Nonequilibrium Statistical Physics and the ASEP

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LAPTh, ANNECY, March 13, 2014

- 1. Thermodynamics and Equilibrium Statistical Physics
- 2. Out of Equilibrium
- 3. Fluctuations far from equilibrium

EQUILIBRIUM STATISTICAL MECHANICS

Lars Onsager (1903-1976)



'As in other kinds of book-keeping, the trickiest questions that arise in the application of thermodynamics deal with the proper identification and classification of the entries; the arithmetics is straightforward' (Onsager, 1967).

THERMODYNAMICS is the science of ENERGY CONVERSIONS:

- IDENTIFY correctly the various forms of energy involved in a process and WRITE a balance (First Principle).
- Different type of energies are NOT necessarily EQUIVALENT. Converting energy from one form to another involves a *compensation fee* called the ENTROPY (Second Principle, Clausius).

Classical thermodynamics deals only with equilibrium states that do not change with time: time plays no role as a thermodynamic variable.

 $\Delta U = W + Q$

THE ENERGY OF THE UNIVERSE IS CONSTANT.

Which Sphere is hotter?





Whenever dissipation and heat exchanges are involved, time reversibility seems to be lost SOME EVENTS ARE ALLOWED BY NATURE BUT NOT THE OTHERS!



A criterion for separating allowed processes from impossible one is required.

No process is possible whose *sole* result is the transfer of heat from a cooler body to a hotter body (Clausius).

No process is possible whose *sole* result is the absorption of heat from a reservoir and the conversion of this heat into work (Kelvin-Planck).

A NEW physical concept (Clausius): ENTROPY.

$$S_2 - S_1 \ge \int_{1 \to 2} \frac{\partial Q}{T}$$

Clausius Inequality (1851)

THE ENTROPY OF THE UNIVERSE INCREASES.

The Mistress of the World and Her Shadow

- A system wants to minimize its energy.
- A system wants to maximize its entropy.

This competition between energy and entropy is at the heart of most of everyday physical phenomena (such as phase transitions: ice \rightarrow water).

The two principles of thermodynamics can be embodied simultaneously by the **FREE ENERGY** F :

$$F = U - TS$$

The decrease of free energy represents the maximal work that one can extract from a system.

Free energy: A physical example

Consider a gas enclosed in a chamber with a moving piston. We suppose that the gas evolves from state A to B and that it can exchange heat only with it environment at fixed temperature T.



Because of irreversibility, the Work, W_{useful} , that one can extract from this system is at most equal to to the decrease of free energy:

$$\mathcal{W}_{useful} \leq \! F_{ ext{initial}} - F_{ ext{final}} = -\Delta F$$

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MOLECULAR THEORY OF HEAT





J. C. Maxwell

L. Boltzmann

The statistical mechanics of a system at thermal equilibrium is encoded in the Boltzmann-Gibbs canonical law:

$$P_{
m eq}(\mathcal{C}) = rac{{
m e}^{-E(\mathcal{C})/kT}}{Z}$$

the Partition Function Z being related to the Thermodynamic Free Energy F:

F = -kTLog Z

This provides us with a well-defined prescription to analyze systems *at equilibrium*:

(i) Observables are mean values w.r.t. the canonical measure.

(ii) Statistical Mechanics predicts fluctuations (typically Gaussian) that are out of reach of Classical Thermodynamics.

Thermal Equilibrium: a dynamical state

Equilibrium is a dynamical concept. At the molecular scale things constantly change and a system keeps on evolving through various microscopic configurations:

Thermodynamic observables are nothing but average values of fluctuating, probabilistic, microscopic quantities.





Robert Brown (1773-1858)

K. Mallick

Nonequilibrium Statistical Physics and the ASEP

Physics of Brownian Motion

The Brownian Particle is restlessly shaken by water molecules. Its dynamics resembles that of a drunken-walker.

Suppose that the piece of pollen has a speed v. Then it experiences a friction force $-\gamma v$ with $\gamma = 6\pi \eta a$, η being the viscosity of water (Stokes).



