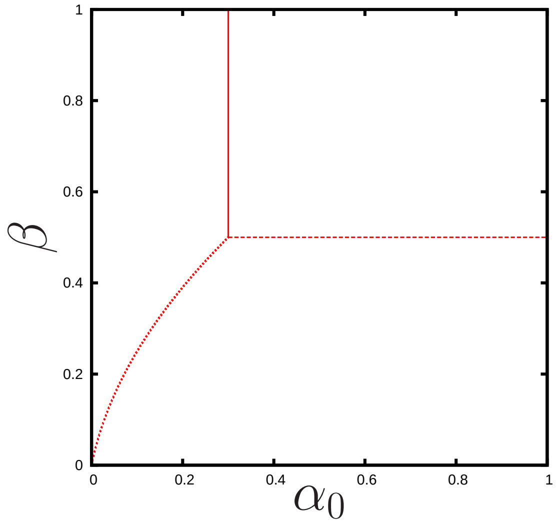
- Consider current-dependent input rate $\alpha(j)$
- Fixed points given by

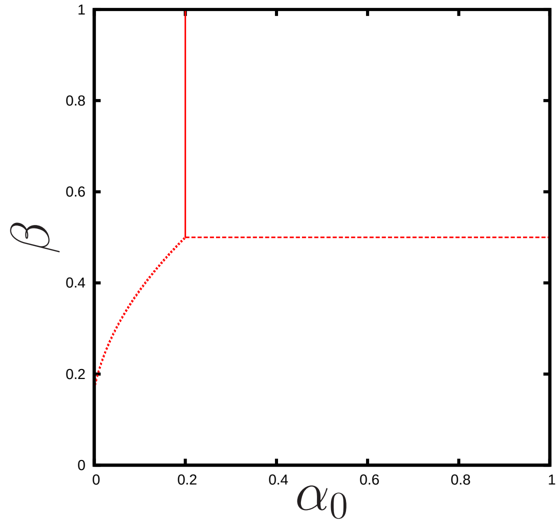
$$j^* = \begin{cases} \frac{1}{4} & \text{for } \alpha(j^*) > \frac{1}{2}, \beta > \frac{1}{2} \\ \alpha(j^*)(1-\alpha(j^*)) & \text{for } \alpha(j^*) < \frac{1}{2}, \beta > \alpha(j^*) \\ \beta(1-\beta) & \text{for } \alpha(j^*) > \beta, \beta < \frac{1}{2} \end{cases}$$

- For example, set $\alpha(j) = \alpha_0 + aj$ (with $a > 0$) [cf. Sharma & Chowdhury '11]:
  - Get modified phase diagram in (α_0, β) plane
  - LD–MC transition at $\alpha_0 = \frac{1}{2} - \frac{a}{4}$
  - LD–HD transition at $\beta = \frac{-(1-a)+\sqrt{(1-a)^2+4a\alpha_0}}{2a}$.

