Exact solution for single-file diffusion

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ICTS, Bangalore, August 2018

Joint work with Takashi Imamura and Tomohiro Sasamoto:

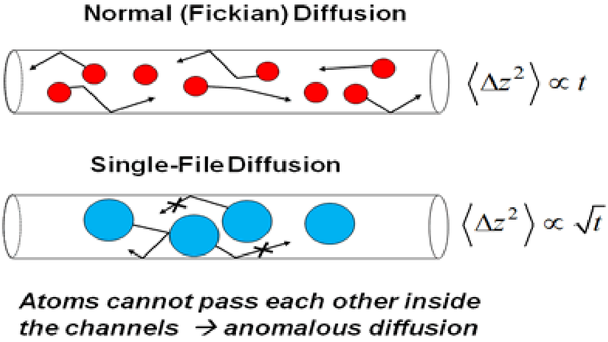
T. Imamura, K. M. and T. Sasamoto, PRL **118**, 160601 (2017)

T. Imamura, K. M. and T. Sasamoto, *in preparation* (2018).

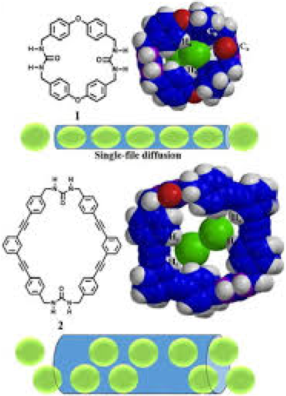
Single-file diffusion

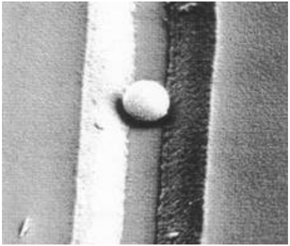
Single-file diffusion is an important phenomena soft-condensed matter (for example, transport through cell membranes).

A pristine model for single-file diffusion is the Symmetric Exclusion Process.



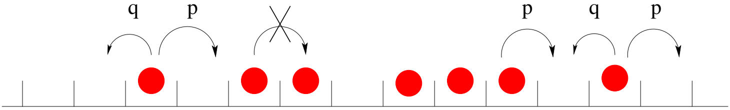
Experimental observations





(C. Bechinger's group in Stuttgart)

The Exclusion Process



The Exclusion Process is an interacting particles system:

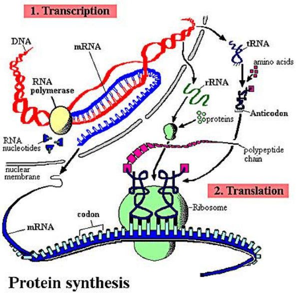
• EXCLUSION: Hard core-interaction, at most 1 particle per site.

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

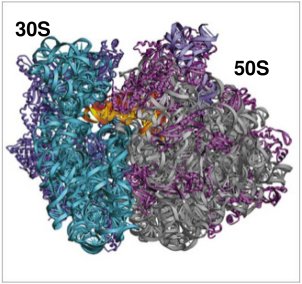
The Exclusion Process plays the role of a Paradigm in contemporary Statistical Physics (*Recall Nuno Romão's Mantras*).

The ASEP appears as a building block in many realistic models of 1d transport and is studied extensively in probability, combinatorics, condensed matter physics...

An Elementary Model for Protein Synthesis



(a)



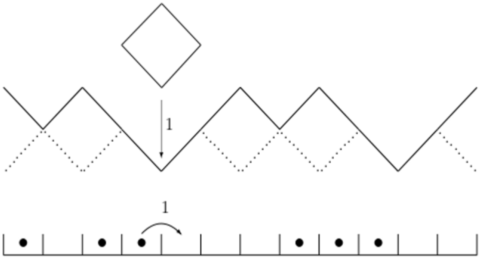
(b)

(c)

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

Relation to Kardar-Parisi-Zhang

The Exclusion Process is equivalent to an interface growth model



For asymmetric jumps, the height $h(x,t)$ satisfies the KPZ equation

$$\frac{\partial h}{\partial t} = \nu \frac{\partial^2 h}{\partial x^2} + \frac{\lambda}{2}\left(\frac{\partial h}{\partial x}\right)^2 + \xi(x,t)$$

The ASEP is a discrete version of the KPZ equation in one-dimension.

The Symmetric Exclusion Process (SEP)

We shall focus the Symmetric Exclusion Process, $(p = q = 1)$, on an infinite one-dimensional line with a finite density ρ of particles. This model was invented by F. Spitzer in 1970.