The Brownian Particle diffuses around its initial position according to a Gaussian Law: $\langle X^2(t) \rangle = 2Dt$

The Einstein Formula



$$D=rac{RT}{6\pi\eta a\,\mathcal{N}}$$

R: Perfect Gas Constant T: Temperature η : viscosity of water a: diameter of the pollen \mathcal{N} : Avogadro Number

'I weighted the Hydrogen Atom'



$$\label{eq:gamma-10} \begin{split} \eta \sim 10^{-3} & a \sim 10^{-7} \quad R \sim 8.3 \\ D \simeq 1 \, \mu m^2/s \end{split}$$

Mass of the Hydrogen Atom:

 $1.6\,10^{-24}$ g

Jean Perrin (1870-1942)

Fluctuation-Dissipation Relation

Suppose that the Brownian Particle is subject to a small force f_{ext} . Balancing with the viscous force $-(6\pi\eta a)v$, we obtain the limiting speed

$$v_{\infty} = \sigma f_{
m ext}$$
 with $\sigma = rac{1}{6\pi\eta a}$

The response coefficient σ is called a susceptibility.

The Einstein Relation can be rewritten as;

 $\sigma = \frac{D}{kT}$

Susceptibility (Linear Response) \equiv Fluctuations at Equilibrium

(Kubo Formula)

Onsager's Reciprocity Relations (1931)



The Conductivity Tensor L remains symmetric even though the crystal does not display any special symmetry

$$L_{ik} = L_{ki}$$

Crucial for Thermoelectric Effects.

The fact that the dynamics converges towards **thermodynamic equilibrium** and **time-reversal invariance** (detailed-balance) are the key-properties behind Einstein and Onsager's Relations.

Thermodynamic equilibrium is characterized by the fact that the average values of all the **fluxes exchanged** between the system and its environment (matter, charge, energy, spin...) **identically vanish**.

Brownian Fluctuations show that Equilibrium is a dynamical concept.

Microscopic Dynamics: a Probabilistic Approach

A convenient manner to model the dynamics of a complex system:

- Enumerate the Micro-states $\{\mathcal{C}_1, \mathcal{C}_2 \dots\}$
- Transition Rates from C to C' between t and t + dt do not depend on the previous history of the system (short time correlations are neglected: Markovian hypothesis).

$\mathcal{C} \to \mathcal{C}'$ with probability $M(\mathcal{C}', \mathcal{C})dt$

Evolution of $P_t(\mathcal{C})$, probability of being in the micro-state \mathcal{C} at time t:

$$\frac{d}{dt}P_t(\mathcal{C}) = \sum_{\mathcal{C}' \neq \mathcal{C}} M(\mathcal{C}, \mathcal{C}')P_t(\mathcal{C}') - \left\{ \sum_{\mathcal{C}' \neq \mathcal{C}} M(\mathcal{C}', \mathcal{C}) \right\} P_t(\mathcal{C})$$

MASTER EQUATION

The Master Equation is a balance equation in a *network* of configurations.

Connecting to Thermodynamics

Impose that the stationary state is given by the Boltzmann-Gibbs canonical law: $P_{eq}(\mathcal{C}) = \frac{e^{-\mathcal{E}(\mathcal{C})/kT}}{Z}$. This condition implies that

$$\sum_{\mathcal{C}' \neq \mathcal{C}} M(\mathcal{C}, \mathcal{C}') \mathrm{e}^{-E(\mathcal{C}')/kT} = \mathrm{e}^{-E(\mathcal{C})/kT} \left\{ \sum_{\mathcal{C}' \neq \mathcal{C}} M(\mathcal{C}', \mathcal{C}) \right\}$$

This is a set of *global constraints* on the rates: Global Balance.



