Macroscopic Fluctuations of Interacting Particles

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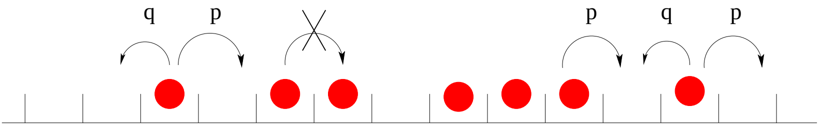
IHP, Alain Comtet, October 14, 2014

P. Krapivsky, K. M. and T. Sadhu, PRL 113, 078101 (2014)
P. Krapivsky, K. M. and T. Sadhu, submitted to J. Phys. A

A Paradigm of non-equilibrium behaviour: ASEP

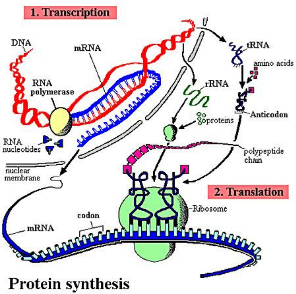


Asymmetric Exclusion Process. A Minimal Model for non-equilibrium Statistical Mechanics.

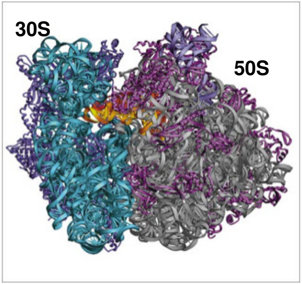
- EXCLUSION: Hard core-interaction; at most 1 particle per site.
- ASYMMETRIC: External driving; breaks detailed-balance
- PROCESS: Stochastic Markovian dynamics; no Hamiltonian.

The ASEP appears as a building block in many realistic models of 1d transport and is studied extensively in probability, combinatorics, statistical physics...
Yet, it was invented in 1968 by molecular biologists.

The central dogma of molecular biology



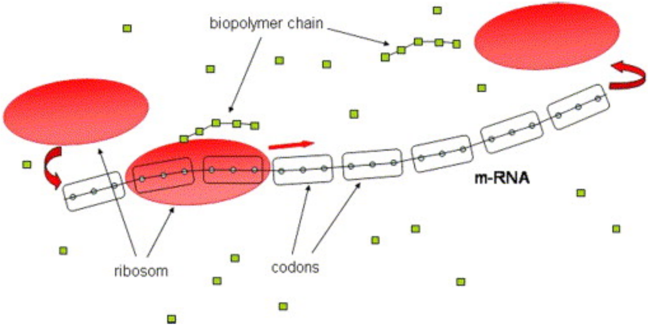
(a)



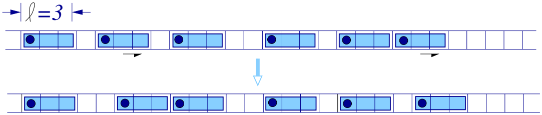
(b)

(c)

An Elementary Model for Protein Synthesis



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



Anomalous diffusion in SEP

Consider the Symmetric Exclusion Process on an infinite one-dimensional line with a 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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- Because of the exclusion condition, a particle displays an anomalous diffusive behaviour:

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

Single-File Diffusion is an important model in soft-condensed matter (e.g., ion transport through cell membranes).

Some open questions

- The quantitative behaviour of the higher cumulants of X_t is not known. Can we calculate the cumulant generating function $\log[\langle e^{\lambda X_T} \rangle]$ or the full distribution of X_t?
- What is the robustness of the $t^{1/4}$? Can tagged particle statistics be determined for more general systems, *without having to use integrability or rely on some combinatorial trick?*
- What is the influence of the initial setting?
- Statistical properties of the tagged particle trajectory? Multiple-time correlations?
- Other important observables (current, total displacement...)?

