# Survival of a target in a gas of diffusing particles with exclusion

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Prof. Giulio Racah 1909-1965 He was born in Firenze, and died here

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# Plan

✓ Macroscopic Fluctuation Theory of diffusive lattice gases

MFT in non-stationary settings: examples

Survival of a target against "searchers"

a. Stationary fluctuations: d>2, long timesb. Non-stationary fluctuations: d=1, and any d for intermediate times

Extensions and summary

Diffusive lattice gases



SSEP: simple symmetric exclusion process

RWs, ZRP:  $\alpha = \alpha(n_i)$ 

random walkers; zero-range process

Large-scale behavior: fluctuating hydrodynamics

$$\partial_t \rho = \nabla \cdot \left[ D(\rho) \nabla \rho + \sqrt{\sigma(\rho)} \xi(\mathbf{x}, t) \right], \quad \begin{array}{c} \xi: \text{Gaussian noise,} \\ \text{delta-correlated in } \mathbf{x} \text{ and } t \end{array}$$

Spohn 1991, Kipnis and Landim 1999

Diffusive lattice gases are fully characterized, at large scales, by the diffusivity  $D(\rho)$  and mobility  $\sigma(\rho)$ 

$$\partial_t \rho = \nabla \cdot \left[ D(\rho) \nabla \rho + \sqrt{\sigma(\rho)} \xi(\mathbf{x}, t) \right]$$

 $D(\rho)$  and  $\sigma(\rho)$  are related to the equilibrium free energy density  $F(\rho)$ :

$$\frac{d^2 F(\rho)}{d\rho^2} = \frac{2D(\rho)}{\sigma(\rho)}$$

When noise is ignored: diffusion equation

 $\partial_t \rho = \nabla \cdot \left[ D(\rho) \nabla \rho \right]$ 

## Macroscopic Fluctuation Theory (MFT)

Bertini, De Sole, Gabrielli, Jona-Lasinio and Landim (2001, ...)

Large parameter: number of particles in a relevant region of space. Generalizes the weak-noise WKB theory of Freidlin and Wentzel to fields

Similar in spirit: Elgart and Kamenev (2004), M and Sasorov (2010) - WKB approximation to master equation for random walk on lattice and *on-site reactions*. Large parameter: number of particles *on a single site* 

MFT can be derived from fluctuating hydrodynamics via saddle-point expansion of a proper path integral (Tailleur, Kurchan, Lecomte 2007). This leads to a minimization problem that can be cast into a classical Hamiltonian field theory for the particle density q(x,t) and conjugate "momentum" density p(x,t):

$$\partial_t q = \nabla \cdot [D(q) \nabla q - \sigma(q) \nabla p)] \qquad \qquad \partial_t q = \delta H / \delta p, \\ \partial_t p = -D(q) \nabla^2 p - \frac{1}{2} \sigma'(q) (\nabla p)^2 \qquad \qquad \partial_t p = -\delta H / \delta q,$$

$$H[q(\mathbf{x},t), p(\mathbf{x},t)] = \int d\mathbf{x} \,\mathcal{H},$$
$$\mathcal{H} = -D(q)\nabla q \cdot \nabla p + \frac{1}{2}\sigma(q)(\nabla p)^2$$

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

Boundary conditions, in x and t, are determined by specific problem.

Mean-field (noiseless) limit: p(x,t)=0: downhill trajectories

$$\partial_t q = \nabla \cdot \left[ D(q) \nabla q \right]$$

Fluctuations:  $p(x,t) \neq 0$ : uphill trajectories, the optimal density history

The probability density of a large deviation is given by the mechanical action along a proper uphill trajectory:

$$-\ln \mathscr{P} \cong S = \int d\mathbf{x} \int_{0}^{T} dt \left[ p(\mathbf{x}, t) \partial_{t} q(\mathbf{x}, t) - \mathscr{H} \right]$$
$$= \frac{1}{2} \int d\mathbf{x} \int_{0}^{T} dt \, \sigma(q) (\nabla p)^{2}$$

If the initial condition is random, one should also find the optimal *initial* density profile and add to S the Boltzmann-Gibbs free energy "cost" of creating it