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:

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

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

Open problems:

- No formulae for higher moments of X_t are available.
- The distribution of X_t at finite time is not known.
- In the long time limit $t \to \infty$, The tracer's position X_t satisfies a Large Deviation Principle (Sethuraman and Varadhan, 2013):

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

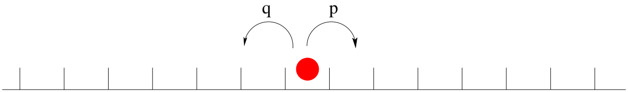
  where $\phi(\xi)$ is the large-deviation (or rate) function. Bounds for $\phi(\xi)$ have been found but its exact expression is unknown.

- What is the influence of the initial setting? For example, what happens out of equilibrium with a step initial profile ?

Exact Tracer Statistics

An elementary case: non-interacting particles

We first discuss the case of a tracer without exclusion, hopping to the right and to the left with rates p and q, respectively: everything can be calculated.



- The characteristic function is given by

$$\langle e^{sX_t} \rangle = e^{-tC_0(s)} \quad \text{with} \quad C_0(s) = q(1 - e^{-s}) - p(e^s - 1)$$

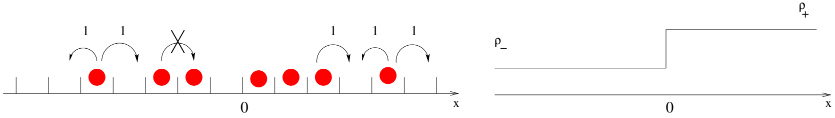
- The Large Deviation Principle, Prob $\left(\frac{X_t}{t} = -\xi\right) \simeq \exp[-t\phi_0(\xi)]$, is satisfied with

$$\phi_0(\xi) = p + q - \sqrt{\xi^2 + 4pq} + \xi \ln \frac{\sqrt{\xi^2 + 4pq} + \xi}{2q}$$

- The functions ϕ_0 and $C_0(s)$ are related by Legendre Transform.
- Here, scalings are linear with time t.

SEP with step profile

Start with a step-like profile (ρ_+, ρ_-) and the tagged particle located at 0. Let the system evolve and call X_t the position of the tracer.



The goal is to calculate the large deviation function (LDF) $\phi(\xi)$ or, equivalently, the characteristic function of X_t, which behaves as

$$\langle e^{sX_t} \rangle \sim e^{-\sqrt{t}C(s)} \quad \text{when} \quad t \to \infty$$

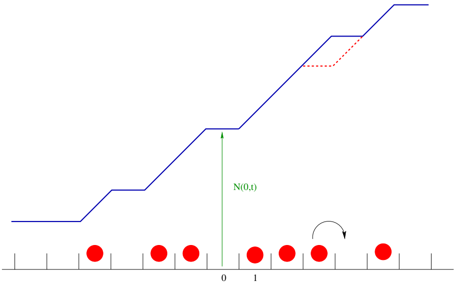
and $C(s)$ generates the cumulants of X_t: $C(s) = -\sum_n \frac{s^n}{n!} \frac{\langle X_t^n \rangle_c}{\sqrt{t}}$

The functions $C(s)$ and $\phi(\xi)$ are related by Legendre transform

$$C(s) = \min_{\xi} \left(2s\xi + \phi(\xi) \right)$$

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.

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

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 have obtained 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

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

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

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

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

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

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

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:

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

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 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

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

By expanding $\mu(\xi, \lambda)$ w.r.t. λ, combinatorial formulae for all the cumulants of the local height function $N(x, t)$ for $t \to \infty$ are found.

Long time limit of the cumulants

Expanding $\mu(\xi, \lambda)$ with respect to λ and identifying the term of order n with the n-th cumulant, we obtain

$$\frac{\langle N(x,t)^n \rangle_c}{\sqrt{t}} = \sum_{l=1}^{n} (-1)^l (l-1)! \left(\alpha_{n,l}(r_+, r_-) \frac{\Xi(-\sqrt{l}\xi)}{\sqrt{l}} - 2\alpha_{n,l}(1,0)\xi\rho_+^l \right)$$

with

$$\alpha_{n,l}(a,b) = \sum_{\substack{\nu \vdash n \\ \nu = 1^{l_1} 2^{l_2} \dots \\ l_1 + l_2 + \dots = l}} \frac{n!}{\prod_{j=1}^{n} l_j!} \prod_{j=1}^{n} \left(\frac{a + (-1)^j b}{j!} \right)^{l_j}$$

The symbol $\nu \vdash n$ means that $\nu = 1^{l_1} 2^{l_2} \cdots$ is a partition of n, *i.e.*, $n = \sum_j j l_j$.