Time-reversal Invariance and Detailed Balance

The master equation can be written in the following manner:

$$\frac{d}{dt}P_t(\mathcal{C}) = \sum_{\mathcal{C}'} \left\{ M(\mathcal{C}, \mathcal{C}') P_t(\mathcal{C}') - M(\mathcal{C}', \mathcal{C}) P_t(\mathcal{C}) \right\} = \sum_{\mathcal{C}'} J_t(\mathcal{C}, \mathcal{C}')$$

At equilibrium, the microscopic dynamics of the system is time-reversible. This symmetry property implies that all *local* currents vanish (Onsager)

$$M(\mathcal{C},\mathcal{C}')P_{ ext{eq}}(\mathcal{C}')=M(\mathcal{C}',\mathcal{C})P_{ ext{eq}}(\mathcal{C})$$

DETAILED BALANCE

Detailed balance is a **strong property** that goes beyond the laws of classical thermodynamics:

All local currents $J_t(\mathcal{C}, \mathcal{C}')$ between pairs of configurations vanish at thermodynamic equilibrium.

We are now going to show that Detailed Balance is equivalent to Time-Reversal Invariance.

The main idea is to construct a measure on time-trajectories of the system.

• Probability of remaining in C during a time interval τ :

$$\lim_{dt\to 0} \left(1 + M(\mathcal{C},\mathcal{C})dt\right)^{\frac{\tau}{dt}} = \mathrm{e}^{M(\mathcal{C},\mathcal{C})\tau}$$

where $M(\mathcal{C},\mathcal{C}) = -\sum_{\mathcal{C}' \neq \mathcal{C}} M(\mathcal{C}',\mathcal{C})$ represents the exit rate from \mathcal{C} .

• Probability of going from C to C during dt: M(C', C)dt



Probability $Pr\{C(t)\}$ of observing a trajectory C(t):

$$\Pr\{\mathcal{C}(t)\} = e^{\mathcal{M}(\mathcal{C}_n,\mathcal{C}_n)(\mathcal{T}-t_n)} \mathcal{M}(\mathcal{C}_n,\mathcal{C}_{n-1}) dt_n e^{\mathcal{M}(\mathcal{C}_{n-1},\mathcal{C}_{n-1})(t_n-t_{n-1})} \dots \\ \mathcal{M}(\mathcal{C}_2,\mathcal{C}_1) dt_2 e^{\mathcal{M}(\mathcal{C}_1,\mathcal{C}_1)(t_2-t_1)} \mathcal{M}(\mathcal{C}_1,\mathcal{C}_0) dt_1 e^{\mathcal{M}(\mathcal{C}_0,\mathcal{C}_0)t_1} \mathcal{P}_{eq}(\mathcal{C}_0)$$

Weight of the reversed Trajectory

TIME-REVERSED TRAJECTORY C(T-t)



$$\Pr\{\hat{\mathcal{C}}(t)\} = e^{\mathcal{M}(\mathcal{C}_0,\mathcal{C}_0)t_1} \mathcal{M}(\mathcal{C}_0,\mathcal{C}_1)dt_1 e^{\mathcal{M}(\mathcal{C}_1,\mathcal{C}_1)(t_2-t_1)} \cdots e^{\mathcal{M}(\mathcal{C}_{n-1},\mathcal{C}_{n-1})(t_n-t_{n-1})} \mathcal{M}(\mathcal{C}_{n-1},\mathcal{C}_n)dt_n e^{\mathcal{M}(\mathcal{C}_n,\mathcal{C}_n)(\mathcal{T}-t_n)} \mathcal{P}_{eq}(\mathcal{C}_n)$$

Detailed Balance and Time Reversal

Ratio of the forward-backward Probabilities:

$$\frac{\Pr\{\mathcal{C}(t)\}}{\Pr\{\hat{\mathcal{C}}(t)\}} = \frac{M(\mathcal{C}_n, \mathcal{C}_{n-1})M(\mathcal{C}_{n-1}, \mathcal{C}_{n-2})\dots M(\mathcal{C}_1, \mathcal{C}_0) P_{eq}(\mathcal{C}_0)}{M(\mathcal{C}_0, \mathcal{C}_1) M(\mathcal{C}_1, \mathcal{C}_2) \dots M(\mathcal{C}_{n-1}, \mathcal{C}_n) P_{eq}(\mathcal{C}_n)}$$