Current-dependent TASEP, phase diagram

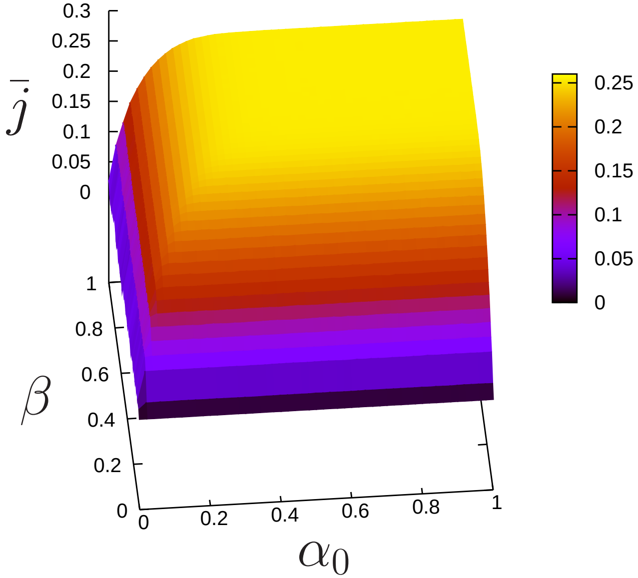
$$\alpha(j) = \alpha_0 + aj$$

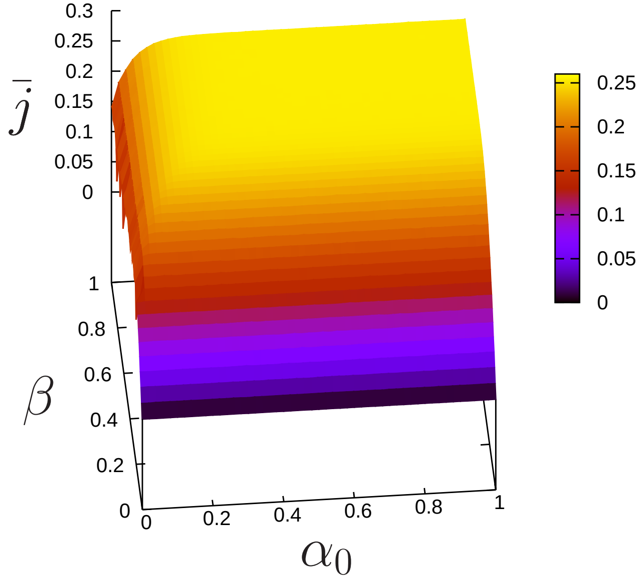




$a = 0.8$

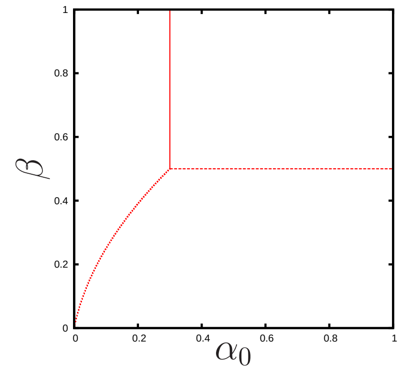
$a = 1.2$

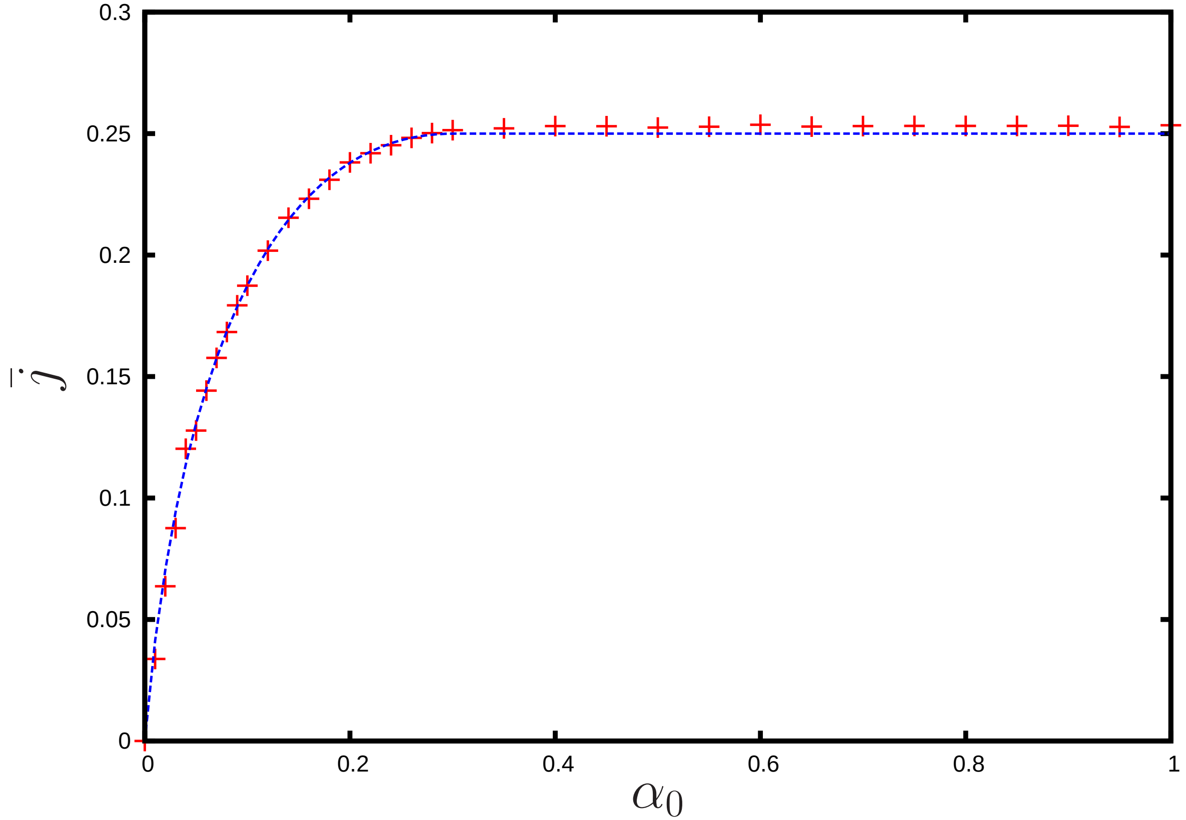




Current-dependent TASEP, mean current

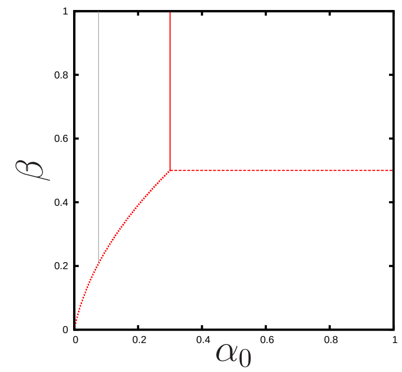
- Fixed point j^* determines mean current in different phases
- In LD phase have $j^* = \frac{-(2\alpha_0 a + 1 - a) + \sqrt{(1-a)^2 + 4\alpha_0 a}}{2a^2}$
- Simulation for $\beta = 0.6$, $a = 0.8$:

