Exact solution for single-file diffusion

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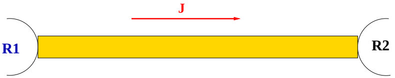
Joint work with Takashi Imamura and Tomohiro Sasamoto:

T. Imamura, K. M. and T. Sasamoto, PRL **118**, 160601 (2017).

T. Imamura, K. M. and T. Sasamoto, *submitted to CMP, July 2020*.

Equilibrium versus non-equilibrium

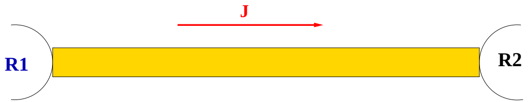
Consider a conductor in contact with two reservoirs at temperatures T_1 and T_2 (or chemical, or electric, potentials μ_1, μ_2).



- If $T_1 = T_2$: Equilibrium Statistical Mechanics. The state of the system, characterized by very few parameters, is determined by optimizing the relevant thermodynamic potential and leads to an equation of state. This allows us to study phase transitions, universality classes, statistical fluctuations (generically Gaussian).
- When $|T_1 - T_2| \ll T_1$: linear response theory. A stationary current sets in, proportional to the temperature gradient. The conductivity determined by quadratic correlations at equilibrium.
  Here, the flow of the current implies that some entropy is continuously generated and keeps on increasing with time. (Linear response theory may be reformulated in terms of optimal entropy *production rate*, cf. Prigogine's school).

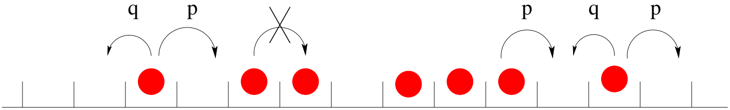
Far from equilibrium

The fundamental picture of a non-equilibrium system is thus a long pipe in contact with two distant reservoirs at very different "potentials" (densities, temperatures...).



We are interested in the flow of current, the variation of local densities, correlations and fluctuations. Because the system is far from equilibrium, the above framework of Equilibrium Statistical Mechanics no more valid.

A minimal mathematical model is provided by the asymmetric exclusion process (ASEP):



The Exclusion Process: a paradigm

The Exclusion Process is stochastic interacting particles process: random walkers on a lattice with the exclusion constraint, i.e. a site can be occupied by at most one "particle" at a given time.

• EXCLUSION: Hard core-interaction, at most 1 particle per site. ASEP is a genuine N-body system.

• NON-VANISHING CURRENT: produced by boundary or initial conditions, and/or by an external driving field (when $p \neq q$, jumps are asymmetric).

• PROCESS: Stochastic Markovian dynamics; no Hamiltonian : no way of defining Gibbs measures.

The Exclusion Process plays the role of a Paradigm in contemporary Statistical Physics, as as a building block in many realistic models of low-dimensional transport.

ASEP is integrable

The exclusion process is a continuous time Markov process defined on the lattice $\mathbb{Z}$. The state of ASEP at time t is given by the collection of binary variables $\{\eta_x(t)\}_{x\in\mathbb{Z}}$, such that $\eta_x(t) = 1$ (resp. 0) if site x is occupied (resp. empty) at time t.

The evolution is defined with the Markov generator L (acting on fonctions f on the state space):

$$Lf = \sum_{x\in\mathbb{Z}} (p\eta_x(1-\eta_{x+1}) + q(1-\eta_x)\eta_{x+1})[f(\eta^{x,x+1}) - f(\eta)]$$

Using spin variables, the local update operator on the bond $(x, x+1)$ reads

$$p\mathbf{S}_x^+\mathbf{S}_{x+1}^- + q\mathbf{S}_x^-\mathbf{S}_{x+1}^+ + \frac{p+q}{4}\mathbf{S}_x^z\mathbf{S}_{x+1}^z - \frac{1}{4}$$

The Exclusion Process is an integrable non-hermitian spin chain as realized by D. Dhar and and L. Gwa & H. Spohn, with many remarkable combinatorial properties.

Integrability methods can be used (or generalized) to answer some relevant questions in non-equilibrium statistical physics.

Outline

1. **Exact tracer statistics: statement of the problem and results**

2. **Integrable probabilities**

    a. Duality
    b. Exact formula for q-Moments (Bethe without Ansatz)
    c. Combinatorics of pole expansions
    d. The symmetric limit: Fredholm determinant and asymptotics

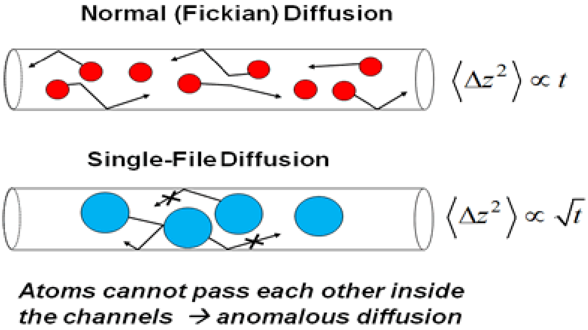
3. **Physical consequences: large deviations and fluctuating hydrodynamics (MFT)**