These formulae for the height can be translated as properties of the tracer's position.

But, first, we describe the strategy of the calculation.

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

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

DUALITY (Proof)

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.

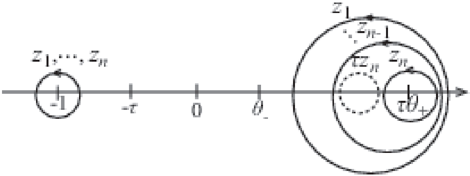
The n-th correlation function, although more contrived, is analyzed along similar lines. The key point is to check the adjacency conditions.

2. INTEGRABLE PROBABILITIES

Using that ASEP is an integrable model, solvable by Bethe Ansatz, the τ-correlation functions can be expressed as multiple contour integrals in the complex plane (Schütz, Tracy-Widom, Borodin-Corwin-Sasamoto).

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

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



Proof of the contour integrals

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

For the master equation, we use

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

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

For the initial condition, one has to perform a residue calculation at $t=0$ by evaluating the residue at θ_+ or θ_- depending on whether x_i is positive or negative.

3. Symmetric limit

For finite values of x and t, the symmetric exclusion case is obtained by performing the $\tau \to 1$ limit in the contour integrals.
This requires a combinatorial calculation in which the nested contours are disentangled by taking recursively the residues at poles :

$$\langle \tau^{n N_{\mathbf{ASEP}}} \rangle = \sum_{k=0}^{n} (-1)^k \prod_{i=n-k+1}^{n} \left(1 - \frac{r_-}{\tau^i r_+}\right)$$
$$\times \sum_{\substack{P \subset \{1,\dots,n\} \\ |P|=k}} \tau^{v(P)} \int_{-1} \cdots \int_{-1} f_P(z_1,\dots,z_k) \prod_{i=1}^{k} dz_i \cdot \prod_{i=1}^{n-k} e^{\Lambda_i}$$

Here P corresponds to which poles are taken, $v(P)$ is the exponent of τ depending on P, and

$$e^{\Lambda_i} = \left(\frac{1+\tau^i\theta_+}{1+\tau^{i-1}\theta_+}\right)^x e^{\Lambda(\tau^i{}_+)t}$$

Now, in these expressions, the $\tau \to 1$ limit can (safely) be carried out.

4. Determinant and Large time limit

Once the residues have evaluated, and the $\tau \to 1$ limit taken, the remaining n-fold integral becomes

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

where C_0 is a small contour around the origin. Using some identities on symmetric functions, this integral can be rewritten as a determinant

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

This expression leads to the exact finite time formula for the characteristic function as a Fredholm determinant; finally, the asymptotic analysis of this determinant yields the explicit formula for $\mu(\xi, \lambda)$.

Back to 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 $m = q\sqrt{t}$.

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 the SEP (P. Ferrari, S. Goldstein and J. L. Lebowitz, 1985).

Cumulants of the tracer

From the knowledge of $\phi(\xi)$, the cumulants of the tracer can be calculated explicitly for $t \to \infty$:

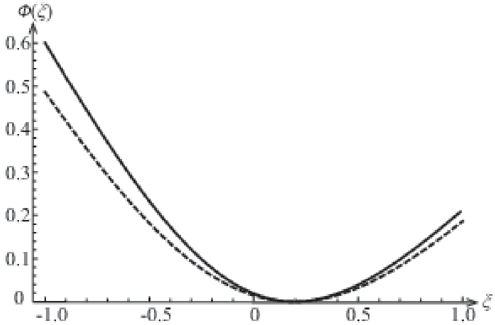
- Variance : $\langle X_t^2 \rangle = 2\frac{1-\rho}{\rho}\sqrt{\frac{Dt}{\pi}}$ (Arratia)
- Fourth order :

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

- At order 6:

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

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

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

This result can be obtained by hydrodynamics.

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

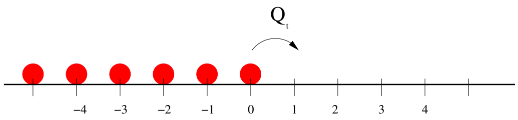
$$\mathrm{Var}(X_t) = \frac{4K(\rho_+ - \rho_-)^2 A(\xi_0)\sqrt{t}}{(\rho_+\,\mathrm{erfc}\,(\xi_0) + \rho_-\,\mathrm{erfc}\,(-\xi_0))^2}$$

with

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

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 current Q_t cumulant generating function 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 $\Xi(\xi) = \int_\xi^\infty \mathrm{erfc}\,(u)\mathrm{d}u$.