MFT emerged in the context of non-equilibrium steady states of lattice gases



*Expected* density profile solves the steady-state mean-field problem

$$D(\overline{\rho}) d\overline{\rho} / dx = \text{const}$$
$$\overline{\rho}(\mathbf{x} = 0) = \rho_{-} \qquad \overline{\rho}(\mathbf{x} = \mathbf{L}) = \rho_{+}$$

Density fluctuations  $\mathscr{F}[\rho(x)] \sim \exp\{-LF[\rho(x/L)]\}$  L>>1

 $F[\rho(x/L)]$  large deviation functional

Reviews: Derrida 2007, Jona-Lasinio 2010, Bertini et al 2014

#### MFT emerged in the context of non-equilibrium steady states of lattice gases



Fluctuations of current  $\mathcal{F}(J) \sim \exp[-LS(J, \rho_{-}, \rho_{+})], L >> 1$ 

 $S(J, 
ho_{-}, 
ho_{+})$  large deviation function

What is the most probable density profile for given  $\mathcal{J}$ ?

Reviews: Derrida 2007, Jona-Lasinio 2010, Bertini et al. 2014

MFT emerged in the context of non-equilibrium steady states of lattice gases



- Non-locality: long range correlations
- Uphill trajectory is different from time-reversed downhill trajectory
- Non-smooth parameter dependence of large deviation function/functional: "phase transitions"

Reviews: Derrida 2007, Jona-Lasinio 2010, Bertini et al. 2014

#### Non-stationary settings are also interesting

# Example 1: Formation of void of size L at time T in an initially uniform gas

Krapivsky, M and Sasorov 2012



$$\mathcal{F}(L,T) \sim \exp[-T^{d/2}S_d(\frac{L}{\sqrt{T}},n)], \quad T >> 1, L >> 1$$

d: dimension of space  $S_d(\frac{L}{\sqrt{T}},n)$  large deviation function; Most probable density history

#### Non-stationary settings are also interesting

#### Example 2: Fluctuations of mass/energy transfer in finite time

Derrida and Gerschenfeld 2009a,2009b, Sethuraman and Varadhan 2011, Krapivsky and M 2012, M and Sasorov 2013, 2014, Vilenkin, M and Sasorov 2014

$$\begin{array}{c} \rho_{-} \\ \hline \\ \rho_{+} \\ \hline \\ M_{T} = \int_{0}^{\infty} [\rho(x,T) - \rho(x,0)] \, dx \\ \langle M_{T} \rangle = \frac{\rho_{-} - \rho_{+}}{\sqrt{\pi}} \sqrt{T}, \quad T >> 1 \quad \begin{array}{c} \text{for Random Walkers} \\ (\text{RWs}), \text{SSEP and KMP} \\ \mathcal{P}(M_{T}) \sim \exp[-\sqrt{T} S(\frac{M_{T}}{\sqrt{T}}, \rho_{-}, \rho_{+})], \quad T >> 1 \\ \end{array}$$
Large deviation function  $S(\frac{M_{T}}{\sqrt{T}}, \rho_{-}, \rho_{+}) = ? \text{ Even } \rho_{-} = \rho_{+} \text{ is nontrivial} \\ \text{What is the most probable history of the density field conditional on } M_{T}? \end{array}$ 

#### Non-stationary settings

Example 3 (this talk): Target survival problem



What is the probability that *no particle* hit the target until t=T? What is the most probable density history of the gas conditional on the non-hitting? For a given lattice gas, the answers depend on three parameters:

$$l = \frac{R}{\sqrt{DT}}, d, n_0$$

The T→∞ asymptotic of the target survival probability is known for ideal gas (RWs), see references in Bray, Majumdar and Schehr, Adv. Phys. 62, 225 (2013)

$$-\frac{\ln \mathcal{P}_{\rm RW}(T)}{n_0} \simeq \begin{cases} \frac{2(DT)^{1/2}}{\sqrt{\pi}}, & d = 1, \\ \frac{4\pi DT}{\ln(DT/R^2)}, & d = 2, \\ \frac{2(d-2)\pi^{d/2} R^{d-2} DT}{\Gamma(d/2)}, & d > 2, \end{cases}$$

