Large Deviations of the Current in the Open Exclusion Process

K. Mallick

Institut de Physique Théorique, CEA Saclay (France)

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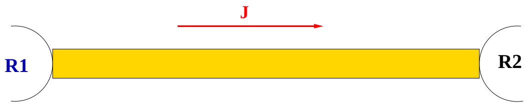
Systems far from equilibrium

Consider a Stationary Driven System in contact with reservoirs at different potentials: no microscopic theory is yet available.



- What are the relevant macroscopic parameters?
- Which functions describe the state of a system?
- Do Universal Laws exist? Can one define Universality Classes?
- Can one postulate a general form for the microscopic measure?
- What do the fluctuations look like ('non-gaussianity')?

In the steady state, a non-vanishing macroscopic current J flows.

Our aim is to study the statistics of this current and its large deviations starting from a microscopic model.

Large Deviations of the Total Current

Let Y_t be the total charge transported through the system (total current) between time 0 and time t.

In the stationary state, a non-vanishing mean-current: $\frac{Y_t}{t} \to J$

The fluctuations of Y_t obey a Large Deviation Principle:

$$P\left(\frac{Y_t}{t} = j\right) \sim e^{-t\Phi(j)}$$

$\Phi(j)$ being the *large deviation function* of the total current.

Equivalently, the moment-generating function, which when $t \to \infty$, behaves as

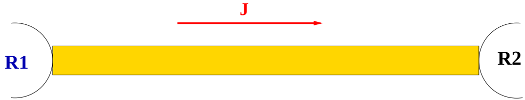
$$\left\langle \mathrm{e}^{\mu Y_t} \right\rangle \simeq \mathrm{e}^{E(\mu)t}$$

They are related by Legendre transform: $\boxed{E(\mu) = \max_j\left(\mu j - \Phi(j)\right)}$

Large deviation functions play an important role in non-equilibrium statistical mechanics (*Fluctuation Theorem*).

Classical Transport in 1d: ASEP

A paradigm of a non-equilibrium system



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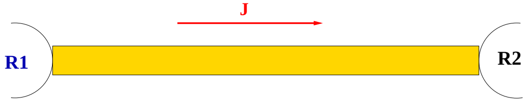
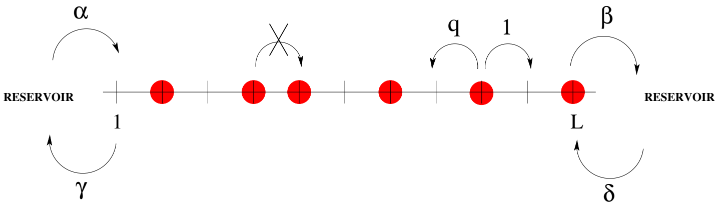
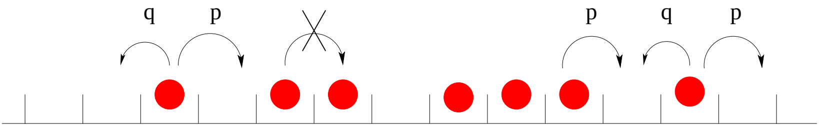


The asymmetric exclusion model with open boundaries



The Exclusion Process



Asymmetric Exclusion Process. A paradigm for non-equilibrium Statistical Mechanics.

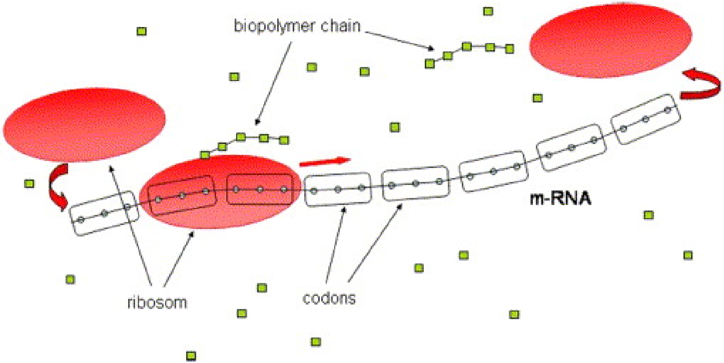
- EXCLUSION: Hard core-interaction; at most 1 particle per site.
- ASYMMETRIC: External driving; breaks detailed-balance
- PROCESS: Stochastic Markovian dynamics; no Hamiltonian.