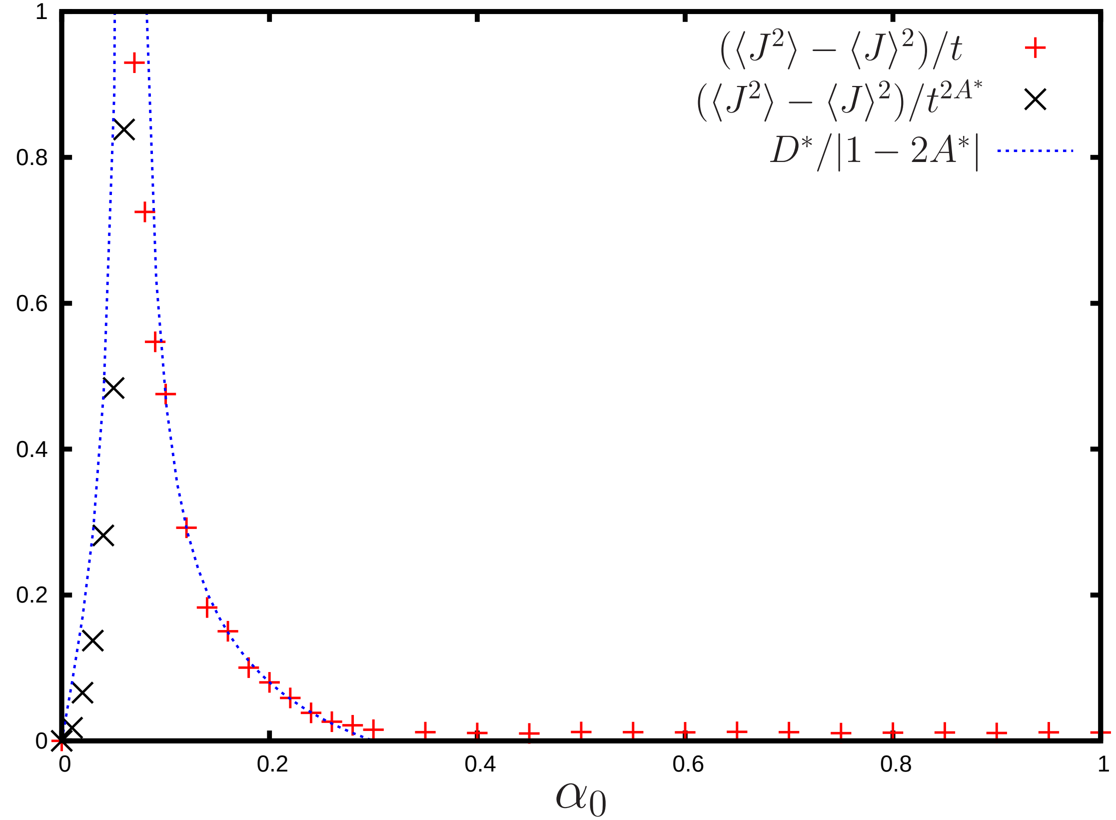




Current-dependent TASEP, fluctuations

- In LD phase, have $A^* = 1 - \sqrt{(1-a)^2 + 4a\alpha_0}$
- Fluctuations superdiffusive for $\alpha_0 < \alpha_c = \frac{1/4-(1-a)^2}{4a}$
- Simulation for $\beta = 0.6$, $a = 0.8$, $\alpha_c \approx 0.066$:



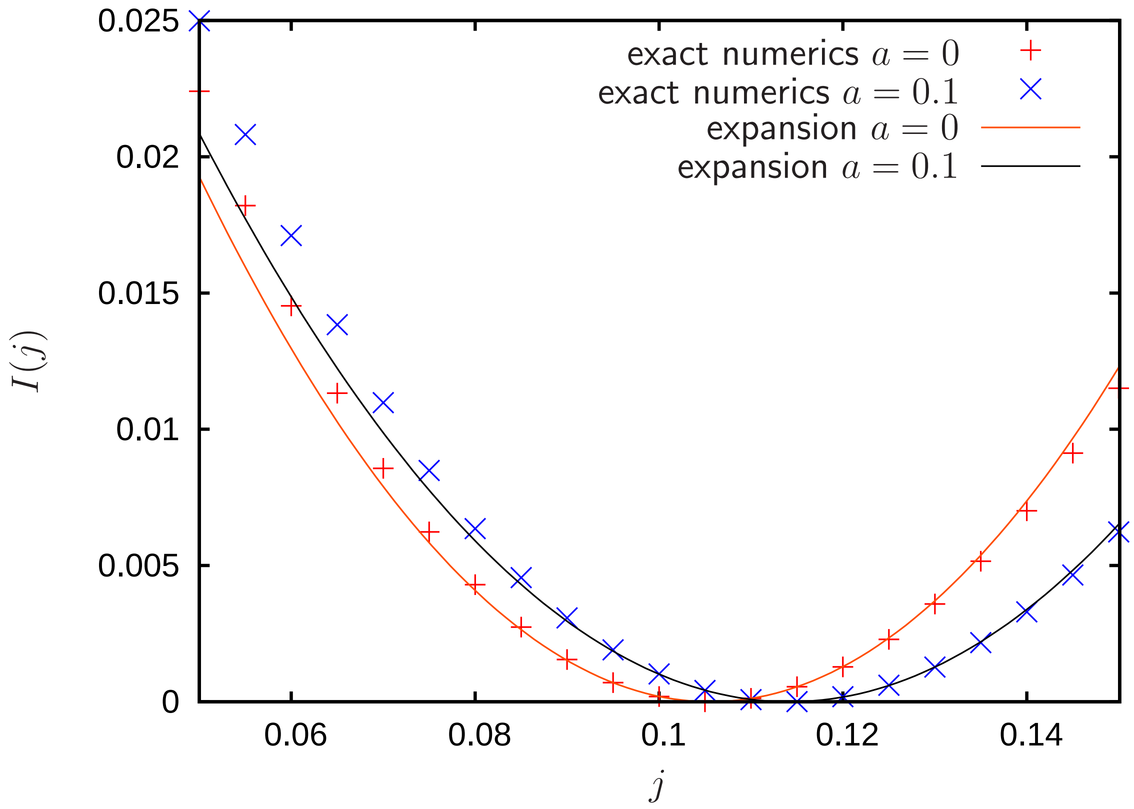


Current-dependent TASEP, comparison with exact numerics

- $L \to \infty$ limit for current fluctuations in low-density phase [Lazarescu & Mallick '11]:

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

- Can Legendre transform this to get $I(j)$ and then solve E-L equations numerically
- Comparison for $\alpha(j) = \alpha_0 + aj$ with $\alpha_0 = 0.12$:



Fluctuation symmetry for current-dependent processes?

- Second-order expansion about fixed point yields

$$\frac{\text{Prob}(\mathcal{J}_t/t = -j)}{\text{Prob}(\mathcal{J}_t/t = j)} \sim \begin{cases} \exp\left[-\frac{2(1-2A^*)j^*}{D^*} \times jt\right] & \text{for } A^* < \frac{1}{2} \\ \exp\left[-\frac{2(2A^*-1)j^*}{D^*} t_0^{2A^*-1} \times jt^{2-2A^*}\right] & \text{for } A^* > \frac{1}{2} \end{cases}$$

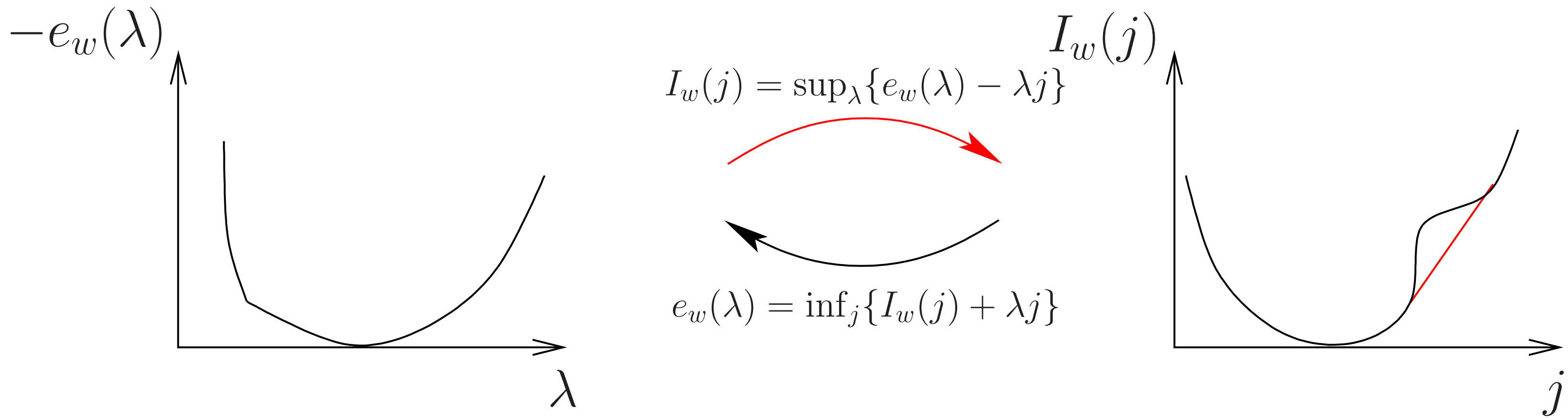
- Cf. modified symmetry for anomalous dynamics found in [Chechkin & Klages '09]

- *Open question: does symmetry still hold in tails of distribution?*

  – Answer from structure of E-L equations?

Non-convex rate functions

- For $e_w(\lambda)$ non-differentiable, Legendre transform *only* yields convex envelope of $I_w(j)$



- 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 explicitly, e.g., for zero-range process with current-dependence?

Summary and outlook

- General approach to current fluctuations in systems with memory-dependent rates
  - "Temporal additivity principle"
  - Expansion about fixed points
- For totally asymmetric exclusion process, with input rate $\alpha(j) = \alpha_0 + aj$, predict superdiffusive regime in phase diagram
- 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 (e.g., in ZRP with bounded rates)
- Outlook:
  - More work on fluctuation theorems for non-Markovian systems
  - Hydrodynamic limit
  - Intrinsically non-Markovian processes...

Harder problem

- Suppose rates at time t depend not on $j(t)$ but on full history, i.e., $j(\tau)$ for $0 \leq \tau \leq t$.
- Now have an intrinsically non-Markovian problem
- For example, take rates at time t which depend on $j(t/2)$
  - 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...