1. Exact Tracer Statistics

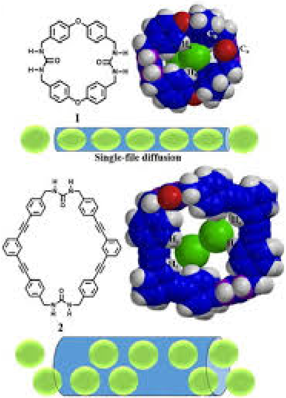
Single-file diffusion

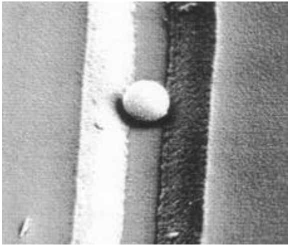
Single-file diffusion is an important phenomena soft-condensed matter (for example, transport through cell membranes).

A pristine model for single-file diffusion is the Symmetric Exclusion Process (SEP) on $\mathbb{Z}$.



Experimental observations





(C. Bechinger's group in Stuttgart)

The Symmetric Exclusion Process (SEP) on Z.

Consider the Symmetric Exclusion Process, $(p = q = 1)$ on $\mathbb{Z}$ with a uniform finite density ρ of particles.

Suppose that we tag and observe a particle that was initially located at site 0 and monitor its position X_t with time.

On the average $\langle X_t \rangle = 0$ but how large are its fluctuations?

- If the particles were non-interacting (no exclusion constraint), each particle would diffuse normally $\langle X_t^2 \rangle = Dt$.

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- If the particles were non-interacting (no exclusion constraint), each particle would diffuse normally $\langle X_t^2 \rangle = Dt$.
- Because of the exclusion condition, a particle displays an anomalous diffusive behaviour: when $t \to \infty$, we have

$$\langle X_t^2 \rangle = 2\frac{1-\rho}{\rho}\sqrt{\frac{Dt}{\pi}} + o(t^{1/2}) \qquad \text{(Arratia, 1983)}$$

T.E. Harris, *J. Appl. Prob.* (1965). F. Spitzer, *Adv. Math.* (1970). R. Arratia, *Ann. Prob.* (1983).

Open problems:

- No asymptotic formulae for higher moments of X_t were available.
- It has been proved (Sethuraman and Varadhan, 2013) that in the long time limit $t \to \infty$, the tracer's position X_t satisfies a Large Deviation Principle :

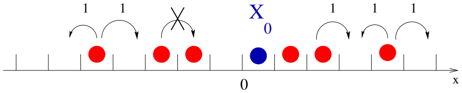
$$\text{Prob}\left(\frac{X_t}{\sqrt{4t}} = -\xi\right) \sim \exp[-\sqrt{t}\phi(\xi)].$$

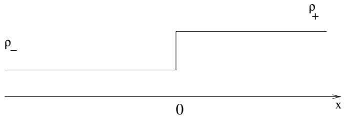
  where $\phi(\xi)$ is the large-deviation (or rate) function. Bounds for $\phi(\xi)$ have been found but its exact expression is unknown.

- What is the influence of the initial setting? For example, what would happen out of equilibrium with a step initial profile ?
- The exact finite-time distribution of X_t is not known.
- *What happens in the asymmetric case* $(p \neq q)$*?*

SEP with step profile

Consider SEP with a step-like Bernoulli initial condition with density ρ_- (resp. ρ_+) to the left (resp. right). The tagged particle (or tracer) is initially located at 0. Let the system evolve: X_t denotes the position of the tracer at time t.





The goal is to determine the statistics of of the position of the tracer X_t and to extract asymptotics in the long time limit.

Finite time distribution of the tracer

The distribution function of the tracer X_t is given, at all times, in terms of a Fredholm determinant:

$$\mathbb{P}[X_t \leq x] = \int_{C_0} \frac{dz}{1-z} \det(1 + \omega K_{x,t})_{L_2(C_0)} W_0(z)$$

where

$$\omega(z) = \rho_+(z^{-1} - 1) + \rho_-(z - 1) + \rho_+\rho_-(z^{-1} - 1)(z - 1)$$

$$K_{t,x}(\xi_1, \xi_2) = \frac{\xi_1^{|x|} e^{\epsilon(\xi_1)t}}{\xi_1\xi_2 + 1 - 2\xi_2} \quad \text{with} \quad \epsilon(\xi) = \xi + \xi^{-1} - 2$$

$$W_0(\lambda) = \left(1 + \rho_\epsilon(z^{-\epsilon} - 1)\right)^{|x|} \text{ with } \epsilon = \text{sgn}(x)$$

The ω variable expresses fundamental symmetries of the model : parity and time-reversal. (It appears recurrently in calculations for SEP).

The Kernel $K_{t,x}$ originates from the Bethe Ansatz.

The function W_0 carries 'Poisson-like' boundary conditions.