Most probable density histories have not been found even for ideal gas. For *non-ideal* gases such as SSEP there are no previous results, except for some bounds. MFT formulation is similar to that for the mass transfer:

$$\partial_{t}q = \nabla \cdot [D(q)\nabla q - \sigma(q)\nabla p)]$$

$$+ \text{ spherical symmetry}$$

$$\partial_{t}p = -D(q)\nabla^{2}p - \frac{1}{2}\sigma'(q)(\nabla p)^{2}$$

Boundary condition: q(r=R,t)=0

The process is conditional on N absorbed particles by time T:

$$\frac{2\pi^{d/2}}{\Gamma(d/2)}\int_{R}^{\infty} dr \ r^{d-1}[n_0 - q(r,T)] = N \qquad \text{M and Redner 2014}$$

This integral constraint calls for a Lagrangian multiplier  $\lambda$  and leads to additional boundary condition (in time) coming from the minimization of action:

$$p(r,t=T) = \lambda \theta(r-R)$$

The parameter  $\lambda$  is ultimately fixed by N=0

Deterministic, or quenched, initial condition  $q(r > R, t = 0) = n_0$ 

Once q(r,t) and p(r,t) found:

$$-\ln \mathscr{P} \cong \mathbf{S}(\mathbf{N}) = \frac{\pi^{d/2}}{\Gamma(d/2)} \int_{0}^{T} dt \int_{R}^{\infty} dr \ r^{d-1} \sigma(q) (\partial_{r} p)^{2}$$

Random, or annealed initial condition introduces two changes:

• the initial condition becomes p-dependent:

$$p(r,0) - 2 \int_{n_0}^{q(r,0)} dq_1 \, \frac{D(q_1)}{\sigma(q_1)} = \lambda \theta(r-R) \quad (1)$$

(Derrida and Gerschenfeld 2009)

• when evaluating the probability, one should add to S the Boltzmann-Gibbs free energy "cost" of creating the optimal initial density profile q(r,0) described by Eq. (1)

Dynamic scaling of the absorption probability

MFT equations are invariant under rescaling  $t/T \to t$ ,  $\mathbf{x}/\sqrt{DT} \to \mathbf{x}$ The radius of absorber becomes  $l = R/\sqrt{DT}$ 

$$-\ln \mathscr{P} \cong \mathbf{S} = (DT)^{d/2} s \left[ l, \frac{N}{(DT)^{d/2}}, n_0 \right],$$
  

$$s = \frac{\pi^{d/2}}{\Gamma(d/2)} \int_0^1 dt \int_l^\infty dr \ r^{d-1} \sigma(q) (\partial_r p)^2$$
We are interested in the limit N->0

d=1: S is independent of R, so s doesn't depend on  $\ell$  leading to survival probability

 $-\ln \mathscr{P} \cong (DT)^{1/2} s_1(n_0)$  for all diffusive lattice gases

The  $T^{1/2}$  scaling signals that the 1d-problem is non-stationary. An important consequence is that  $s_1(n_0)$  depends on whether the initial condition is deterministic or random. Long-time asymptotics for d>2: stationary fluctuations

$$-D(q)\frac{dq}{dr} + \sigma(q)v = 0 \quad \text{zero flux at all times}$$
$$\frac{D(q)}{r^{d-1}}\frac{d}{dr}(r^{d-1}v) + \frac{1}{2}\sigma'(q)v^2 = 0, \quad v \equiv dp/dr$$

#### This leads to a single nonlinear ODE for q(r):

$$\nabla_r^2 q + \left(\frac{D'}{D} - \frac{\sigma'}{2\sigma}\right) \left(\frac{dq}{dr}\right)^2 = 0, \text{ where}$$
$$\nabla_r^2 q = \frac{1}{r^{d-1}} \frac{d}{dr} \left(r^{d-1} \frac{d}{dr}\right)$$

### SSEP

$$D(q) = D = \text{const}, \qquad \sigma(q) = 2Dq(1-q)$$

The nonlinear ODE becomes

$$\nabla_r^2 q + \frac{2q-1}{2q(1-q)} \left(\frac{dq}{dr}\right)^2 = 0.$$

A simple change of variables  $q(r) = \sin^2 u(r)$  brings this equation to

$$\nabla_r^2 u = 0.$$

The solution, in the variable q, is

$$q(r) = \sin^2 \left[ \left( 1 - \frac{l^{d-2}}{r^{d-2}} \right) \arcsin \sqrt{n_0} \right], \quad l = \frac{R}{\sqrt{DT}}, \ d > 2$$