The probability $P_t(\mathcal{C})$ to find the system in the microscopic configuration $\mathcal{C}$ at time t satisfies

$$\frac{dP_t(\mathcal{C})}{dt} = MP_t(\mathcal{C})$$

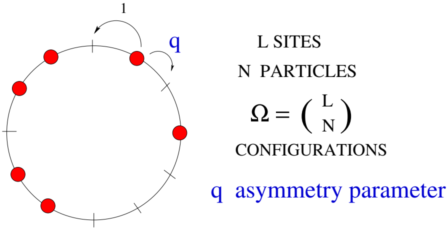
The Markov Matrix M encodes transitions rates amongst configurations.

Elementary Model for Protein Synthesis



C. T. MacDonald, J. H. Gibbs and A.C. Pipkin, Kinetics of biopolymerization on nucleic acid templates, *Biopolymers* (1968).

Current Fluctuations on a ring



The total current, Y_t, corresponds to the total distance covered by all the N particles, hopping on a ring of size L, between time 0 and time t.

The moment-generating function defined as

$$\left\langle \mathrm{e}^{\mu Y_t} \right\rangle \simeq \mathrm{e}^{E(\mu)t}$$

can be identified to the dominant eigenvalue of a μ-deformed process:

On a ring this is solvable by Bethe Ansatz.

Totally Asymmetric Case (Derrida Lebowitz 1998)

For $q = 0$ on a ring, $E(\mu)$ is calculated thanks to the decoupling property of the Bethe equations.

The structure of the solution is given by a parametric representation of the cumulant generating function $E(\mu)$:

$$\begin{aligned} \mu &= -\frac{1}{L}\sum_{k=1}^{\infty} \frac{[kL]!}{[kN]!\,[k(L-N)]!}\frac{B^k}{k}\,, \\ E &= -\sum_{k=1}^{\infty} \frac{[kL-2]!}{[kN-1]!\,[k(L-N)-1]!}\frac{B^k}{k}\,. \end{aligned}$$

Mean Total current:

$$J = \lim_{t\to\infty} \frac{\langle Y_t \rangle}{t} = \frac{N(L-N)}{L-1}$$

Diffusion Constant:

$$D = \lim_{t\to\infty} \frac{\langle Y_t^2 \rangle - \langle Y_t \rangle^2}{t} = \frac{LN(L-N)}{(L-1)(2L-1)} \frac{C_{2L}^{2N}}{\left(C_L^N\right)^2}$$

Exact expressions for the large deviation function.

The General Case (K. M. and S. Prolhac, 2010)

For arbitrary asymmetry q on a ring, The function $E(\mu)$ is found by functional Bethe Ansatz, again in a parametric form:

$$\mu = -\sum_{k\geq 1} C_k \frac{B^k}{k} \quad \text{and} \quad E = -(1-q)\sum_{k\geq 1} D_k \frac{B^k}{k}$$

C_k and D_k are combinatorial factors enumerating some tree structures. There exists an auxiliary function

$$W_B(z) = \sum_{k\geq 1} \phi_k(z) \frac{B^k}{k}$$

such that C_k and D_k are given by complex integrals along a small contour that encircles 0 :

$$C_k = \oint_{\mathcal{C}} \frac{dz}{2\,i\,\pi} \frac{\phi_k(z)}{z} \quad \text{and} \quad D_k = \oint_{\mathcal{C}} \frac{dz}{2\,i\,\pi} \frac{\phi_k(z)}{(z+1)^2}$$

The function $W_B(z)$ contains all information about the current statistics.