C_0 is a small enough complex contour around 0 (poles from the denominator of the kernel are excluded).

Fredholm determinant (aparte)

Let $K = (K_{ij})$ be a finite matrix. Then, the following expansion holds:

$$\det(I + \omega K) =$$

$$1 + \omega \sum_i K_{ii} + \frac{\omega^2}{2!} \sum_{i_1, i_2} \begin{vmatrix} K_{i_1 i_1} & K_{i_1 i_2} \\ K_{i_2 i_1} & K_{i_2 i_2} \end{vmatrix} + \frac{\omega^3}{3!} \sum_{i_1, i_2, i_3} \begin{vmatrix} K_{i_1 i_1} & K_{i_1 i_2} & K_{i_1 i_3} \\ K_{i_2 i_1} & K_{i_2 i_2} & K_{i_2 i_3} \\ K_{i_3 i_1} & K_{i_3 i_2} & K_{i_3 i_3} \end{vmatrix} + \dots$$

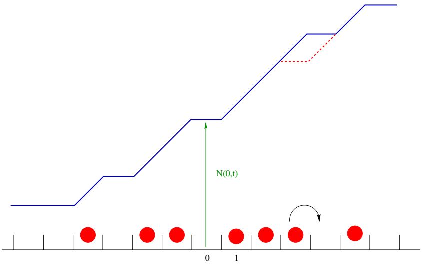
For a compact trace-class operator with kernel $K(x, y)$, we do the following replacement (i.e. discretize)

$$\sum_i K_{ii} \to \int dx\, K(x, x)$$

$$\sum_{i_1, i_2} \begin{vmatrix} K_{i_1 i_1} & K_{i_1 i_2} \\ K_{i_2 i_1} & K_{i_2 i_2} \end{vmatrix} \to \int \int dxdy \begin{vmatrix} K(x, x) & K(x, y) \\ K(y, x) & K(y, y) \end{vmatrix} \quad \text{etc...}$$

Mapping to an interface model

We represent the exclusion process by an interface model



$N(0,t)$ represents the total current through $(0,1)$ in the duration t. By convention, *left going current is counted positively.*

$$N(x,t) = N(0,t) + \begin{cases} \sum_{y=1}^{x} \eta_y(t)\,, & x > 0 \\ 0, & x = 0 \\ -\sum_{y=x+1}^{0} \eta_y(t)\,, & x < 0 \end{cases}$$

Note that $N(x,t)$ is related to the KPZ height via $h(x,t) = N(x,t) - \frac{x}{2}$

Tracer's position versus the height N(x,t)

Because the tracer is continuously moving, it is useful to relate its position X_t to a local observable such as $N(x,t)$.

Using particle number conservation, one can show

$$\text{Prob}\left(X_t > x\right) = \text{Prob}\left(N(x,t) \leq 0\right)$$

Or, equivalently,

$$\text{Prob}\left(X_t \leq x\right) = \text{Prob}\left(N(x,t) > 0\right)$$

This relates the statistical properties of X_t and those of the height $N(x,t)$. In particular, one can deduce the large deviation function and the cumulants of X_t from the corresponding quantities for $N(x,t)$.

Hence, we'll first focus on $N(x,t)$.

Exact expression of the generating function

We shall derive a formula for the characteristic function of the height $N(x,t)$, exact at any finite-time, in terms of a Fredholm determinant:

$$\langle e^{\lambda N(x,t)} \rangle = \det(1 + \omega K_{t,x}) W_0(\lambda)$$

where

$$\omega(\lambda) = \rho_+(e^{\lambda} - 1) + \rho_-(e^{-\lambda} - 1) + \rho_+\rho_-(e^{\lambda} - 1)(e^{-\lambda} - 1)$$

$$K_{t,x}(\xi_1, \xi_2) = \frac{\xi_1^{|x|} e^{\epsilon(\xi_1)t}}{\xi_1\xi_2 + 1 - 2\xi_2} \quad \text{with} \quad \epsilon(\xi) = \xi + \xi^{-1} - 2$$

$$W_0(\lambda) = \left(1 + \rho_\pm(e^{\pm\lambda} - 1)\right)^{|x|} \text{ with } \pm = \mathrm{sgn}(x)$$

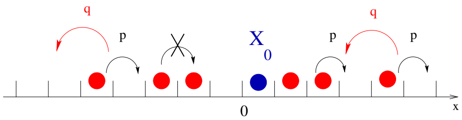
From this result, information about the tracer will be deduced.

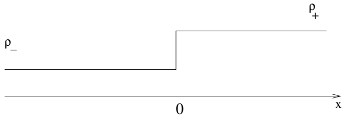
We now outline the strategy to solve the problem.

