Nested Matrix Ansatz for the Exclusion Process

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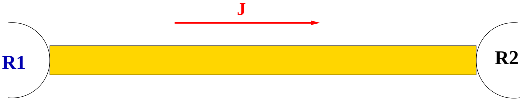
Introduction

A stationary driven system in contact with reservoirs is out of equilibrium:



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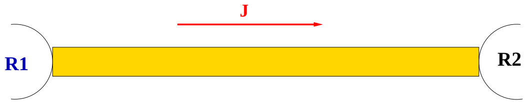
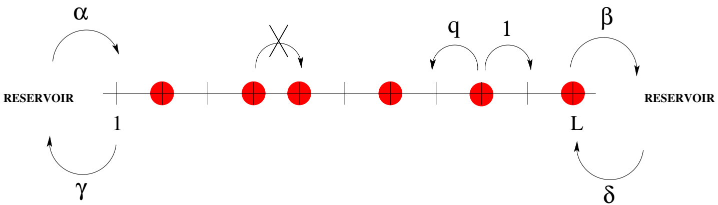
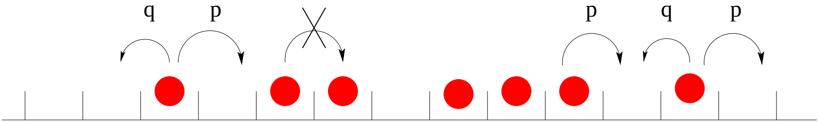


The asymmetric exclusion model (ASEP)



Thousands of articles devoted to this model in the last 20 years: A paradigm for non-equilibrium statistical physics.

ASEP



Asymmetric Exclusion Process. A paradigm 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

An Elementary Model for Protein Synthesis

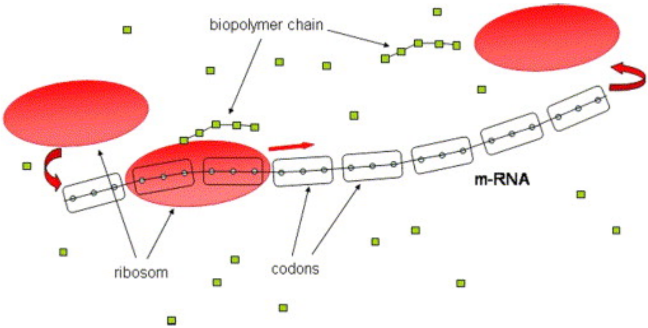


Figure: courtesy of Andreas Schadscheider

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

An ubiquitous minimal model

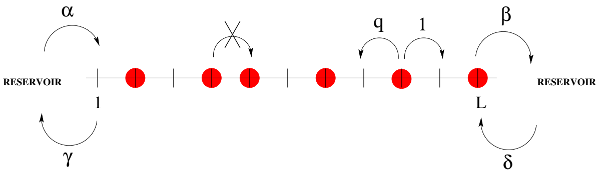
ORIGINS

- Interacting Brownian Processes (Spitzer, Harris, Liggett).
- Driven diffusive systems (Katz, Lebowitz and Spohn).
- Transport of Macromolecules through thin vessels.
  Motion of RNA templates.
- Hopping conductivity in solid electrolytes.
- Directed Polymers in random media. Reptation models.
- Interface dynamics. KPZ equation

APPLICATIONS

- Traffic flow.
- Sequence matching.
- Brownian motors.

Matrix Ansatz for ASEP (DEHP, 1993)



The key to the solution of the ASEP is the Matrix Product Representation of the stationary probabilities. The weight of a configuration $\mathcal{C}$ is given by:

$$P(\mathcal{C}) = \frac{1}{Z_L} \langle W| \prod_{i=1}^{L} (\tau_i D + (1 - \tau_i) E) |V\rangle$$

where $\tau_i = 1$ (or 0) if the site i is occupied (or empty) and the normalization constant is $Z_L = \langle W| (D + E)^L |V\rangle$

The weights of the system satisfy exact recursion relations between size L and size $L - 1$. This combinatorial structure will be encoded in the algebra generated by D, E, $\langle W|$ and $|V\rangle$.