The function $W_B(z)$ is the solution of a functional Bethe equation:

$$\boxed{W_B(z) = -\ln\Big(1 - BF(z)e^{X[W_B](z)}\Big)}$$

where

$$\boxed{F(z) = \frac{(1+z)^L}{z^N}}$$

The operator X is a integral operator

$$X[W_B](z_1) = \oint_{\mathcal{C}} \frac{dz_2}{\imath 2\pi\, z_2} W_B(z_2) K(z_1, z_2)$$

with the kernel

$$\boxed{K(z_1, z_2) = 2\sum_{k=1}^{\infty} \frac{q^k}{1-q^k} \left\{ \left(\frac{z_1}{z_2}\right)^k + \left(\frac{z_2}{z_1}\right)^k \right\}}$$

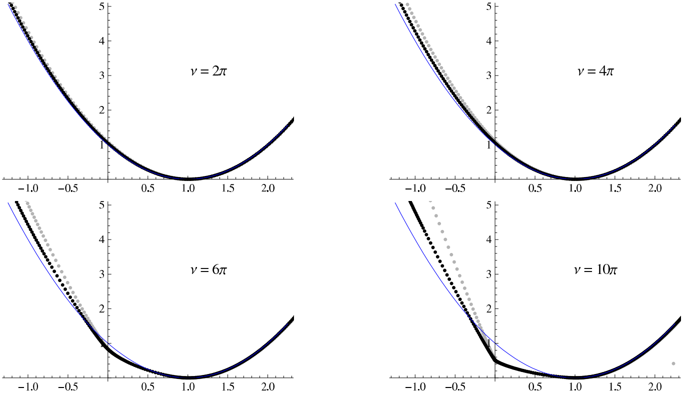
Solving this Functional Bethe Ansatz equation to all orders enables us to calculate cumulant generating function. For $x = 0$, the TASEP result is readily retrieved.

The function $W_B(z)$ also contains information on the 6-vertex model associated with the ASEP.

From the Physics point of view, the solution allows one to

- Classify the different universality classes (KPZ, EW).
- Study the various scaling regimes.
- Investigate the hydrodynamic behaviour.

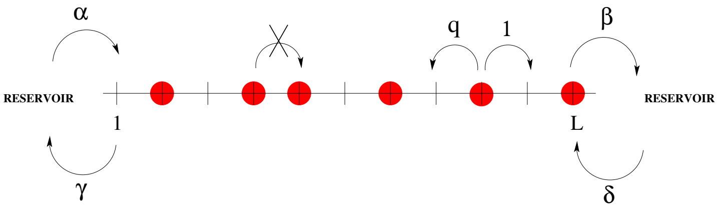
Full large deviation function (weak asymmetry)



$$E\left(\frac{\mu}{L}\right) \simeq \frac{\rho(1-\rho)(\mu^2+\mu\nu)}{L} - \frac{\rho(1-\rho)\mu^2\nu}{2L^2} + \frac{1}{L^2}\psi[\rho(1-\rho)(\mu^2+\mu\nu)]$$

with $$\psi(z) = \sum_{k=1}^{\infty} \frac{B_{2k-2}}{k!(k-1)!} z^k$$

The ASEP with Open Boundaries



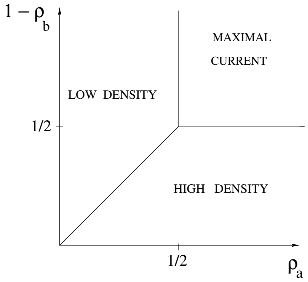
The stationary probability of a configuration $\mathcal{C}$ is given by a Matrix Product Representation (DEHP 1993):

$$P(\mathcal{C}) = \frac{1}{Z_L} \langle W | \prod_{i=1}^{L} \left(\tau_i D + (1-\tau_i) E \right) | V \rangle \,.$$

where $\tau_i = 1$ (or 0) if the site i is occupied (or empty).
The operators D and E, the vectors $\langle W|$ and $|V\rangle$ satisfy

$$\begin{aligned} D\,E - qE\,D &= D + E \\ (\beta\,D - \delta\,E)\,|V\rangle &= |V\rangle \\ \langle W|(\alpha\,E - \gamma\,D) &= \langle W| \end{aligned}$$

The Phase Diagram



$\rho_a = \frac{1}{a+1}$: effective left reservoir density.
$\rho_b = \frac{b}{b+1}$: effective right reservoir density.

$$a = \frac{(1-q-\alpha+\gamma)+\sqrt{(1-q-\alpha+\gamma)^2+4\alpha\gamma}}{2\alpha}$$

$$b = \frac{(1-q-\beta+\delta)+\sqrt{(1-q-\beta+\delta)^2+4\beta\delta}}{2\beta}$$

Current Fluctuations in the Open ASEP

The observable Y_t counts the total number of particles exchanged between the system and the left reservoir between times 0 and t.