Use recursively the detailed balance condition:

$$M(\mathcal{C}_1,\mathcal{C}_0)P_{\rm eq}(\mathcal{C}_0)=P_{\rm eq}(\mathcal{C}_1)M(\mathcal{C}_0,\mathcal{C}_1)$$

Detailed Balance and Time Reversal

Ratio of the forward-backward Probabilities:

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Use recursively the detailed balance condition:

$$M(\mathcal{C}_1, \mathcal{C}_0)P_{\mathrm{eq}}(\mathcal{C}_0) = P_{\mathrm{eq}}(\mathcal{C}_1)M(\mathcal{C}_0, \mathcal{C}_1)$$

$$\frac{\Pr\{\mathcal{C}(t)\}}{\Pr\{\hat{\mathcal{C}}(t)\}} = 1$$

Detailed balance implies that the dynamics is time reversible. The converse property is true.

A system is in equilibrium if and only if its dynamics satisfies detailed balance.

OUT OF EQUILIBRIUM

In Nature, many systems are far from thermodynamic equilibrium and keep on exchanging matter, energy, information with their surroundings. There is no general conceptual framework to study such systems.

Systems far from equilibrium

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



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



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

In the steady state, a non-vanishing macroscopic current J flows. What can we say about the properties of this current from the point of view of Statistical Physics?

Rare Events and Large Deviations

Let $\epsilon_1, \ldots, \epsilon_N$ be N independent binary variables, $\epsilon_k = \pm 1$, with probability p (resp. q = 1 - p). Their sum is denoted by $S_N = \sum_{1}^{N} \epsilon_k$.

- The Law of Large Numbers implies that $S_N/N \rightarrow p-q$ a.s.
- The Central Limit Theorem implies that $[S_N N(p-q)]/\sqrt{N}$ converges towards a Gaussian Law.

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- The Law of Large Numbers implies that $S_N/N \rightarrow p-q$ a.s.
- The Central Limit Theorem implies that $[S_N N(p-q)]/\sqrt{N}$ converges towards a Gaussian Law.

One can show that for -1 < r < 1, in the large N limit,

$$\operatorname{Proba}\left(\frac{S_N}{N}=r\right)\sim \mathrm{e}^{-N\,\Phi(r)}$$

where the positive function $\Phi(r)$ vanishes for r = (p - q).

The function $\Phi(r)$ is a Large Deviation Function: it encodes the probability of rare events (*use Stirling's Formula*)

$$\Phi(r) = \frac{1+r}{2} \ln\left(\frac{1+r}{2p}\right) + \frac{1-r}{2} \ln\left(\frac{1-r}{2q}\right)$$

Local density fluctuations in a gas at thermal equilibrium



Mean Density $ho_0 = \frac{N}{V}$ In a volume v s. t. $1 \ll v \ll V$ $\langle \frac{n}{v} \rangle = \rho_0$

The local density varies around ρ_0 . Typical fluctuations scale as $\sqrt{v/V}$.

The probability of observing large fluctuations is given by

Proba
$$\left(\frac{n}{v} = \rho\right) \sim e^{-v \Phi(\rho)}$$
 with $\Phi(\rho_0) = 0$

The Large Deviation Function for density fluctuations is given by

$$\Phi(\rho) = \beta \left(f(\rho, T) - f(\rho_0, T) - (\rho - \rho_0) \frac{\partial f}{\partial \rho_0} \right)$$

We can ask the more general question of the large deviation of a density profile: cover the large box with K = V/v small boxes and calculate the probability of having a density ρ_1 in the first box, ρ_2 in the second box ...

Proba
$$(\rho_1, \rho_2, \dots, \rho_K) \simeq e^{-V \mathcal{F}(\rho_1, \rho_2, \dots, \rho_K)}$$

In the limit $V
ightarrow \infty$,, we obtain

$$\mathcal{F}(\rho_1,\rho_2,\ldots\rho_K)=\frac{\beta}{K}\sum_{k=1}^K (f(\rho_i,T)-f(\rho_0,T))$$

where ρ_0 is the average density.