Quadratic Algebra

The Matrix Ansatz will represent the steady state weights if the operators D and E, the vectors $\langle W|$ and $|V\rangle$ satisfy

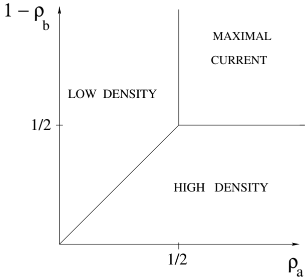
$$\begin{aligned} D\,E - qE\,D &= (1-q)(D + E) \\ (\beta\,D - \delta\,E)\,|V\rangle &= |V\rangle \\ \langle W|(\alpha\,E - \gamma\,D) &= \langle W| \end{aligned}$$

(B. Derrida, M. R. Evans, V. Hakim and V. Pasquier, 1993)

The Matrix Ansatz allows one to derive the Phase Diagram in the infinite size limit and to calculate many Stationary State Properties such as currents, correlations, fluctuations, finite size corrections, large deviations of the density profile... (see the review of R. Blythe and M. R. Evans).

Note that the recursions can also be encoded through generating functions (Derrida, Domany and Mukamel, 1992: $q = 0, \alpha = \beta = 1$; Schütz and Domany, 1993: $q = 0$ arbitrary α, β).

The Phase Diagram



$\rho_a = \frac{1}{a_+ + 1}$: effective left reservoir density.

$\rho_b = \frac{b_+}{b_+ + 1}$: effective right reservoir density.

$$a_\pm = \frac{(1 - q - \alpha + \gamma) \pm \sqrt{(1 - q - \alpha + \gamma)^2 + 4\alpha\gamma}}{2\alpha}$$

$$b_\pm = \frac{(1 - q - \beta + \delta) \pm \sqrt{(1 - q - \beta + \delta)^2 + 4\beta\delta}}{2\beta}$$

Representations of the quadratic algebra

$D = 1 + d$ where d is a q-destruction operator.

$E = 1 + e$ where e is a q-creation operator.

$$d = \begin{pmatrix} 0 & \sqrt{1-q} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{1-q^2} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{1-q^3} & \dots \\ & & & \ddots & \ddots \end{pmatrix} \quad \text{and} \quad e = d^\dagger$$

Nested Matrix Ansatz

1. Multispecies Exclusion Processes

2. Large deviations of the current in the Open ASEP

1. Multispecies Models

The dynamical rules

We consider the N-TASEP model on a periodic RING. There are N classes of particles and holes.
During an infinitesimal time step dt, the following processes take place on each bond with probability dt:

$$I\ 0 \to 0\ I \qquad \text{for} \quad I \neq 0$$
$$I\ J \to J\ I \qquad \text{for} \quad 1 \leq I < J \leq N$$

Hierarchical priority rules: First-class particles have highest priority and overtake all the others; Second-class particles overtake all the other ones except first class particles etc... Note that particles can always overtake holes (= 0-th class particles).

There are P_I particles of class I. Total number of configurations:

$$\Omega = \frac{L!}{P_0!P_1!P_2!\dots P_N!}$$

What is the Stationary Measure ?

The Two Species case

If there is single species the stationary measure is uniform.

Matrix Product for the Stationary Measure *(Derrida, Janowski, Lebowitz and Speer, 1993)*:

A Configuration is represented by a string e.g. 01220211. The corresponding Stationary Weight is given by

$$p(01220211) = \frac{1}{Z} \mathrm{Tr}(EDAAEADD)$$

where E, D and A, operators belong to a *quadratic algebra*

$$\begin{aligned} DE &= D + E \\ DA &= A \\ AE &= A \end{aligned}$$

This Matrix Ansatz leads to steady state properties. This invariant measure *is not a Boltzmann-Gibbs measure* (E. Speer).