# SSEP, d>2

$$q(r) = \sin^{2} \left[ \left( 1 - \frac{l^{d-2}}{r^{d-2}} \right) \arcsin \sqrt{n_{0}} \right], \quad l = \frac{R}{\sqrt{DT}}$$
$$v(r) \equiv \frac{dp}{dr} = \frac{1}{2q(1-q)} \frac{dq}{dr} = \frac{2(d-2)l^{d-2} \arcsin \sqrt{n_{0}}}{r^{d-1} \sin \left[ 2 \left( 1 - \frac{l^{d-2}}{r^{d-2}} \right) \arcsin \sqrt{n_{0}} \right]}$$

$$q(r-l \ll l) \cong (d-2)^2 \arcsin^2\left(\sqrt{n_0}\right) \left(\frac{r}{l} - 1\right)^2$$

quadratic so that the flux to the target is zero  $v(r-l \ll l) = \frac{1}{l-r}$ 

singular at all times; doesn't depend on  $n_0$ 

# SSEP, d>2

$$q(r) = \sin^{2} \left[ \left( 1 - \frac{l^{d-2}}{r^{d-2}} \right) \arccos \sqrt{n_{0}} \right], \quad l = \frac{R}{\sqrt{DT}}$$
$$v(r) \equiv \frac{dp}{dr} = \frac{1}{2q(1-q)} \frac{dq}{dr} = \frac{2(d-2)l^{d-2} \arcsin \sqrt{n_{0}}}{r^{d-1} \sin \left[ 2\left( 1 - \frac{l^{d-2}}{r^{d-2}} \right) \arccos \sqrt{n_{0}} \right]}$$

Taking n<sub>0</sub><<1 we get the results for ideal gas"

$$q(r) = n_0 \left( 1 - \frac{l^{d-2}}{r^{d-2}} \right)^2, \quad l = \frac{R}{\sqrt{DT}}$$
$$v(r) = \frac{dp}{dr} = \frac{d-2}{r} \left[ \left( \frac{r}{l} \right)^{d-2} - 1 \right]^{-1}$$

# Survival probability for SSEP

$$-\ln \mathcal{P} \simeq \frac{2(d-2) \pi^{d/2} R^{d-2} DT \arcsin^2 \sqrt{n_0}}{\Gamma(d/2)}, \quad d > 2.$$

differs from the result for ideal gas only by the density dependence. The LDF increases much faster with the density, but remains finite.



The stationary solution does not satisfy the boundary conditions in time. As a result, boundary layers at t=0 and t=1 develop

Numerical solution: iterations of q forward in time, p backward in time Chernykh and Stepanov 2001



# The stationary solution also implies that the survival probability is independent, at d>2 and $\ell$ <1, on whether the initial condition is quenched or annealed

For ideal gas (RWs) this prediction is verified by microscopic calculations M,Vilenkin and Krapivsky 2014

### d=2: critical dimension for long-time asymptotic

$$q(r) = \begin{cases} \sin^2 \left( \frac{\ln \frac{r}{\ell} \arcsin \sqrt{n_0}}{\ln \frac{L}{\ell}} \right), & \ell \le r \le L, \\ n_0, & r > L. \end{cases}$$

$$v(r) = \begin{cases} \frac{2 \arcsin \sqrt{n_0}}{r \ln \frac{L}{\ell} \sin \left(\frac{2 \ln \frac{r}{\ell} \arcsin \sqrt{n_0}}{\ln \frac{L}{\ell}}\right)}, & \ell \le r \le L, \\ 0, & r > L. \end{cases}$$

#### L~1. In the original variables L~(DT)<sup>1/2</sup> Logarithmic accuracy

$$-\ln \mathcal{P} \simeq S \simeq \frac{2\pi DT \operatorname{arcsin}^2 \sqrt{n_0}}{\ln \frac{\sqrt{DT}}{R}}, \qquad R \ll \sqrt{DT}.$$

# d=1: Non-stationary fluctuations, SSEP



We have been unable to solve the complete non-stationary problem analytically

- 1. We solved it in the ideal gas limit  $n_0 \ll 1$
- 2. We calculated finite-density corrections perturbatively
- 3. We solved the problem numerically for different gas densities and determined  $s_1(n_0)$ .