2. Integrable Probabilities

The general problem: a tracer in ASEP

It will prove useful to study the tracer problem in the more general setting of the *asymmetric exclusion process* with jump rates p and q with $p \leq q$:





This provides us with the extra-parameter τ:

$$\tau = \frac{p}{q} \leq 1$$

The moving tracer position X_t has been traded for the localized height variables $N(x,t)$, which form an infinite set of highly correlated observables. *We need to restore finiteness.*

a. DUALITY for ASEP

For the Asymmetric Exclusion Process, with asymmetry parameter $\tau = p/q < 1$, the observable $N(x,t)$ satisfies a remarkable self-duality property.

For $x_1 < x_2 < \ldots < x_n$, τ-correlations of the type,

$$\phi(x_1, \ldots, x_n; t) = \langle \tau^{N(x_1,t)} \ldots \tau^{N(x_n,t)} \rangle$$

follow the same dynamical equations as the ASEP with a finite number n of particles located at $x_1, \ldots, x_n$.

Duality results from a quantum group invariance of the process (G. Schütz, T Imamura and T. Sasamoto, C. Giardina et al.)

It can be understood in an elementary manner using stochastic (Poisson) calculus.

DUALITY (Proof)

Consider $\phi(x;t) = \langle \tau^{N(x,t)} \rangle$. Between t and $t + dt$, its variation is

$$\phi(x;t+dt) - \phi(x;t) = \langle \tau^{N(x,t+dt)} - \tau^{N(x,t)} \rangle = \langle \tau^{N(x,t)} \left(\tau^{dN(x,t)} - 1 \right) \rangle$$

We observe that between t and $t + dt$, we have

$$\tau^{dN(x,t)} - 1 = \begin{cases} \tau - 1\,, & \text{with prob.} \quad \eta_{x+1}(t)(1 - \eta_x(t))dt \\ \frac{1}{\tau} - 1\,, & \text{with prob.} \quad \tau\eta_x(t)(1 - \eta_{x+1}(t))dt \\ 0\,, & \text{otherwise.} \end{cases}$$

leading to

$$\begin{aligned} \frac{d\phi(x;t)}{dt} &= (\tau - 1)\langle \tau^{N(x,t)} (\eta_{x+1}(t) - \eta_x(t)) \rangle \\ &= \phi(x+1;t) + \tau\phi(x-1;t) - (1+\tau)\phi(x;t) \end{aligned}$$

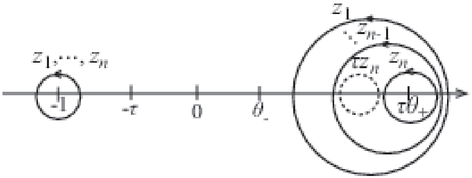
The last identity results from the fact that the local occupation is a binary variable. This is the evolution of a single particle under ASEP dynamics.

The n-th correlation function, although more contrived, is analyzed along similar lines. The key point is to check the adjacency conditions.

Inspired by the fact that ASEP is integrable by "Bethe Ansatz", the τ-correlation functions can be expressed as multiple contour integrals in the complex plane:

$$\langle \tau^{\sum_i N(x_i,t)} \rangle = \tau^{\sum_i i - \frac{x_i}{2}} \prod_{i=1}^{n} \left(1 - \frac{r_-}{\tau^i r_+}\right) \int \cdots \int \prod_{i<j} \frac{z_i - z_j}{z_i - \tau z_j} \prod_{i=1}^{n} \frac{e^{\Lambda_{x_i,t}(z_i)}}{(1 - \frac{z_i}{\tau\theta_+})(z_i - \theta_-)} \mathrm{d}z_i$$

with $r_\pm = \rho_\pm(1-\rho_\mp)$, $\theta_\pm = \rho_\pm/(1-\rho_\pm)$ and $e^{\Lambda_{x,t}(z)} = \left(\frac{1+z}{1+z/\tau}\right)^x e^{-\frac{q(1-\tau)^2 z}{(1+z)(\tau+z)} t}$



Contour integrals (Proof)

The complex integral formula for the τ-correlations is proved by showing that it solves the dynamical ASEP master equation *and the initial condition.*

The following identities

$$-\frac{q(1-\tau)^2 z}{(1+z)(\tau+z)} = p\frac{1+z/\tau}{1+z} + q\frac{1+z}{1+z/\tau} - (p+q)$$

$$\frac{(p-q)(z_1-\tau z_2)}{(1+z_1/\tau)(1+z_2/\tau)} = q\frac{(1+z_1)(1+z_2)}{(1+z_1/\tau)(1+z_2/\tau)} + p - \frac{1+z_2}{1+z_2/\tau}$$

allow us to prove that these conplex integrals obey the master equation (the nesting conditions on the contours are crucial).

The initial condition at $t=0$ is checked by a residue calculation.

Contour integral formulas were initially inspired by the Bethe Ansatz (Schütz, Tracy-Widom). Yet, they are *not* an Ansatz: they are exact representations of the correlators. The z_i's are dummy integration variables, not Bethe roots (there are no Bethe equations here).