If we let the number K of boxes go to infinity, then the question we are asking is the probability of observing a given density profile $\rho(x)$ in the big volume V. The large deviation function \mathcal{F} becomes a functional of the density profile:

$$\mathcal{F}[\rho(\mathbf{x})] = \beta \int d\mathbf{x} \left(f(\rho(\mathbf{x}), T) - f(\rho_0, T) \right)$$

 $f = -\log Z(\rho, T)$ being, as above, the *free energy per unit volume*.

The Free Energy of Thermodynamics can be viewed as a Large Deviation Function

Conversely, large deviation functions *may* play the role of potentials in non-equilibrium statistical mechanics. Indeed, they can be defined for very general processes, even far from equilibrium.

Large Deviations of the Total Current



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

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

The fluctuations of Y_t obey a Large Deviation Principle:

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

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

Note that $\Phi(j)$ is positive, vanishes at j = J and is convex (in general).

Large Deviations of a Non-Equilibrium profile



What is the probability of observing an atypical density profile in the steady state? What does the functional $\mathcal{F}(\{\rho(x)\})$ look like for such a non-equilibrium system? Recall that in the equilibrium case, this functional is the free energy.

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

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

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

A Symmetry of the Large Deviation Function

Large deviation functions obey remarkable identities that remain valid far from equilibrium: *The Fluctuation Theorem of Gallavotti and Cohen.*

Large deviation functions obey a symmetry that remains valid far from equilibrium:

$$\Phi(r) - \Phi(-r) = Ar$$

The coefficient A is a constant, e.g. $A = \ln q/p$ in the example of the walker above.

This Fluctuation Theorem of Gallavotti and Cohen is deep and general: it reflects covariance properties under time-reversal.

In the vicinity of equilibrium the Fluctuation Theorem yields the fluctuation-dissipation relation (Einstein), Onsager's relations and linear response theory (Kubo).

Generalized Detailed Balance

Is there a 'natural way' of breaking detailed balance? What happens to detailed balance for a system connected to different reservoirs?

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Is there a 'natural way' of breaking detailed balance? What happens to detailed balance for a system connected to different reservoirs?

For a system at contact with reservoirs at different temperatures, detailed balance is generalized as follows:

$$M_{\Delta E_1,\Delta E_2}(\mathcal{C}\to\mathcal{C}')=M_{-\Delta E_1,-\Delta E_2}(\mathcal{C}'\to\mathcal{C})\,\mathrm{e}^{-\frac{\Delta E_1}{kT_1}-\frac{\Delta E_2}{kT_2}}$$

with $\Delta E_i = E_i(\mathcal{C}') - E_i(\mathcal{C})$.

This relation is 'derived' by applying detailed balance to the global system $S + R_1 + R_2$ and tracing out the degrees of freedom of the reservoirs.

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More generally, suppose that during an elementary transition $\mathcal{C} \to \mathcal{C}'$, an time-odd quantity y (charge, energy, entropy...) is transfered, and let γ_0 be a constant,

$$M_{+y}(\mathcal{C}
ightarrow \mathcal{C}') = M_{-y}(\mathcal{C}'
ightarrow \mathcal{C}) \, \mathrm{e}^{\gamma_0 y}$$

GENERALIZED DETAILED BALANCE

Generalized Detailed Balance versus Time Reversal



$$\frac{\Pr\{\mathcal{C}(t)\}}{\Pr\{\hat{\mathcal{C}}(t)\}} = e^{\gamma_0 \, \boldsymbol{Y}\{\mathcal{C}(t)\}} \quad \frac{P_{\mathrm{stat}}(\mathcal{C}_0)}{P_{\mathrm{stat}}(\mathcal{C}_n)}$$

where $Y\{C(t)\} = y_1 + y_2 + \ldots y_n$ is total charge transfered when the system follows the trajectory C(t) between 0 and t. By time-reversal, we have

$$Y\{\hat{\mathcal{C}}(t)\} = -Y\{\mathcal{C}(t)\}$$

The Gallavotti-Cohen Theorem

By summing over all trajectories, one shows that Y_t has the following statistical property:

$$\left\langle \mathrm{e}^{(\gamma-\gamma_0)Y_t} \right\rangle \simeq \left\langle \mathrm{e}^{-\gamma Y_t} \right\rangle \ \ \, \mathrm{when} \ t
ightarrow \infty$$