Hence, $Y_{t+dt} = Y_t + y$ with

- $y = +1$ if a particle enters at site 1 (at rate α),
- $y = -1$ if a particle exits from 1 (at rate γ)
- $y = 0$ if no particle exchange with the left reservoir has occurred during dt.

These three mutually exclusive types of transitions lead to a three parts decomposition of the Markov Matrix: $M = M_+ + M_- + M_0$.

The cumulant-generating function $E(\mu)$ when $t \to \infty$, $\langle \mathrm{e}^{\mu Y_t} \rangle \simeq \mathrm{e}^{E(\mu)t}$, is the dominant eigenvalue of the deformed matrix

$$\boxed{M(\mu) = M_0 + \mathrm{e}^{\mu} M_+ + \mathrm{e}^{-\mu} M_-}$$

$E(\mu)$ could not be obtained by Bethe Ansatz for the open system:

We developed a Generalized Matrix Product Method.

Generalized Matrix Ansatz

We have proved that the dominant eigenvector of the deformed matrix $M(\mu)$ is given by the following matrix product representation:

$$F_{\mu}(\mathcal{C}) = \frac{1}{Z_L^{(k)}} \langle W_k | \prod_{i=1}^{L} (\tau_i D_k + (1-\tau_i) E_k) | V_k \rangle + \mathcal{O}\left(\mu^{k+1}\right)$$

The matrices D_k and E_k are the same as above

$$\begin{aligned} D_{k+1} &= (1 \otimes 1 + d \otimes e) \otimes D_k + (1 \otimes d + d \otimes 1) \otimes E_k \\ E_{k+1} &= (1 \otimes 1 + e \otimes d) \otimes E_k + (e \otimes 1 + 1 \otimes e) \otimes D_k \end{aligned}$$

The boundary vectors $\langle W_k|$ and $|V_k\rangle$ are constructed recursively:

$$|V_k\rangle = |\beta\rangle|\tilde{V}\rangle|V_{k-1}\rangle \quad \text{and} \quad \langle W_k| = \langle W^{\mu}|\langle \tilde{W}^{\mu}|\langle W_{k-1}|$$

$$[\beta(1-d) - \delta(1-e)]\,|\tilde{V}\rangle = 0$$

$$\langle W^{\mu}|[\alpha(1 + \mathrm{e}^{\mu}\, e) - \gamma(1 + \mathrm{e}^{-\mu}\, d)] = (1-q)\langle W^{\mu}|$$

$$\langle \tilde{W}^{\mu}|[\alpha(1 - \mathrm{e}^{\mu}\, e) - \gamma(1 - \mathrm{e}^{-\mu}\, d)] = 0$$

Structure of the solution I

For arbitrary values of q and $(\alpha, \beta, \gamma, \delta)$, and for any system size L the parametric representation of $E(\mu)$ is given by

$$\mu = -\sum_{k=1}^{\infty} C_k(q; \alpha, \beta, \gamma, \delta, L) \frac{B^k}{2k}$$

$$E = -\sum_{k=1}^{\infty} D_k(q; \alpha, \beta, \gamma, \delta, L) \frac{B^k}{2k}$$

The coefficients C_k and D_k are given by contour integrals in the complex plane:

$$C_k = \oint_{\mathcal{C}} \frac{dz}{2\, i\, \pi} \frac{\phi_k(z)}{z} \quad \text{and} \quad D_k = \oint_{\mathcal{C}} \frac{dz}{2\, i\, \pi} \frac{\phi_k(z)}{(z+1)^2}$$

There exists an auxiliary function

$$W_B(z) = \sum_{k \geq 1} \phi_k(z) \frac{B^k}{k}$$

that contains the full information about the statistics of the current.