More generally, integrability can be used to give exact formulas for many interesting stochastic processes (Borodin, Corwin, Sasamoto).

c. Combinatorics of the residue expansion

A key step is to disentangle recursively the contours by evaluating the residues at non-essential singularities. This leads to an expansion for the τ-moment of the form

$$\langle \tau^{nN} \rangle = \sum_{k=0}^{n} (\tau\theta_+)^k \prod_{i=1}^{n-k} e^{\Lambda_i} \prod_{j=n-k+1}^{n} (1 - \frac{\theta_-}{\tau^j \theta_+}) \int_{-1} \prod_{i=1}^{k} \frac{e^{\Lambda_{x,t}(z_i)} dz_i}{z_i - \theta_-} \prod_{1 \le i < j \le k} \frac{z_i - z_j}{z_i - \tau z_j} F_k^{(n)}(\{z_i\}; \theta_+)$$

where the the functions $F_k^{(n)}$ are non-vanishing for $0 \le k \le n$ and satisfy the following recursion relation (starting with $F_0^{(0)} = 1$):

$$F_k^{(n)}(z_1, \ldots, z_k; \theta_+) = \tau^{k-1} g_{n-k+1}(z_k, a) F_{k-1}^{(n-1)}(z_1, \ldots, z_{k-1}; \theta_+) + \tau^k F_k^{(n-1)}(z_1, \ldots, z_k; \tau\theta_+)$$

with $g_m(z, \theta_+) = \frac{z - \tau^{m-1}\theta_+}{z - \tau\theta_+} \frac{1}{z - \theta_+}$ for $m \ge 1$

d. Symmetric limit

The results stated up to now are valid for an arbitrary $\tau < 1$. We now specialize to symmetric exclusion case by performing the $\tau \to 1$ limit. More precisely, we have

$$\langle N_{SEP}(x,t)^n \rangle = \lim_{\tau \to 1} \left\langle \left(\frac{1 - \tau^{N_{\mathbf{ASEP}}}}{1-\tau} \right)^n \right\rangle$$

Having performed the pole expansion, this limit can safely be carried out in the contour integrals. One also needs to extract the dominant contribution in the pole recursion relation which, when $\tau \to 1$, becomes a PDE that can be solved. We obtain

$$\langle N_{SEP}(x,t)^n \rangle = \sum_{k=0}^{n} m_{n,k} J_k(x,t)$$

with

$$\sum_{n=0}^{\infty} \frac{\lambda^n}{n!} m_{n,k} = \frac{k}{k!} (1 + \rho_+(e-1))^x$$

Fredholm Determinant

The J_k factors are given by k-fold complex integrals along a small contour C_0 around the origin:

$$J_k = \int_{C_0} \cdots \int_{C_0} \prod_{1 \le i < j \le k} \frac{\xi_i - \xi_j}{\xi_i \xi_j + 1 - 2\xi_j} \prod_{i=1}^{k} \frac{\xi_i^x e^{(\xi_i + 1/\xi_i - 2)t} d\xi_i}{(1-\xi_i)^2}$$

Symmetrizing this integral in the ξ_i's and using some combinatorial identities, we obtain

$$J_k = \int_{C_0} \cdots \int_{C_0} \det(K_{t,x}(\xi_i, \xi_j))_{i,j=1}^k \prod_{i=1}^{k} d\xi_i$$

This expression leads to the exact finite time formula for the characteristic function as a Fredholm determinant:

$$\langle e^{\lambda N(x,t)} \rangle = \det(1 + \omega K_{t,x}) W_0(\lambda)$$

Back to the tracer

The height distribution is the inverse Laplace transform of this characteristic function, and this yields the distribution of the tracer at any given time.

More generally, at $t = 0$, once the particle closest to the origin in the region $x \geq 0$ is selected as the tracer, all the particles in the system can be labeled as :

$$\ldots < X_2 < X_1 < X_0 < X_{-1} < X_{-2} < \ldots$$

Then, the position $X_m(t)$ of the m-th tagged particle at time t is related to the local height variables as follows :

$$\text{Prob}[X_m(t) \leq x] = \text{Prob}[N(x,t) > m]$$

This leads to the finite time distribution of any particle in SEP with two-sided Bernoulli initial condition:

$$\boxed{\mathbb{P}[X_m(t) \leq x] = \int_{C_0} \frac{z^m dz}{1-z} \det(1 + \omega K_{x,t})_{L_2(C_0)} W_0(z)}$$

3. Large deviations and MFT

We now draw some physical consequences of the previous results.

Statistics of the height N(x,t) at long times

In the long time limit, the characteristic function of $N(x,t)$ behaves as

$$\langle e^{\lambda N(x,t)} \rangle \sim e^{-\sqrt{t}\mu(\xi,\lambda)}$$

where $\mu(\xi,\lambda)$ is the cumulant generating function of $N(x,t)$.