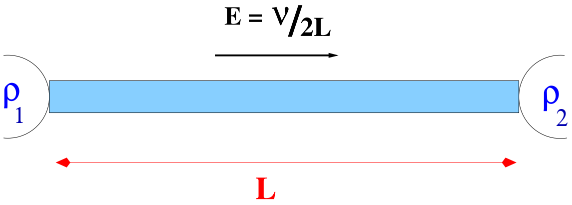
When $\rho_- = 0$, the tracer is the left-most particle of a SEP expanding in a half-empty space: finding the distribution of X_t becomes identical to a problem in extreme value statistics (S. Sabhapandit). The tracer is superdiffusive and follows a Gumbel law. It can be shown that

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

Remark: the $\rho \to 1$ limit can also be retrieved (O. Bénichou et al.).

Hydrodynamic Description

The deterministic hydrodynamic limit



Starting from the microscopic level, define local density $\rho(x,t)$ and current $j(x,t)$ with macroscopic space-time variables $x = i/L, t = s/L^2$ (diffusive scaling). The average coarse-grained evolution of the system is given by (De Masi, Presutti, Spohn, Varadhan)

$$\partial_t \rho(x,t) = -\nabla J(x,t) \quad \text{with} \quad J = -D(\rho)\nabla\rho + \nu\sigma(\rho)$$

For the ASEP, $D(\rho) = 1$ and $\sigma(\rho) = 2\rho(1-\rho)$

How can Fluctuations be taken into account?

The Macroscopic Fluctuation Theory

At a coarse-grained level (under diffusive scaling of space and time), the 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

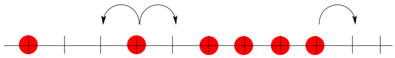
$$D_{ASEP}(\rho) = 1 \quad \text{and} \quad \sigma_{ASEP}(\rho) = 2\rho(1-\rho)$$

Values of Diffusivity and Conductivity

- Independent particles: $D = 1$, $\sigma = 2\rho$
- Simple Exclusion Process: $D_{\mathrm{SEP}} = 1$, $\sigma_{\mathrm{SEP}} = 2\rho(1-\rho)$
- Kipnis-Marchioro-Presutti model: $D_{\mathrm{KMP}} = 1$, $\sigma_{\mathrm{KMP}} = 2\rho^2$
- Repulsion Process: Hops increasing the number of nearest neighbourg pairs are forbidden:

$$D_{\mathrm{RP}} = \begin{cases} \frac{1}{(1-\rho)^2} & \text{if } 0 < \rho < \frac{1}{2} \\ \frac{1}{\rho^2} & \text{if } \frac{1}{2} < \rho < 1 \end{cases} \quad \sigma_{\mathrm{RP}} = \begin{cases} \frac{2\rho(1-2\rho)}{1-\rho} & \text{if } 0 < \rho < \frac{1}{2} \\ \frac{2(1-\rho)(2\rho-1)}{\rho} & \text{if } \frac{1}{2} < \rho < 1 \end{cases}$$

- Exclusion Process with Avalanches: $D_{\mathrm{EPA}} = \frac{1}{(1-2\rho)^3}$, $\sigma_{\mathrm{EPA}} = \frac{2\rho(1-\rho)}{(1-2\rho)^3}$



The MFT Action

For a weakly-driven diffusive system, 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:

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

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.

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.

MFT Equations

An excursion X_t of the position of the Tracer will be produced by an optimal fluctuation that can be obtained by extremalizing the above action.

The corresponding Euler-Lagrange equations, have an Hamiltonian structure and can be rewritten as

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

with suitable boundary conditions that generally embody the constraints. 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 can not be solved analytically in general, a perturbative approach allows us to derive the first few cumulants of X_t (Krapivsky, KM and Sadhu, 2014,2015).

Variance and Kurtosis

- Second Moment:

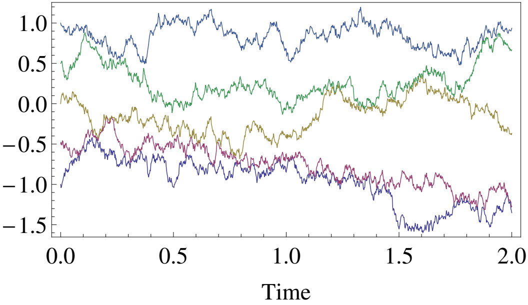
$$\langle X_t^2 \rangle = \frac{2(1-\rho)}{\rho}\sqrt{\frac{t}{\pi}}$$

- Fourth Cumulant:

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

Interacting Brownian Motions

A special case of Single-File diffusion is a system of Interacting Brownian Motions with hard-core reflection. It can be obtained as the limit of SEP in a continuous space with point-particles.