Structure of the solution II

This auxiliary function $W_B(z)$ solves a functional Bethe equation:

$$\boxed{W_B(z) = -\ln\left(1 - BF(z)e^{X[W_B](z)}\right)}$$

- The operator X is a integral operator

$$X[W_B](z_1) = \oint_{\mathcal{C}} \frac{dz_2}{\imath 2\pi\, z_2} W_B(z_2) K\left(\frac{z_1}{z_2}\right)$$

$$\boxed{\text{with kernel} \quad K(z) = 2\sum_{k=1}^{\infty} \frac{q^k}{1-q^k} \left\{z^k + z^{-k}\right\}}$$

- The function $F(z)$ is given by

$$\boxed{F(z) = \frac{(1+z)^L(1+z^{-1})^L(z^2)_\infty(z^{-2})_\infty}{(a_+z)_\infty(a_+z^{-1})_\infty(a_-z)_\infty(a_-z^{-1})_\infty(b_+z)_\infty(b_+z^{-1})_\infty(b_-z)_\infty(b_-z^{-1})_\infty}}$$

where $(x)_\infty = \prod_{k=0}^{\infty}(1 - q^k x)$ and $a_\pm$, $b_\pm$ depend on the boundary rates.

- The complex contour $\mathcal{C}$ encircles 0, $q^k a_+, q^k a_-, q^k b_+$, $q^k b_-$ for $k \geq 0$.

Discussion

- These results are of *combinatorial nature: valid for arbitrary values of the parameters and for any system sizes with no restrictions.*
- *Average-Current:*

$$J = \lim_{t\to\infty} \frac{\langle Y_t \rangle}{t} = (1-q)\frac{D_1}{C_1} = (1-q)\frac{\oint_\Gamma \frac{dz}{2\,i\,\pi}\,\frac{F(z)}{z}}{\oint_\Gamma \frac{dz}{2\,i\,\pi}\,\frac{F(z)}{(z+1)^2}}$$

(cf. T. Sasamoto, 1999.)

- *Diffusion Constant:*

$$\Delta = \lim_{t\to\infty} \frac{\langle Y_t^2 \rangle - \langle Y_t \rangle^2}{t} = (1-q)\frac{D_1 C_2 - D_2 C_1}{2\,C_1^3}$$

where C_2 and D_2 are obtained using

$$\phi_1(z) = \frac{F(z)}{2} \quad \textit{and} \quad \phi_2(z) = \frac{F(z)}{2}\left(F(z) + \oint_\Gamma \frac{dz_2 F(z_2) K(z/z_2)}{2\imath\pi z_2}\right)$$

(TASEP case solved in B. Derrida, M. R. Evans, K. M., 1995)

Asymptotic behaviour in the Phase Diagram

- Maximal Current Phase:

$$\mu = -\frac{L^{-1/2}}{2\sqrt{\pi}} \sum_{k=1}^{\infty} \frac{(2k)!}{k!k^{(k+3/2)}} B^k$$

$$\mathcal{E} - \frac{1-q}{4}\mu = -\frac{(1-q)L^{-3/2}}{16\sqrt{\pi}} \sum_{k=1}^{\infty} \frac{(2k)!}{k!k^{(k+5/2)}} B^k$$

- Low Density (and High Density) Phases:
  Dominant singularity at a_+: $\phi_k(z) \sim F^k(z)$. By Lagrange Inversion:

$$E(\mu) = (1-q)(1-\rho_a)\frac{\mathrm{e}^{\mu} - 1}{\mathrm{e}^{\mu} + (1-\rho_a)/\rho_a}$$

(cf de Gier and Essler, 2011).

Current Large Deviation Function:

$$\boxed{\Phi(j) = (1-q)\left\{\rho_a - r + r(1-r)\ln\left(\frac{1-\rho_a}{\rho_a}\frac{r}{1-r}\right)\right\}}$$

where the current j is parametrized as $j = (1-q)r(1-r)$.

Matches the predictions of Macroscopic Fluctuation Theory in the Weak Asymmetry Limit, as observed by T. Bodineau and B. Derrida.