Macroscopic Fluctuation Theory

Study the system at a coarse-grained hydrodynamical level.
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:

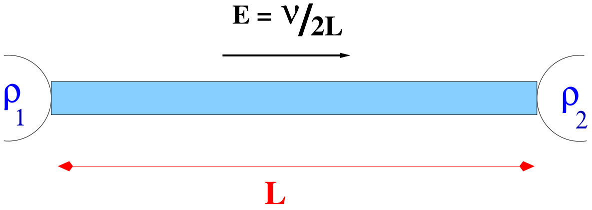
$$\mathrm{Pr}\{j(x,t), \rho(x,t)\} \sim \mathrm{e}^{-\mathcal{I}(j,\rho)}$$

The rate functional $\mathcal{I}(j, \rho)$ is the optimum of a variational problem (L. Bertini, D. Gabrielli, A. De Sole, G. Jona-Lasinio and C. Landim)

$$\mathcal{I}(j,\rho) = \min_{\rho,j} S(j,\rho) \text{ with } S(j,\rho) = \int_0^T dt \int_{-\infty}^{+\infty} \frac{(j - \nu\sigma(\rho) + D(\rho)\nabla\rho)^2 \, dx}{2\sigma(\rho)}$$

with the constraint: $\partial_t \rho = -\nabla . j$
The transport coefficients $D(\rho)$ (Diffusivity) and $\sigma(\rho)$ (Conductivity) carry the relevant information from the microscopic level to the macroscopic stage. *They must be calculated using the microscopic dynamical rules.*
From $\mathcal{I}(j, \rho)$, the distribution of any functional of j and ρ can be derived, in principle.

The Hydrodynamic Limit: deterministic case



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 hydrodynamic evolution of the system is given by:

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

How can Fluctuations be taken into account?

Fluctuating Hydrodynamics

Let Y_t be the integrated current of particles transferred from the left reservoir to the right reservoir during time t.

- $\lim_{t\to\infty} \frac{\langle Y_t \rangle}{t} = D(\rho)\frac{\rho_1 - \rho_2}{L} + \sigma(\rho)\frac{\nu}{L}$ for $(\rho_1 - \rho_2)$ small
- $\lim_{t\to\infty} \frac{\langle Y_t^2 \rangle}{t} = \frac{\sigma(\rho)}{L}$ for $\rho_1 = \rho_2 = \rho$ and $\nu = 0$.

Then, the equation of motion is obtained as:

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

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

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

For the symmetric exclusion process, the 'phenomenological' coefficients are given by

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

Values of Diffusivity and Conductivity

- Independent particles: $D = 1$, $\sigma = 2\rho$

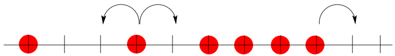
- Simple Exclusion Process: $D_{\mathrm{SEP}} = 1$, $\sigma_{\mathrm{SEP}} = 2\rho(1-\rho)$

- 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:

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

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



Katz-Lebowitz-Spohn model (Driven Ising Model)

The Katz-Lebowitz-Spohn model is a driven lattice gas where the hopping rates depend on the neighbouring sites:

$$0100 \underset{1+\delta}{\overset{1+\delta}{\leftrightarrows}} 0010 \quad 1101 \underset{1-\delta}{\overset{1-\delta}{\leftrightarrows}} 1011 \quad 1100 \underset{1+\epsilon}{\overset{1-\epsilon}{\leftrightarrows}} 1010 \quad 0101 \underset{1-\epsilon}{\overset{1+\epsilon}{\leftrightarrows}} 0011$$

$$\sigma_{\rm KLS} = 2\frac{\lambda(\rho)[1+\delta(1-2\rho)]-2\epsilon\sqrt{\rho(1-\rho)}}{\lambda(\rho)^3} \text{ with } \lambda(\rho) = \frac{1+\sqrt{1-8\epsilon\rho(1-\rho)/(1+\epsilon)}}{2\sqrt{\rho(1-\rho)}}$$

The diffusivity is given by $D_{\rm KLS}(\rho) = \frac{1}{2}\chi(\rho)\,\sigma_{\rm KLS}(\rho)$, where $\chi(\rho)$ is obtained by eliminating the parameter h between the two equations:

$$\chi = \frac{1}{4}\,\frac{1+\epsilon}{1-\epsilon}\,\frac{\cosh h}{\left(\sinh^2 h + \frac{1+\epsilon}{1-\epsilon}\right)^{3/2}}$$

$$\rho = \frac{1}{2}\left(1 + \frac{\sinh h}{\sqrt{\sinh^2 h + \frac{1+\epsilon}{1-\epsilon}}}\right)$$