Equivalently, $N(x,t)$ satisfies a Large Deviation Principle for $t \to \infty$

$$\text{Prob}\left(\frac{N(x,t)}{\sqrt{t}} = q\right) \simeq \exp[-\sqrt{t}\Phi(\xi,q)] \quad \text{with} \quad \xi = -\frac{x}{\sqrt{4t}}$$

The functions $\Phi(\xi,q)$ and $\mu(\xi,\lambda)$ are Legendre transforms of each other

$$\Phi(\xi,q) = \max_{\lambda}\left(\mu(\xi,\lambda) + \lambda q\right)$$

In particular: $\Phi(\xi,0) = \max_{\lambda} \mu(\xi,\lambda)$

Explicit formula for $\mu(\xi,\lambda)$:

The large-time asymptotics analysis of the Fredholm determinant yields the cumulant generating function $\mu(\xi,\lambda)$:

$$\mu(\xi,\lambda) = \sum_{n=1}^{\infty} \frac{(-\omega)^n}{n^{3/2}} A(\sqrt{n}\,\xi) \; + \xi \log \frac{1+\rho_+(e^{\lambda}-1)}{1+\rho_-(e^{-\lambda}-1)}$$

where, again,

$$\omega(\lambda) = \rho_+(e^{\lambda}-1) + \rho_-(e^{-\lambda}-1) + \rho_+\rho_-(e^{\lambda}-1)(e^{-\lambda}-1)$$

and

$$A(u) = \Xi(\xi) + \xi \quad \text{with } \Xi(\xi) = \int_{\xi}^{\infty} \mathrm{erfc}\,(u)\mathrm{d}u$$

Expanding $\mu(\xi,\lambda)$ w.r.t. λ gives explicit formulae for the cumulants of $N(x,t)$ for $t \to \infty$.

Large deviations of the Tracer

Recall that the observables X_t and $N(x,t)$ are related by

$$\text{Prob}\left(X_t \leq x\right) = \text{Prob}\left(N(x,t) > 0\right)$$

Besides, both X_t and $N(x,t)$ satisfy the Large Deviation Principle:

$$\text{Prob}\left(\frac{X_t}{\sqrt{4t}} = -\xi\right) \sim \exp[-\sqrt{t}\phi(\xi)] \quad \text{and} \quad \text{Prob}\left(\frac{N(x,t)}{\sqrt{t}} = q\right) \sim \exp[-\sqrt{t}\Phi(\xi,q)]$$

Combining these facts, one deduces the following relation between the Large Deviation Functions

$$\boxed{\phi(\xi) = \Phi(\xi, q=0) = \max_\lambda \mu(\xi,\lambda)}$$

This gives a parametric formula for the LDF of the tracer.

More generally, one can show that $\Phi(\xi,q)$ represents the Large Deviation Function of the particle with label m scaling as $m = q\sqrt{t}$.

Cumulants of the tracer

The knowledge of the LDF $\phi(\xi)$ allows the cumulants of the tracer to be calculated explicitly for $t \to \infty$.
For uniform density $\rho_+ = \rho_- = \rho$, we find

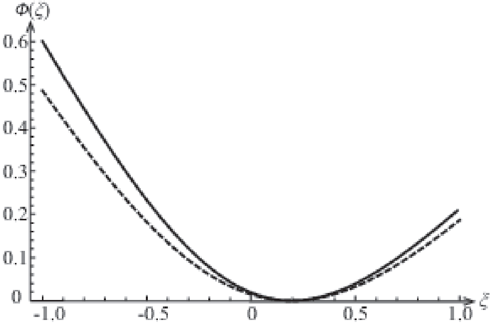
- Variance : $\langle X_t^2 \rangle = 2\frac{1-\rho}{\rho}\sqrt{\frac{Dt}{\pi}}$ (Arratia)
- Fourth order :

$$\frac{\langle X_t^4 \rangle_c}{\sqrt{4t}} = \frac{1-\rho}{\sqrt{\pi}\rho^3}[1 - (4 - (8 - 3\sqrt{2})\rho)(1-\rho) + \frac{12}{\pi}(1-\rho)^2]$$

- At order 6:

$$\begin{aligned}\frac{\langle X_t^6 \rangle_c}{\sqrt{4t}} = \frac{1-\rho}{\pi^{5/2}\rho^5}\Big[& \left(1020 - 450\pi + 45\pi^2\right) \\ & - \left(4800 - \pi(2700 - 540\sqrt{2}) + \pi^2(270 - 45\sqrt{2})\right)\rho \\ & + \left(6120 - \pi(5250 - 1620\sqrt{2}) + \pi^2(570 - 225\sqrt{2} + 40\sqrt{3})\right)\rho^2 \\ & - \left(4080 - \pi(4200 - 1620\sqrt{2}) + \pi^2(480 - 300\sqrt{2} + 80\sqrt{3})\right)\rho^3 \\ & + \left(1020 - \pi(1200 - 540\sqrt{2}) + \pi^2(136 - 120\sqrt{2} + 40\sqrt{3})\right)\rho^4 \Big]\end{aligned}$$

A plot of the Large Deviation Function



The large deviation function $\phi(\xi)$ of the tracer position in the SEP is plotted for the non-equilibrium initial conditions $\rho_+ = 0.3$ and $\rho_- = 0.15$.