The TASEP case

Here $q = \gamma = \delta = 0$ and (α, β) are arbitrary.
The parametric representation of $E(\mu)$ is

$$\mu = -\sum_{k=1}^{\infty} C_k(\alpha, \beta) \frac{B^k}{2k}$$

$$E = -\sum_{k=1}^{\infty} D_k(\alpha, \beta) \frac{B^k}{2k}$$

with

$$C_k(\alpha, \beta) = \oint_{\{0,a,b\}} \frac{dz}{2i\pi} \frac{F(z)^k}{z} \quad \text{and} \quad D_k(\alpha, \beta) = \oint_{\{0,a,b\}} \frac{dz}{2i\pi} \frac{F(z)^k}{(1+z)^2}$$

where

$$F(z) = \frac{-(1+z)^{2L}(1-z^2)^2}{z^L(1-az)(z-a)(1-bz)(z-b)}, \qquad a = \frac{1-\alpha}{\alpha}, \qquad b = \frac{1-\beta}{\beta}$$

A special TASEP case

In the case $\alpha = \beta = 1$, a parametric representation of the cumulant generating function $E(\mu)$:

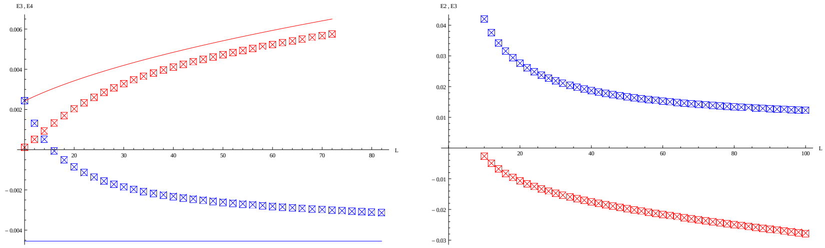
$$\mu = -\sum_{k=1}^{\infty} \frac{(2k)!}{k!} \frac{[2k(L+1)]!}{[k(L+1)]!\,[k(L+2)]!} \frac{B^k}{2k},$$

$$E = -\sum_{k=1}^{\infty} \frac{(2k)!}{k!} \frac{[2k(L+1)-2]!}{[k(L+1)-1]!\,[k(L+2)-1]!} \frac{B^k}{2k}.$$

First cumulants of the current

- Mean Value : $J = \frac{L+2}{2(2L+1)}$
- Variance : $\Delta = \frac{3}{2} \frac{(4L+1)![L!(L+2)!]^2}{[(2L+1)!]^3(2L+3)!}$
- Skewness :
  $E_3 = 12 \frac{[(L+1)!]^2[(L+2)!]^4}{(2L+1)[(2L+2)!]^3} \left\{ 9 \frac{(L+1)!(L+2)!(4L+2)!(4L+4)!}{(2L+1)![(2L+2)!]^2[(2L+4)!]^2} - 20 \frac{(6L+4)!}{(3L+2)!(3L+6)!} \right\}$
  For large systems: $E_3 \to \frac{2187-1280\sqrt{3}}{10368}\pi \sim -0.0090978...$

Numerical results (DMRG)



Left: **Max. Current** ($q = 0.5$, $a_+ = b_+ = 0.65$, $a_- = b_- = 0.6$), Third and Fourth cumulant.

Right: **High Density** ($q = 0.5$, $a_+ = 0.28$, $b_+ = 1.15$, $a_- = -0.48$ and $b_- = -0.27$), Second and Third cumulant.

A. Lazarescu and K. Mallick, J. Phys. A 44, 315001 (2011).

M. Gorissen, A. Lazarescu, K.M., C. Vanderzande, PRL **109** 170601 (2012).

Conclusion

Systems out of equilibrium are ubiquitous in nature. They break time-reversal invariance.

Often, they are characterized by non-vanishing stationary currents.

Large deviation functions (LDF) appear as the right generalization of the thermodynamic potentials: convex, optimized at the stationary state, and non-analytic features can be interpreted as phase transitions.

The LDF's are very likely to play a key-role in constructing a non-equilibrium statistical mechanics.

Finding Large Deviation Functions is a very important current issue. This can be achieved through experimental, mathematical or computational techniques.

The results given here are one of very few exact analytically exact formulae known for Large Deviation Functions.

C. Arita, A, Ayyer, M. Evans, P. Ferrari, O. Golinelli, M. Gorissen, A. Lazarescu, S. Prolhac, and C. Vanderzande