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 j_i:

$$\begin{aligned} &p(j_N, \sigma_N, t | j_0, \sigma_0, t_0) \\ &= \sum_{\substack{j_1,\ldots,j_{N-1} \\ \sigma_1,\ldots,\sigma_{N-1}}} p(j_N, \sigma_N, t | j_{N-1}, \sigma_{N-1}, t_{N-1}) \cdots p(j_2, \sigma_2, t_2 | j_1, \sigma_1, t_1) p(j_1, \sigma_1, t_1 | j_0, \sigma_0, t_0) \end{aligned}$$

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

$$p(j_N, t | j_0, t_0) = \sum_{j_1,\ldots,j_{N-1}} p(j_N, t | j_{N-1}, t_{N-1}) \cdots p(j_2, t_2 | j_1, t_1) p(j_1, t_1 | j_0, t_0)$$

Sketch of argument for temporal additivity principle

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

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

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

6. So using *Markovian* large deviation principle have

$$p(j_{n+1}, t_{n+1}|j_n, t_n) \approx A_n e^{-\Delta\tau I_{w(j_n)}(j_{\Delta\tau}^{(n)})}$$

7. Putting all the slices together gives

$$p(j_N, t|j_0, t_0) \approx A \sum_{j_1,\ldots,j_{N-1}} e^{-\sum_{n=0}^{N-1} \Delta\tau I_{w(j_n)}(j_{\Delta\tau}^{(n)})}.$$

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

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

Sketch of argument for temporal additivity principle

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

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

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

10. To make t-dependence more explicit write

$$\text{Prob}(\mathcal{J}_t/t = j) \sim e^{-t^{\alpha}\tilde{I}(j)},$$

If $\tilde{I}(j)$ exists and is not everywhere zero then have large deviation principle.

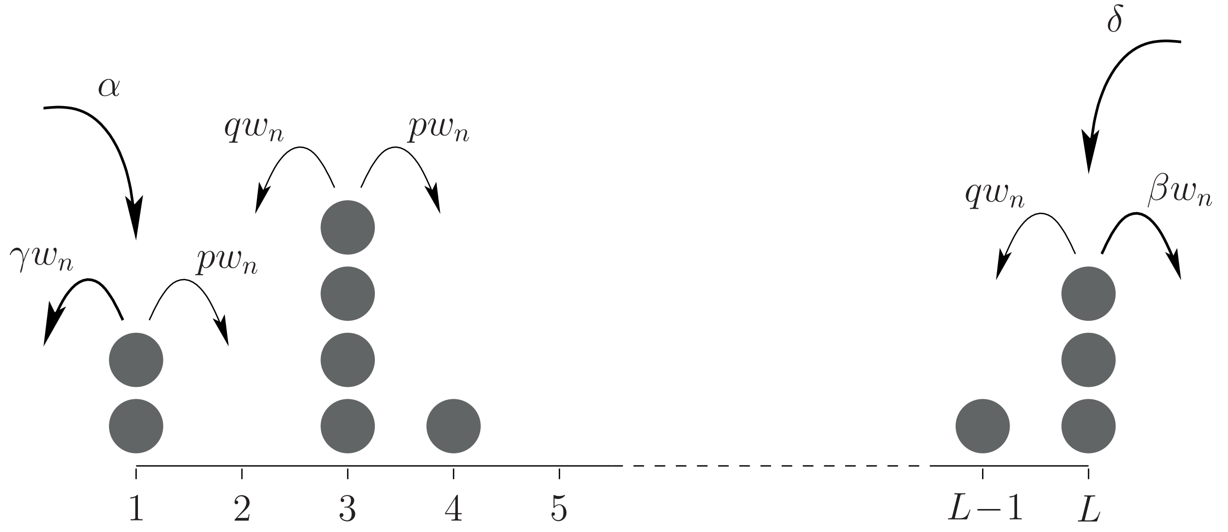
$$\tilde{I}(j) = \lim_{t\to\infty} \min_{j(\tau)} \frac{1}{t^{\alpha}} \int_{t_0}^{t} I_{w(j)}(j + \tau j')\, d\tau.$$

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

- But very few analytically solvable examples...

Example: Zero-Range Process

- 1d *open-boundary* ZRP [Levine et al. '05]:



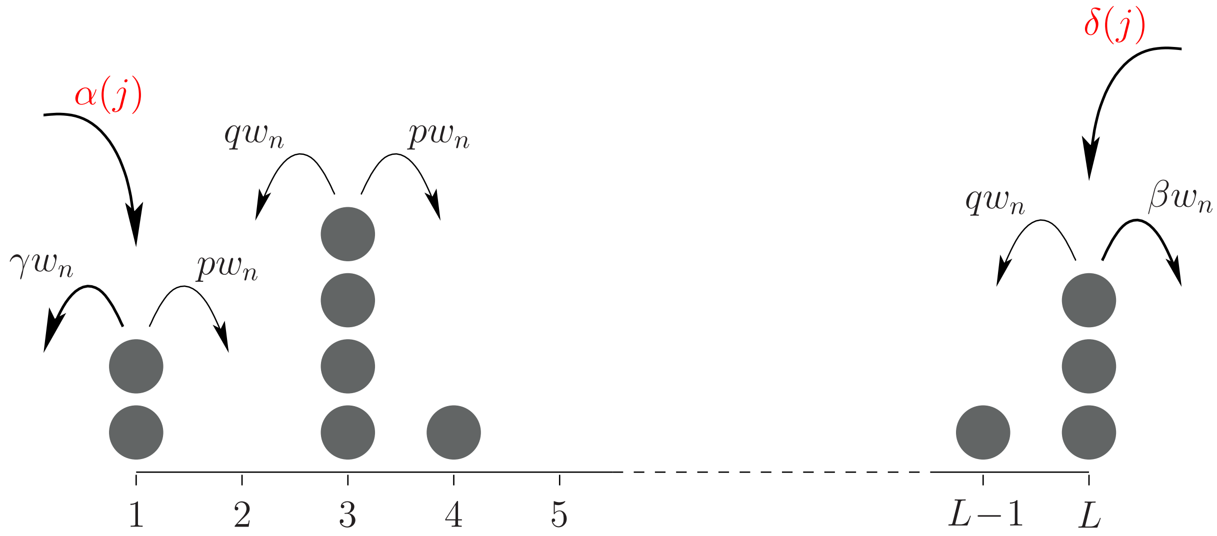
- No condensation if $w_n \to \infty$ as $n \to \infty$
- Current rate function known in Markovian case