A Laplace-Legendre transform yields the Gallavotti-Cohen Fluctuation Theorem:

$$\Phi(j) = \Phi(-j) - \gamma_0 j$$

From the definition of the Large Deviation Function this implies

$$\frac{\Pr\left(\frac{Y_t}{t}=j\right)}{\Pr\left(\frac{Y_t}{t}=-j\right)} \simeq e^{\gamma_0 j t}$$

This relation is true **far from equilibrium**. It has been proved rigorously in various contexts (chaotic systems, Markov/Langevin dynamics...).

Another Surprise: The Jarzynski Identity

Remember the maximal work inequality:

$$\langle W \rangle \leq F_A - F_B = -\Delta F$$

We put brackets to emphasize that we consider the average work: Statistical Physics has taught us that physical observables fluctuate.

Another Surprise: The Jarzynski Identity

Remember the maximal work inequality:

$$\langle W \rangle \leq F_A - F_B = -\Delta F$$

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It was found very recently that there exists a remarkable equality that *underlies* this classical inequality.

$$\left\langle \mathrm{e}^{\frac{W}{kT}} \right\rangle = \mathrm{e}^{-\frac{\Delta F}{kT}}$$

The Jarzynski Identity



$$\left\langle \mathrm{e}^{\frac{W}{kT}} \right\rangle = \mathrm{e}^{-\frac{\Delta F}{kT}}$$

Jarzynski's Work Theorem (1997)

1. Jarzynski's identity mathematically implies the good old maximal work inequality.

 $2. \ {\rm But}, \ {\rm in \ order} \ {\rm to \ have \ an \ EQUALITY}, \ {\rm there \ must \ exist \ some \ occurrences \ in \ which}$

 $W > -\Delta F$

There must be instances in which the classical inequality which results from the Entropy Principle is 'violated'.

3. Jarzynski's identity can be used to calculate chemical free energies of biopolymer configurations: it has experimental applications in biophysics or at the nanoscale.

4. The relation of Crooks: a refinement Jarzynski's identity that allows us to quantify precisely the 'transient violations of the second principle'.

$$\frac{\mathrm{P}^{\mathrm{F}}(W)}{\mathrm{P}^{\mathrm{R}}(-W)} = \mathrm{e}^{\frac{W-\Delta F}{kT}} \qquad \text{(Crooks,1999)}$$

Graphical representation of the Crooks' relation

Crooks' Relation allows us to quantify precisely the 'transient violations' of the Second Principle and can be checked experimentally on single RNA folding/unfolding experiments (Bustamante et al.)



FLUCTUATIONS

FAR FROM EQUILIBRIUM

A Paradigm: The Exclusion Process

The fundamental non-equilibrium system



A Paradigm: The Exclusion Process

The fundamental non-equilibrium system



A paradigm: The asymmetric exclusion model with open boundaries (ASEP) $% \left(ASEP\right) =0$



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

The Periodic Ring



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

WHAT IS THE STATISTICS of Y_t ?

The moment-generating function defined as

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

is the Legendre Transform of the Large Deviation Function. On a ring, $E(\mu)$ can be calculated by Bethe Ansatz (XXZ model).

General Solution on a ring (S. Prolhac, K.M.)

 $E(\mu)$ is found in a parametric form:

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

 C_k and D_k are combinatorial factors enumerating some tree structures. They are given by complex integrals along a small contour encircling 0:

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

The auxiliary function $W_B(z)$ defined as

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

contains all information about the current statistics.