(Y. Kafri et al., 2013)

Tagged particle as a macroscopic observable

How to write 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:

$$\int_{X_T}^{+\infty} \rho(x,t) = \int_0^{+\infty} \rho(x,0)$$

This defined the functional $X_T[\rho]$, whose statistics we can study by MFT.

$$\langle \mathrm{e}^{\lambda X_T} \rangle = \int \mathcal{D}\rho_0(x) \mathcal{P}[\rho_0] \int \mathcal{D}\rho(x,t) \mathcal{D}j(x,t) \mathrm{e}^{\lambda X_T[\rho] - S_{MFT}[j,\rho]} \delta(\partial_t \rho + \nabla . j)$$

The initial profile ρ_0, distributed according to $\mathcal{P}[\rho_0]$ can be fixed (quenched) or fluctuate w.r.t. some chosen measure (annealed).

Scaling shows that the effective action grows as $\sqrt{T} \to$ Saddle-Point.

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

M. F. T. Equations

Evaluating the effective action at the saddle-point (j^*, ρ^*) gives

$$\langle \mathrm{e}^{\lambda \mathrm{X_T}} \rangle \simeq \mathrm{e}^{\sqrt{4\mathrm{T}}\mu(\lambda)}$$

$\sqrt{4T}\mu(\lambda)$ being the cumulant generating function: $\mu(\lambda) = \sum_n \frac{\lambda^n}{n!} \frac{\langle X_T^n \rangle_c}{\sqrt{4T}}$

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The optimization is performed by solving Euler-Lagrange equations, better reformulated as a Hamiltonian structure in terms of two conjugate variables (p, q) that satisfy coupled PDE's (setting $\nu = 0$):

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

where $q(x, t)$ is the optimal density-field and $p(x, t)$ is the conjugate field with Hamiltonian: $H[p, q] = -D(q) \partial_x q \partial_x p + \frac{\sigma(q)}{2} (\partial_x p)^2$
The parameter λ appears through the boundary conditions at $t = 0$ and $t = T$.

A Formula for the variance

In the general case, the MFT equations can not be solved analytically but a perturbative approach w.r.t. λ is possible, providing us with the first few cumulants of X_T.

- Quenched case:

$$\langle X_T^2 \rangle = \frac{\sigma(\rho)}{\rho^2}\sqrt{\frac{T}{\pi D(\rho)}}$$

- Annealed case:

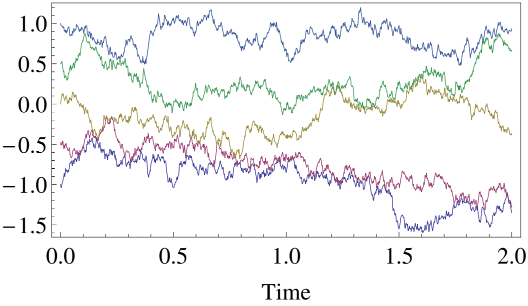
$$\langle X_T^2 \rangle = \frac{\sigma(\rho)}{\rho^2}\sqrt{\frac{\mathbf{2}T}{\pi D(\rho)}}$$

Note the *everlasting effect* of the initial conditions.
For SEP, we also obtain a formula for the 4th 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.