$$I(j) = \frac{(p-q)[\alpha\beta(p/q)^{L-1}+\gamma\delta]}{\gamma(p-q-\beta)+\beta(p-q+\gamma)(p/q)^{L-1}} - \sqrt{j^2 + \frac{4\alpha\beta\gamma\delta(p/q)^{L-1}(p-q)^2}{[\gamma(p-q-\beta)+\beta(p-q+\gamma)(p/q)^{L-1}]^2}}$$
$$- j\ln\left[\frac{2\alpha\beta(p/q)^{L-1}(p-q)}{\gamma(p-q-\beta)+\beta(p-q+\gamma)(p/q)^{L-1}}\right] + j\ln\left[j + \sqrt{j^2 + \frac{4\alpha\beta\gamma\delta(p/q)^{L-1}(p-q)^2}{[\gamma(p-q-\beta)+\beta(p-q+\gamma)(p/q)^{L-1}]^2}}\right].$$

[RJH, Rákos and Schütz, '05]

Current-dependent ZRP

- Choose current-dependent input rates



- Solve Euler-Lagrange equations numerically with

$$\alpha(j) = \alpha e^{a(j-j_c)} \qquad \text{and} \qquad \delta(j) = \delta e^{-a(j-j_c)}$$

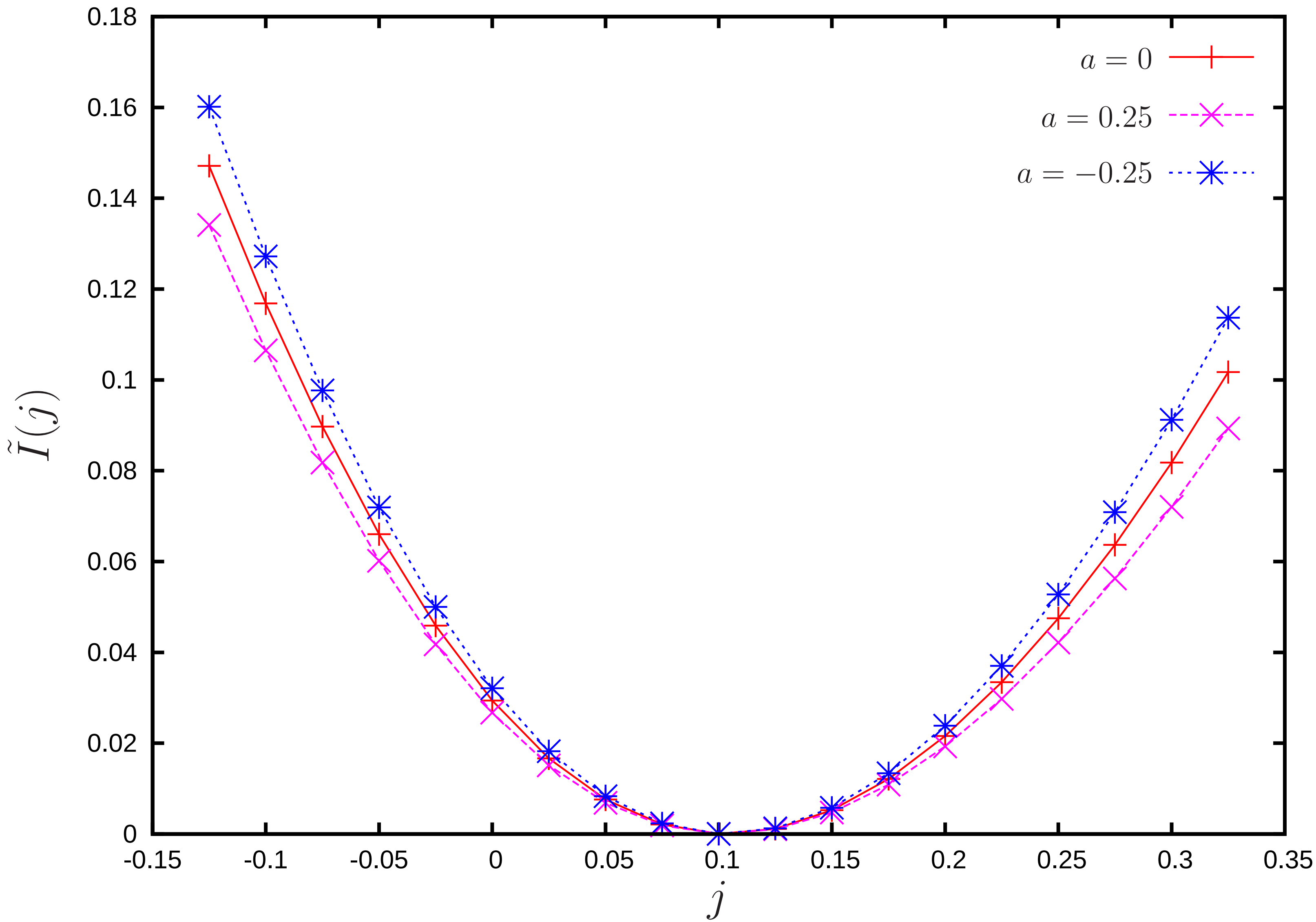
- For all values of a have fixed point at

$$j^* = j_c = \frac{\alpha\beta - \gamma\delta}{\beta + \gamma}$$

- Numerical parameters: $\alpha = 1$, $b = 1.5$, $c = 1$, $d = 1$, $p = 1.1$, $q = 1$, $L = 5$