The dashed curve shows the limit of reflective Brownian particles with the same $\rho_\pm$.

Non-equilibrium "drift"

For non-equilibrium initial conditions, $\rho_+ > \rho_- > 0$, the tracer "drifts" away from the origin as

$$\frac{\langle X_t \rangle}{\sqrt{4t}} = -\xi_0 \quad \text{with} \quad 2\xi_0 \rho_- = (\rho_+ - \rho_-) \int_{\xi_0}^{\infty} \text{erfc}\,(u) \mathrm{d}u$$

This result can be obtained by hydrodynamics. Note that the tracer drifts as $\sqrt{t}$ with a "speed" $-2\xi_0$ proportional to the boundary densities mismatch.

The variance of the tracer is given by the following exact formula:

$$\mathrm{Var}(X_t) = \frac{4K(\rho_+ - \rho_-)^2 A(\xi_0)\sqrt{t}}{(\rho_+\,\text{erfc}\,(\xi_0) + \rho_-\,\text{erfc}\,(-\xi_0))^2}$$

with

$$K = \frac{\rho_+^3 + \rho_-^3 - 3\rho_+^2\rho_- - 3\rho_+\rho_-^2 + 4\rho_+\rho_-}{(\rho_+ + \rho_-)(\rho_+ - \rho_-)^2} - \frac{A(\sqrt{2}\,\xi_0)}{\sqrt{2}A(\xi_0)}.$$

Gallavotti-Cohen relation for the Tracer

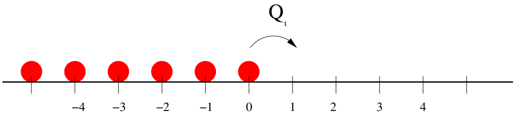
The large deviation function $\phi(\xi)$ of the tracer X_t satisfies the Fluctuation Theorem of Gallavotti and Cohen, that reflects an underlying invariance of the dynamics by time-reversal

$$\phi(\xi) - \phi(-\xi) = 2\xi \log \frac{1-\rho_+}{1-\rho_-}$$

This implies that the Einstein relation is true for single-file diffusion (SEP) (P. Ferrari, S. Goldstein and J. L. Lebowitz, 1985) *despite the fact that the time scaling is anomalous.*

A special case: Current fluctuation at the origin

The observable $N(0,t)$ is nothing but the total current Q_t that has flown through the origin



If one starts with initial step profile (ρ_+, ρ_-), the cumulant generating function of the current Q_t is

$$\mu(0,\lambda) = \frac{1}{\pi}\sum_{n=1}^{\infty}\frac{(-\omega)^n}{n^{3/2}} = \frac{1}{2\pi}\int_0^{\infty} \mathrm{dk}\, \log\left(1 + \omega \mathrm{e}^{-\mathrm{k}^2}\right)$$

with $\omega(\lambda) = \rho_+(e^{\lambda}-1) + \rho_-(e^{-\lambda}-1) + \rho_+\rho_-(e^{\lambda}-1)(e^{-\lambda}-1)$

This result was first obtained by (Derrida and Gerschenfeld, 2011).

Low density limit: Reflecting Brownian particles

In the low density limit $\rho_-, \rho_+ \ll 1$, the SEP becomes equivalent to an ensemble of reflecting Brownian particles. This can be viewed as independent Brownian motions that exchange their labels when they collide and has been solved exactly using various techniques.

The large deviation function of a tracer in the reflecting Brownian limit is

$$\phi(\xi) = \left\{ \sqrt{\rho_+ \Xi(\xi)} - \sqrt{\rho_- \Xi(-\xi)} \right\}^2$$

where $\Xi(\xi) = \int_\xi^\infty \mathrm{erfc}\,(u)\mathrm{d}u$.

When $\rho_- = 0$, the tracer is the left-most particle of a SEP expanding in a half-empty space: finding the distribution of X_t becomes identical to a problem in extreme value statistics (S. Sabhapandit). The tracer is superdiffusive and follows a Gumbel law. It can be shown that

$$\langle X_t \rangle \sim \sqrt{t \log t} \quad \text{and} \quad \mathrm{Var}(X_t) \sim \frac{t}{\log t}$$

Description from Fluctuating hydrodynamics

At a coarse-grained level (under diffusive scaling of space and time), the symmetric exclusion process can be described as a fluid governed by a stochastic hydrodynamic equation (here $\nu = 0$):

$$\partial_t \rho = -\partial_x j \quad \text{with} \quad j = -D(\rho)\nabla\rho + \sqrt{\sigma(\rho)}\xi(x,t)$$

where $\xi(x,t)$ is a Gaussian white noise with variance

$$\langle \xi(x',t')\xi(x,t)\rangle = \frac{1}{L}\delta(x-x')\delta(t-t')$$

where the transport coefficients $D(\rho)$ (Diffusivity) and $\sigma(\rho)$ (Conductivity) must be calculated from the microscopic dynamics for each model. For the exclusion process we have

$$D(\rho) = 1 \quad \text{and} \quad \sigma(\rho) = 2\rho(1-\rho)$$

In the limit of large systems sizes, the noise becomes vanishingly week, and the dominant paths of this stochastic PDE can be described as instantons and related to a classical (non-linear) field theory: MFT.