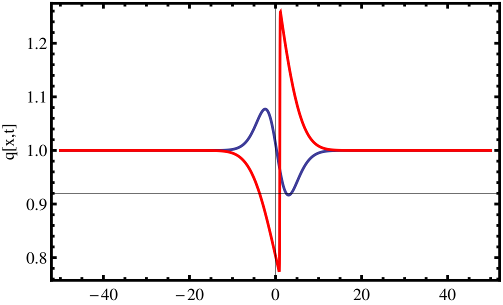


F. Spitzer, *Adv. Math.* (1970).

In this case: $D = 1$, $\sigma = 2\rho$. The MFT equations can be solved exactly.

Shape of the optimal profiles

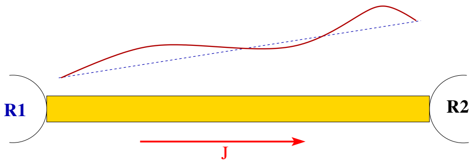
MFT provides you with the statistical properties but also with an understanding of the dynamical process leading to a given atypical fluctuation.



Profil dynamics (Annealed case)

Conclusion

Fluctuations far from equilibrium



What is the distribution of the density profile in the steady state? What is the probability of the current J? Can we determine the corresponding Large Deviation Functions?

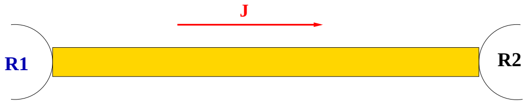
More generally, the probability to observe an atypical current $j(x,t)$ and the corresponding density profile $\rho(x,t)$ during $0 \leq s \leq L^2\, T$ (L being the size of the system) is given by

$$\mathrm{Pr}\{j(x,t),\rho(x,t)\} \sim \mathrm{e}^{-L\,\mathcal{I}(j,\rho)}$$

Could one calculate this large deviation functional for systems out of equilibrium?

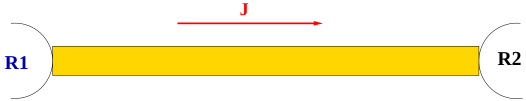
Classical Transport in 1d: ASEP

A picture of a non-equilibrium system

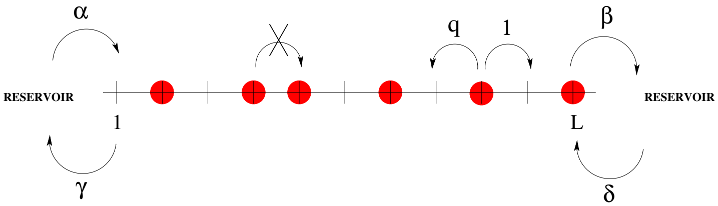


Classical Transport in 1d: ASEP

A picture of a non-equilibrium system



The asymmetric exclusion model



A building block in many realistic models of 1d transport, also studied extensively in probability, combinatorics...

Thousands of articles devoted to this model in the last 20 years.

INTEGRABILITY

Many exact results about large deviations have been obtained thanks to the **integrability** of ASEP, which can be mapped to a non-hermitian deformation of the XXZ spin chain.

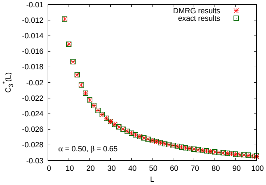
Today, we talked about tracer dynamics.

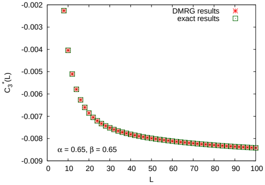
But, for example, the FCS of the ASEP current has also been calculated

$$F(\chi) = (1-q)(1-\rho_a)\frac{e^{i\chi}-1}{e^{i\chi}+(1-\rho_a)/\rho_a}$$

and it yields (by Legendre Transform) the current distribution

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





HYDRODYNAMICS (MFT)

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.

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

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

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

- However, the only non-trivial solutions of the MFT equations have in fact been obtained by using integrability at the microscopic level.
- Could classical integrability help us understand the structure of these equations?
- The analysis of this new set of non-linear 'hydrodynamic equations' has just begun!