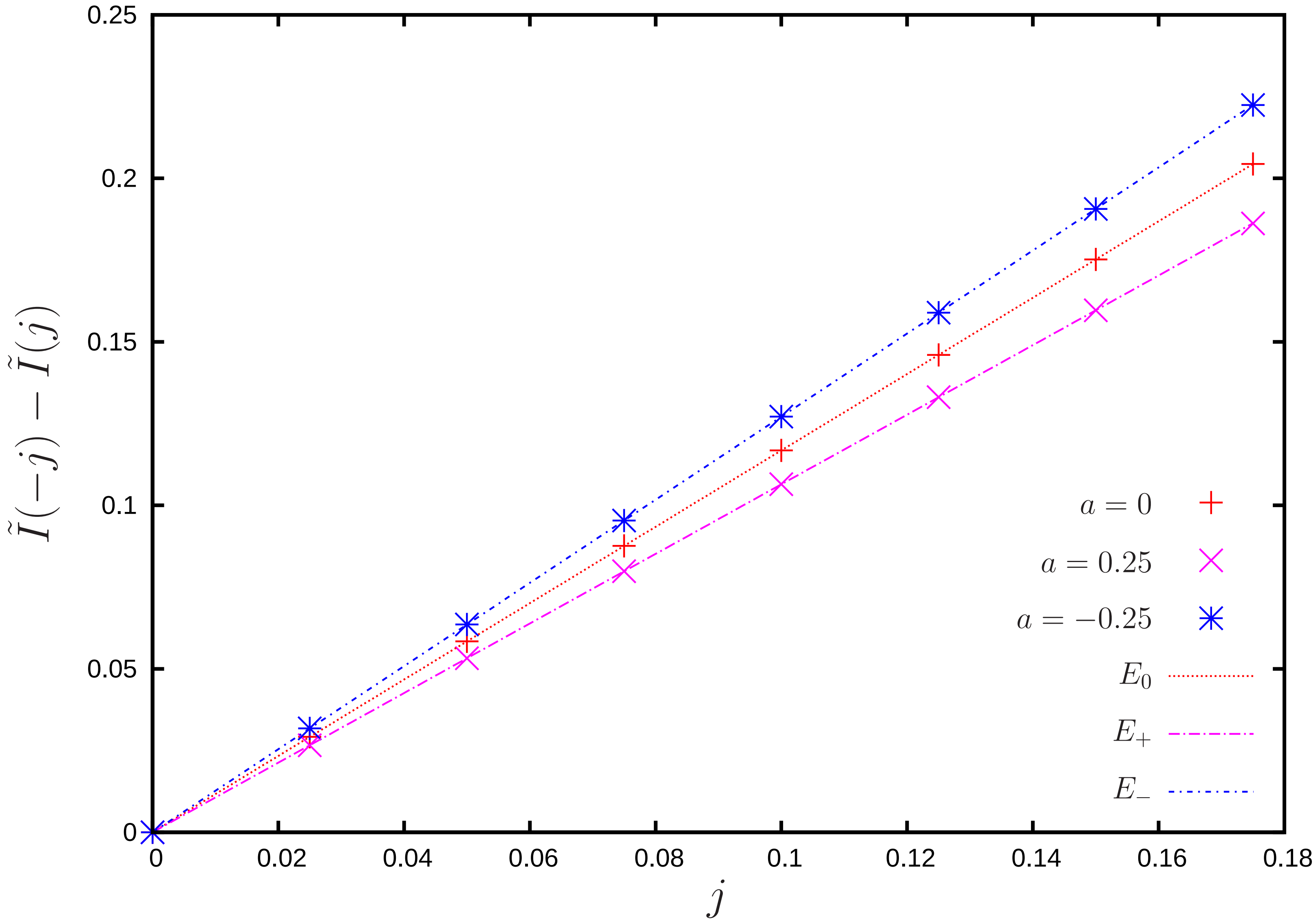
Current-dependent ZRP, rate function

- Numerical solution beyond Gaussian regime:



Current-dependent ZRP, fluctuation symmetry

- Test of fluctuation symmetry $\tilde{I}(-j) - \tilde{I}(j) = Ej$

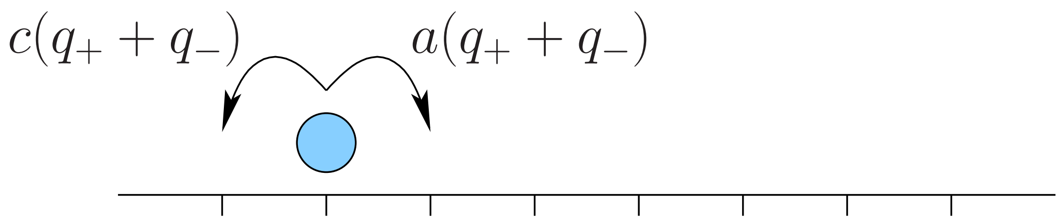


Example: Bi-directional random walk with activity dependent rates

- 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"