The Macroscopic Fluctuation Theory (MFT)

For a weakly-driven diffusive system, G. Jona-Lasinio and his colleagues (L. Bertini, D. Gabrielli, A. De Sole and C. Landim) have shown that the probability to observe a current $j(x,t)$ and a density profile $\rho(x,t)$ during a time T takes a large deviation form:

$$\mathrm{Pr}\{j(x,t),\rho(x,t)\} \sim \mathrm{e}^{-\,S_{MFT}(j,\rho)}$$

where

$$S_{MFT}(j,\rho) = \int_0^T dt \int_{-\infty}^{+\infty} \frac{(j + D(\rho)\nabla\rho)^2\, dx}{2\sigma(\rho)}$$

with $\partial_t \rho = -\nabla . j$

(L. Bertini, D. Gabrielli, A. De Sole, G. Jona-Lasinio and C. Landim).

For a given problem, the dominant paths will be obtained by optimizing this action under constraints. Here the constraint will be the displacement of the tracer.

Tagged particle as a macroscopic observable

How to define the position X_t of the Tagged Particle macroscopically? In Single-File Diffusion, particles can not overtake, *i.e.* the ordering of the particle is conserved:

$$\int_0^{+\infty} (\rho(x,t) - \rho(x,0))\, \mathrm{d}x = \int_0^{X_t} \rho(x,t)\, \mathrm{d}x$$

This defines a functional $X_t[\rho]$, whose statistics we can study by MFT that provides us with a measure for $\rho(x,t)$.

The calculation becomes an optimization problem: Find the optimal path (j^*, ρ^*) that generates a given fluctuation of X_t.

HYDRODYNAMICS (MFT equations)

The MFT leads to a Hamiltonian system for two conjugate fields:

$$\partial_t q = \partial_x[D(q)\partial_x q] - \partial_x[\sigma(q)\partial_x p]$$
$$\partial_t p = -D(q)\partial_{xx} p - \frac{1}{2}\sigma'(q)(\partial_x p)^2$$

The information of the microscopic dynamics relevant at the macroscopic scale is embodied in the 'transport coefficients' $D(q)(=1)$ and $\sigma(q)(=2q(1-q)$.

Here $q(x,t)$ is the optimal density-field and $p(x,t)$ is the conjugate field with Hamiltonian: $H[p,q] = -D(q)\partial_x q \partial_x p + \frac{\sigma(q)}{2}(\partial_x p)^2$

Although these MFT equations have not been solved analytically in general, a perturbative approach allows us to derive the first few cumulants of X_t (Krapivsky et al. 2014, 2015).

Variance and Kurtosis

- Second Moment:

$$\langle X_t^2 \rangle = \frac{2(1-\rho)}{\rho}\sqrt{\frac{t}{\pi}}$$

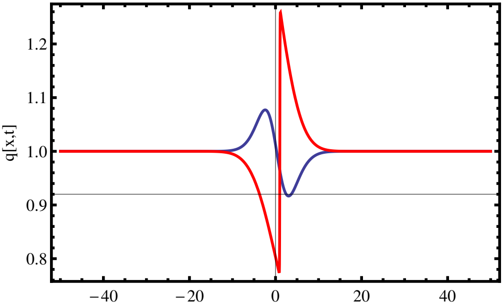
- Fourth Cumulant:

$$\langle X_t^4 \rangle_c = \frac{[1-\rho][1-\left(4-(8-3\sqrt{2})\rho\right)(1-\rho)+\frac{12}{\pi}(1-\rho)^2]}{\rho^3}\sqrt{\frac{4t}{\pi}}$$

The Macroscopic Fluctuation Theory is a general and versatile framework, that does not rely on integrability, allowing in principle to calculate large deviation functions directly at the macroscopic level. It gives a physical picture of how a non-reversible fluctuation can be generated whereas combinatorial approaches seem to miss this dynamical picture.

Shape of the optimal profiles

MFT provides you with the statistical properties but also with an understanding of the dynamical process leading to a given atypical fluctuation. Here we plot the case of Brownian reflecting particles with (annealed initial conditions).



Profil dynamics (Annealed case)

Conclusion

The solution of the elementary problem of a Tracer Motion in SEP has required the use of the main technologies available for studying this class of models: mappings to growth models, duality, integrable probabilities, determinant asymptotics...

The result for the Large Deviation Function is rather simple (it involves Gaussians and Error Functions): Is there a simpler derivation?

As in the KPZ case, other initial conditions may be considered (flat; quenched/annealed).

We are also intrigued by the fact that MFT equations helped us to guess the structure of the problem. It may happen that they could be solvable.