# Ideal gas limit: non-interacting Random Walkers (RWs) $D(q) = 1, \ \sigma(q) = 2q$ $\partial_t q = \nabla \cdot (\nabla q - 2q\nabla p)$ $\partial_t p = -\nabla^2 p - (\nabla p)^2$ Hopf-Cole canonical transformation $Q = qe^{-p}, \ P = e^q$ $\int dx \ \Phi(q, P) = \int dx \ q \ln P$

New Hamiltonian

$$H[Q(\mathbf{x},t), P(\mathbf{x},t)] = \int d\mathbf{x} \,\overline{\mathcal{H}},$$
$$\overline{\mathcal{H}} = -\nabla Q \cdot \nabla P$$

New Hamilton equations

$$\partial_t Q = \nabla^2 Q$$
$$\partial_t P = -\nabla^2 P$$

are linear and uncoupled

Solution for ideal gas, quenched initial condition



Action for ideal gas, quenched initial condition:

$$s_{RW} = -2n_0 \int_0^\infty d\mu \operatorname{erf} \mu = -\Lambda_1 n_0, \quad \Lambda_1 = 2.06883...$$
$$-\ln P = \Lambda_1 n_0 \sqrt{T}$$

This is different from  $-\ln P = \frac{2}{\sqrt{\pi}} n_0 \sqrt{T}$  obtained for annealed initial condition

The two results (quenched and annealed) can be also obtained from the microscopic model:

Example of quenched initial condition: particles are arranged periodically in space.

Annealed initial condition: random distribution.

The microscopic theory also gives pre-exponential factors

M, Vilenkin and Krapivsky 2014

Solution for ideal gas, annealed initial condition

 $q(x,t) = n_0 \operatorname{erf}\left(\frac{x}{\sqrt{4t}}\right) \operatorname{erf}\left[\frac{x}{\sqrt{4(1-t)}}\right]$ 

 $v(x,t) = \frac{\partial p}{\partial x} = \frac{e^{-\frac{x^2}{4(1-t)}}}{\sqrt{\pi (1-t)} \operatorname{erf}\left[\frac{x}{\sqrt{4(1-t)}}\right]}$ 

symmetric around t=1/2, no overshot

same as for quenched



$$v(x,t) = \frac{1}{x}, \quad x \ll \sqrt{1-t}$$

A singularity of v at x=0 is present at all times; universal asymptotic, solves steady state eqn. for p:

$$0 = -p'' - (p')^2$$

#### Finite density correction

Split the SSEP Hamiltonian

$$\mathcal{H} = -\partial_x q \,\partial_x p + q(1-q)(\partial_x p)^2 \qquad \text{D=1}$$

in two parts: the ideal gas Hamiltonian,  $h_0 = -\partial_x q \,\partial_x p + q (\partial_x p)^2$ 

and small correction  $h_1 = -q^2 (\partial_x p)^2$ 

coming from exclusion interaction. The small correction to action can be computed perturbatively. For the quenched initial condition:

$$\delta s = -\int_0^1 dt \int_0^\infty dx \, h_1[q_0(x,t), p_0(x,t)]$$
$$= \int_0^1 dt \int_0^\infty dx \, q_0^2(x,t) v_0^2(x,t),$$

where the integration is over unperturbed (that is, ideal gas) trajectory. The final result is  $\int_{\infty}^{\infty}$ 

$$s = -\Lambda_1 n_0 + \Lambda_2 n_0^2 + \dots, \quad \Lambda_1 = 2 \int_0^\infty d\mu \operatorname{erf} \mu = 2.06883..., \quad \Lambda_2 = 1.08337...$$
$$-\ln P = \sqrt{T} s$$

#### Finite density correction

Split the SSEP Hamiltonian

$$\mathcal{H} = -\partial_x q \,\partial_x p + q(1-q)(\partial_x p)^2 \qquad \text{D=1}$$