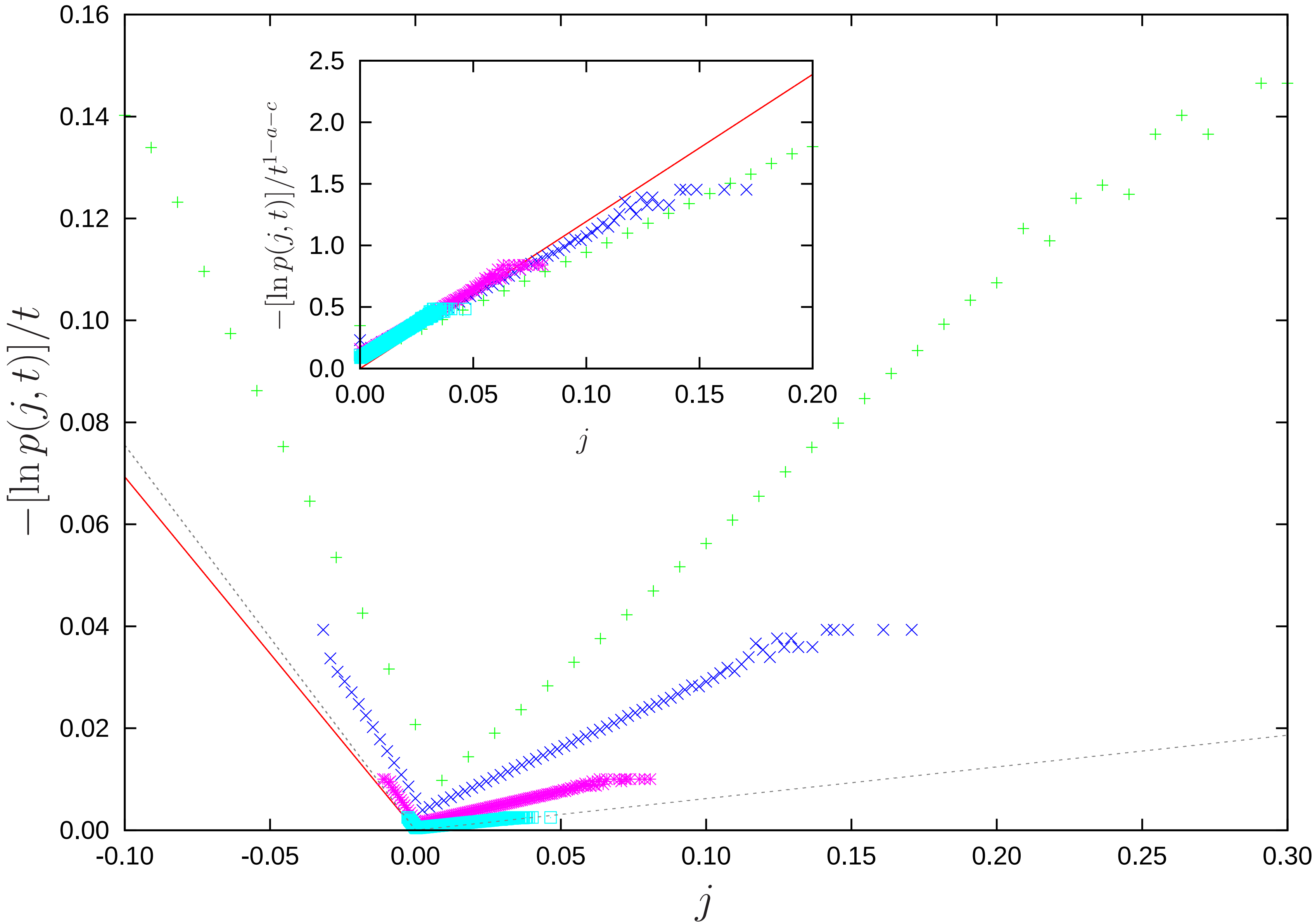
- Without loss of generality take $a > c$, i.e., drive to right
- For $a + c < 1$ there is a stationary state with

$$\text{Prob}(\mathcal{Q}_t/t = j) \sim \begin{cases} \exp[-jt_0^{a+c}\left(\frac{a+c}{a-c}\right)t^{1-a-c}] & \text{for } j \geq 0 \\ \exp[j(\ln\frac{a}{c})t + jt_0^{a+c}\left(\frac{a+c}{a-c}\right)t^{1-a-c}] & \text{for } j < 0. \end{cases}$$

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

Example: Bi-directional random walk with activity dependent rates

Comparison with simulation:



Example: Bi-directional random walk with activity dependent rates

- What about fluctuation symmetry?
- Since

$$\text{Prob}(\mathcal{Q}_t/t = j) \sim \begin{cases} \exp[-jt_0^{a+c}\left(\frac{a+c}{a-c}\right)t^{1-a-c}] & \text{for } j \geq 0 \\ \exp[j(\ln\frac{a}{c})t + jt_0^{a+c}\left(\frac{a+c}{a-c}\right)t^{1-a-c}] & \text{for } j < 0. \end{cases}$$

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 no stationary state)