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

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

where

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

The operator X is a integral operator

$$X[W_B](z_1) = \oint_{\mathcal{C}} \frac{dz_2}{i2\pi z_2} W_B(z_2) K(z_1, z_2)$$

with the kernel

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

Full large deviation function (weak asymmetry)



Non-analytical points of the large deviation function correspond to phase transitions in the system.

The Open ASEP case (A. Lazarescu, KM)



The observable Y_t now counts the total number of particles exchanged between the system and the left reservoir between times 0 and t: this is the total (integrated) current.

The cumulant-generating function $E(\mu)$ defined as $\langle e^{\mu Y_t} \rangle \simeq e^{E(\mu)t}$, when $t \to \infty$, was not obtained by Bethe Ansatz for the open system.

We developed an algebraic method based on the Matrix Product Representation of the eigenstates (cf Derrida et al.).

Structure of the solution I

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

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

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

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

There exists an auxiliary function

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

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

Structure of the solution II

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

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

• The operator X is a integral operator

$$X[W_B](z_1) = \oint_{\mathcal{C}} \frac{dz_2}{i2\pi z_2} W_B(z_2) K\left(\frac{z_1}{z_2}\right)$$

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

• The function F(z) is given by

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

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

Current Large Deviation Function:

In the limit of large size systems, the following exact expression is found for the Large Deviation Function of the current:

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

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



SKEWNESS

A special TASEP case

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

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

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

First cumulants of the current

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

A Macroscopic Point of View



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 typical evolution of the system is given by the hydrodynamic behaviour:

$$\partial
ho = rac{1}{2}
abla^2
ho -
u
abla \sigma(
ho) \quad ext{with} \quad \sigma(
ho) =
ho(1-
ho)$$

(Lebowitz, Spohn, Varadhan)

Large Deviations at the Hydrodynamic Level

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

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

A general principle has been found, the macroscopic fluctuation theory (Jona-Lasinio et al.), to express this large deviation functional $\mathcal{I}(j, \rho)$ as an optimal path problem:

$$\mathcal{I}(j,\rho) = \min_{\rho,j} \bigg\{ \int_0^T dt \int_0^1 dx \frac{(j-\nu\sigma(\rho)+D(\rho)\nabla\rho)^2}{2\sigma(\rho)} \bigg\}$$

Knowing $\mathcal{I}(j,\rho)$, one could derive the large deviations of the current and of the density profile. For instance, $\Phi(j) = \min_{\rho} \{\mathcal{I}(j,\rho)\}$

However, at present, the available results for this variational theory are precisely the ones given by exact solutions of the ASEP.

Equations of Macroscopic Fluctuation Theory

Mathematically, one has to solve the corresponding Euler-Lagrange equations. After some transformations, one obtains a set of coupled PDE's (here, we take $\nu = 0$):

$$\partial_t q = \partial_x [D(q)\partial_x q] - \partial_x [\sigma(q)\partial_x p]$$

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

where q(x, t) is the density-field and p(x, t) is a conjugate field. The physical content is encoded in the 'transport coefficients' D(q)(=1)and $\sigma(q)(=2q(1-q))$ that contain the information of the microscopic dynamics relevant at the macroscopic scale. Do note that these equations have a Hamiltonian structure.

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- A general framework but these non-linear MFT equations are very difficult to solve in general. By using them one can in principle calculate large deviation functions directly at the macroscopic level.
- The analysis of this new set of 'hydrodynamic equations' has just begun!

Conclusion

Systems out of equilibrium are ubiquitous in nature. They break time reversal invariance. Often, they are characterized by non-vanishing stationary currents (fluxes).

Large deviation functions (LDF) appear as the right generalization of the thermodynamic potentials: convex, optimized at the stationary state, and non-analytic features can be interpreted as phase transitions. Besides, they satisfy remarkable relations (Gallavotti-Cohen, Jarzynski-Crooks).

The LDF's are very likely to play a key-role in constructing a general theory of non-equilibrium statistical mechanics. Currently, the prominent candidate for such a theory is The Macroscopic Fluctuation Theory of G. Jona-Lasinio et al.

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

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