 $h_0 = -\partial_x q \partial_x p + q(\partial_x p)^2$ in two parts: the ideal gas Hamiltonian,

and small correction  $h_1 = -q^2 (\partial_x p)^2$ 

coming from exclusion interaction. The small correction to action can be computed perturbatively. For the annealed initial condition one also needs to calculate the small correction to the Boltzmann-Gibbs free energy cost. The final result is

$$s_{an}(n_0) = \frac{2}{\sqrt{\pi}} \Big[ n_0 + (\sqrt{2} - 1)n_0^2 + \dots \Big] \quad .$$
$$-\ln P = \sqrt{T} s_{an}(n_0)$$

That is, for d=1 one obtains different  $n_0$ -dependences of the survival probability for the SSEP in the guenched and annealed case

The  $n_0^2$  correction in the annealed case agrees with Santos and Schütz (2001). They solved a different problem: of particle injection into a semi-infinite line. Thei problem, however, is directly related to the target survival problem. Thanks to Gunter Schütz for this comment!

#### Arbitrary densities: numerical solution, quenched initial condition



# 



For the SSEP this becomes

$$s = \frac{2\pi^{d/2} l^{d-1} s_1(n_0)}{\Gamma(d/2)},$$
  
- ln  $\mathscr{P} \cong S \cong \frac{2\pi^{d/2} s_1(n_0) R^{d-1} \sqrt{T}}{\Gamma(d/2)},$  in any dimension

Quenched and annealed are different for any d in this limit!

Extensions to other lattice gases

$$\nabla_r^2 q + \left(\frac{D'}{D} - \frac{\sigma'}{2\sigma}\right) \left(\frac{dq}{dr}\right)^2 = 0$$

Conjecture (cf. with additivity principle of Derrida): if solution obeying  $q(\ell)=0$ and  $q(\infty)=n_0$  exists, it yields  $\mathcal{P}(T)$ 

Example. ZRP with departure rate

$$\alpha(n_i) = \frac{1}{2}n_i^2$$
  

$$\Rightarrow D(q) = q, \quad \sigma(q) = q^2$$
  

$$\Rightarrow \frac{D'}{D} - \frac{\sigma'}{2\sigma} = 0 \Rightarrow \nabla_r^2 q = 0$$

$$q(r) = n_0 \left( 1 - \frac{l^{d-2}}{r^{d-2}} \right), \quad l = \frac{R}{\sqrt{DT}}$$
  

$$v(r) = \frac{d-2}{r} \left[ \left( \frac{r}{l} \right)^{d-2} - 1 \right]^{-1} \qquad -\ln \mathcal{P} \simeq S = \frac{(d-2) \pi^{d/2} R^{d-2} n_0^2 T}{\Gamma(d/2)}, \quad d > 2,$$

Extensions to other lattice gases

$$\nabla_r^2 q + \left(\frac{D'}{D} - \frac{\sigma'}{2\sigma}\right) \left(\frac{dq}{dr}\right)^2 = 0$$

Let 
$$D(q) \sim q^{\alpha}$$
,  $\sigma(q) \sim q^{\beta}$  as  $q \to 0$   
 $\Rightarrow \frac{D'}{D} - \frac{\sigma'}{2\sigma} = \frac{2\alpha - \beta}{2q}$  as  $q \to 0$   
Look for  $q(r - l << l) = \text{const} (r - l)^{\gamma} + ..., \quad \gamma > 0$   
 $q''(r)$  is balanced by thenonlinear term  
 $\Rightarrow \gamma = \frac{2}{2\alpha - \beta + 2}$ , which yields a necessary condition

$$2\alpha - \beta + 2 > 0$$

When this condition is met, the action is bounded

# Summary

MFT makes it possible to evaluate (in some cases, quite easily) the target survival probability for a class of interacting host gases where no previous results existed Possible applications for diffusion-controlled reactions in crowded environments.

One more example of efficiency and versatility of the MFT

One more example of ever-lasting effect of initial condition in 1d

MFT equations are usually hard to solve. More examples should be worked out to gain experience and intuition

Large deviations in non-stationary problems provide a fascinating insight into non-equilibrium stochastic systems

# Thank you