Infinite dimensional Representations

$D = 1 + \delta$ where $\delta =$ is the right-shift

$E = 1 + \epsilon$ where ϵ is the left-shift.

$A = |1\rangle\langle 1| = [\delta, \epsilon]$ (projector on the first coordinate).

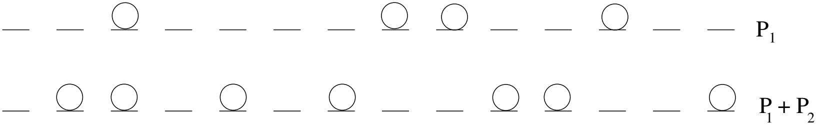
$$D = \begin{pmatrix} 1 & 1 & 0 & 0 & \dots \\ 0 & 1 & 1 & 0 & \\ 0 & 0 & 1 & 1 & \ddots \\ & & & \ddots & \ddots \end{pmatrix}, \; E = D^{\dagger}, \; A = \begin{pmatrix} 1 & 0 & 0 & \dots \\ 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & \dots \\ . & . & . & . \end{pmatrix}$$

This algebra is the same as the one for the open TASEP (with a single species of particles).

The $N \geq 3$ case remained unsolved for more than a decade.

Geometric Construction of the 2-TASEP stationary measure (P. Ferrari, J. Martin)

A procedure to construct a configuration of the 2-TASEP with P_1 First Class Particles and P_2 Second Class Particles starting from two independent configurations of the 1 species TASEP.



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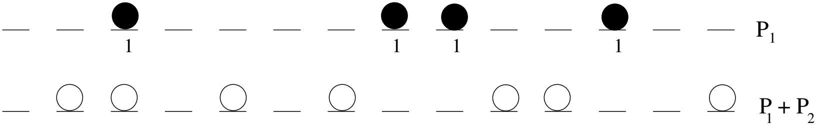

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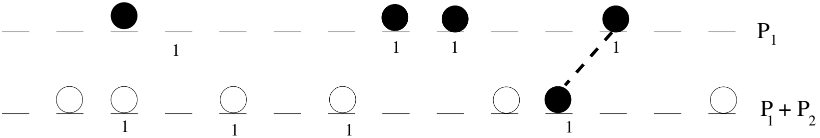

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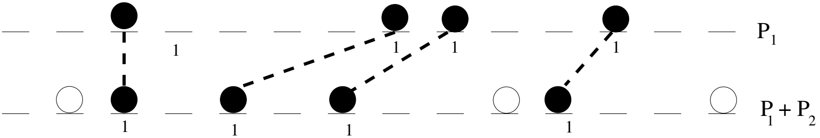

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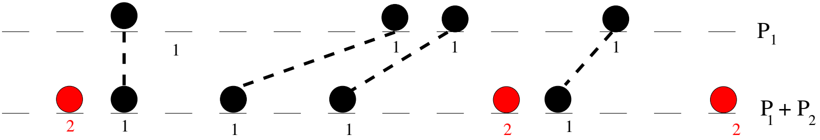
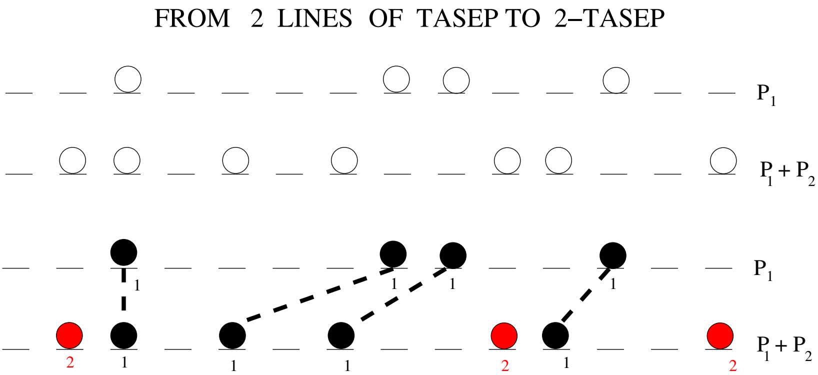


Summary of the construction



This construction is NOT one-to one: different configurations on the 1st line can produce the same configuration on the second line.