A Tracer Statistics: annealed case

For Interacting Brownian Motions, the full statistics of the tracer position, X_t, can be determined. The function $\mu(\lambda)$ is known through a parametric representation:

$$\begin{aligned}
\mu(\lambda) &= \left[\lambda + \rho \frac{1 - e^{B}}{1 + e^{B}}\right] \eta \\
\lambda &= \rho\left(1 - e^{-B}\right)\left[1 + \tfrac{1}{2}\left(e^{B} - 1\right) \mathrm{erfc}(\eta)\right] \\
e^{2B} &= 1 + \frac{2\eta}{\pi^{-1/2} e^{-\eta^2} - \eta\, \mathrm{erfc}(\eta)}
\end{aligned}$$

The first few moments are given by

$$\langle X_T^2 \rangle_c = \frac{2}{\rho\sqrt{\pi}} \sqrt{T},$$

$$\langle X_T^4 \rangle_c = \frac{6\,(4 - \pi)}{\left(\rho\sqrt{\pi}\right)^3} \sqrt{T}$$

$$\langle X_T^6 \rangle_c = \frac{30\left(68 - 30\pi + 3\pi^2\right)}{\left(\rho\sqrt{\pi}\right)^5} \sqrt{T}$$

A Tracer Statistics: quenched case

The function $\mu(\lambda)$ is even simpler in the quenched case

$$\mu(\lambda)=\sqrt{T}\rho\int_{-\infty}^{+\infty}\mathrm{dx}\log\left\{1+2\,\mathrm{erfc}(\mathrm{x})\mathrm{erfc}(-\mathrm{x})\sinh^2\left(\frac{\lambda}{2\rho}\right)\right\}$$

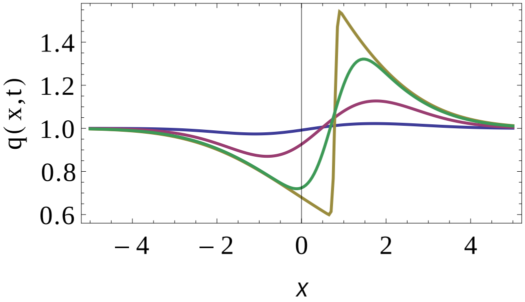
In both cases (annealed and quenched), the large deviation function of the tracer, defined, for $T \to \infty$, via

$$\mathrm{Prob}\left(\frac{X_T}{\sqrt{T}}=\xi\right)\sim\exp\left[-\sqrt{T}\phi(\xi)\right]$$

is obtained by taking the Legendre transform of $\mu(\lambda)$.

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.



Quenched case

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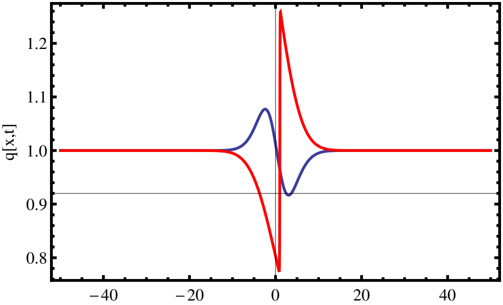
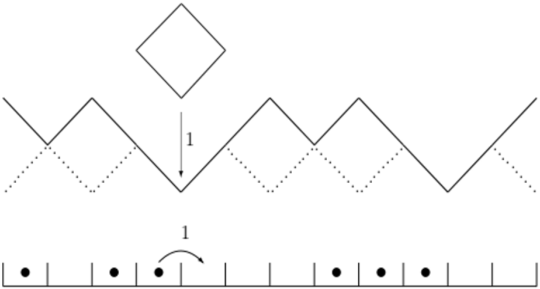


Annealed case

Another observable: Surface swept by an interface



The height of an interface $h(x,t)$ satisfies the generic 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.

Using MFT, the first few moments of the Area swept by the interface have been calculated.

Conclusions

The asymmetric exclusion process is a paradigm for the behaviour of systems far from equilibrium in low dimensions. The ASEP is important for theory but also for its multiple applications.

A tagged particle plays the role of a probe for the dynamics. Single-file in 1d is one of the simplest example of anomalous diffusion.

The Macroscopic Fluctuation Theory is a versatile tool to understand non-equilibrium properties of interacting particle systems. It generalizes the Onsager-Machlup theory of fluctuations close to equilibrium. In particular, it provides us with a physical picture of how a non-reversible fluctuation can be generated. Often, combinatorial approaches miss this picture.

The calculation of the statistics of a tracer in SEP is an important and difficult open problem.