The weight of a 2-TASEP configuration is proportional to the total number of ways you can generate it by this construction.

Relation to the Matrix Ansatz

Characterization of the stationary weights:

- A 1 (on the 1st line) can not be located above a 2 (on the 2nd line).
- **Factorisation Property:** All the 1's (on the 2nd line) situated between two 2's MUST be linked to 1's (on the 1st line) that are located between the positions of the two 2's *(No Crossing Condition)*.
- **'Pushing' Procedure:** The *'ancestors'* of a string of the type 210102 are the strings obtained by pushing the 1's to the right i.e., 210102, 210012, 201102, 201012, 200112.

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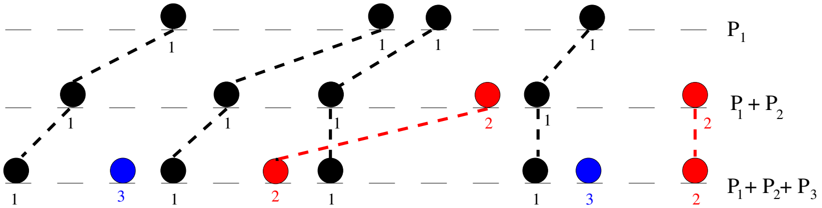
This Geometric Construction is encoded by the Matrix Ansatz:

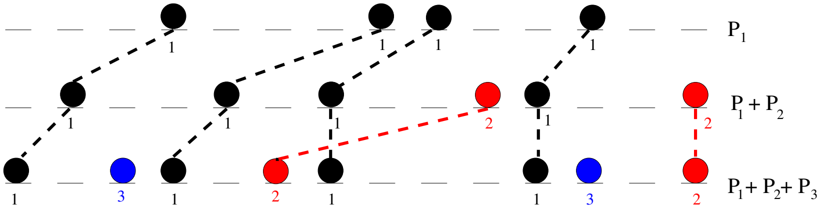
- **Factorisation Property:** A is a **PROJECTOR.**
- **Pushing Procedure:** D and E are **SHIFT OPERATORS** (right-shift and left-shift, respectively).

From 3 lines of TASEP to the 3-TASEP



The weight of a 3-TASEP configuration is proportional to the total number of ways you can generate it by this construction.

From 3 lines of TASEP to the 3-TASEP



The weight of a 3-TASEP configuration is proportional to the total number of ways you can generate it by this construction.

- FIND an ALGORITHM for constructing all ancestors of a given N-TASEP configuration.
- ENCODE this algorithm into an ALGEBRA (Matrix Product Representation).
- CALCULATE the stationary weights $\rightarrow$ TRACES over this algebra.

Nested Matrix Ansatz for the 3-TASEP

Tensor Products of Quadratic Algebras:
Hierarchical construction of representations of ‘nested algebras’ using the D, A and E matrices and the shift operators $\delta = D - 1$ and $\epsilon = E - 1$.

For the 3-species TASEP case:

$$\begin{aligned}
\hat{\mathbf{P}}_0 &= \mathbf{1} \otimes \mathbf{1} \otimes E + \mathbf{1} \otimes \epsilon \otimes A + \epsilon \otimes \mathbf{1} \otimes D\,. \\
\hat{\mathbf{P}}_1 &= \mathbf{1} \otimes \mathbf{1} \otimes D + \delta \otimes \epsilon \otimes A + \delta \otimes \mathbf{1} \otimes E \\
\hat{\mathbf{P}}_2 &= A \otimes \mathbf{1} \otimes A + A \otimes \delta \otimes E \\
\hat{\mathbf{P}}_3 &= A \otimes A \otimes E
\end{aligned}$$

Matrix Ansatz for the N-Species TASEP: M.R. Evans, P. Ferrari, K.M., *J.Stat.Phys, 2009.*

The algebraic proof bypasses the combinatorial pictures: Generalization for the N-Species ASEP, for which no geometric construction exists.

Generalization to the N-ASEP

If backward jumps are allowed (rate $q \neq 0$)

$$\begin{aligned} DE - qED &= (1-q)(D+E) \\ DA - qAD &= (1-q)A \\ AE - qEA &= (1-q)A \end{aligned}$$

$\rightarrow$ Replace the previous shift-operators by **deformed shift-operators:**

$$\boxed{\delta\epsilon = 1 \rightarrow \delta\epsilon - q\epsilon\delta = 1}$$

Recursive Matrix Ansatz:

$$X_J^{(N)} = \sum_{M=0}^{N-1} a_{JM}^{(N)} \otimes X_M^{(N-1)} \quad \text{for } 0 \leq J \leq N \text{ with } X_0^{(1)} = X_1^{(1)} = 1$$

Matrix Ansatz for the N-Species TASEP: M.R. Evans, K.M., S. Prolhac *J.Phys.A, 2009.*

Transfer Matrix

The operators $a_{JM}^{(N)}$ define a Transfer Matrix between the (N-1)-species ASEP and the N-ASEP:

$$|\Omega_N\rangle = T_{N-1\to N}\ |\Omega_{N-1}\rangle$$

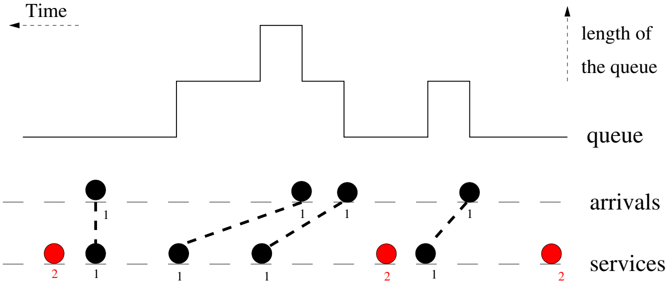
$T_{N-1\to N}$ lifts the (N-1)-ASEP into the N-ASEP, allowing to construct whole sectors of the spectrum ('inverts' the identification operator).

The operators $a_{JM}^{(N)}$ generate a quadratic algebra, that can be expressed in a Yang-Baxter form, using the local update Markov matrix:

$$M_{\mathrm{Loc}}^{(N)}(\mathbf{a}\otimes\mathbf{a}) - (\mathbf{a}\otimes\mathbf{a})M_{\mathrm{Loc}}^{(N-1)} = \mathbf{a}\otimes\widehat{\mathbf{a}} - \widehat{\mathbf{a}}\otimes\mathbf{a}$$

A. Ayyer, KM: *J. Phys. A, 2010.*
C. Arita, A. Ayyer, KM, S. Prolhac: *J. Phys. A, 2011; 2012.*
C. Arita, KM: *J. Phys. A 2013.*

Queueing Theory Interpretation



The matrices D and E act on $|n\rangle$ the length of the queue:

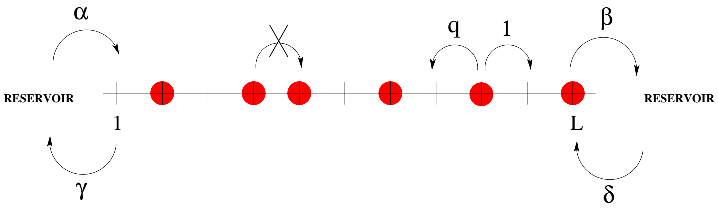
Service Time: $D|n\rangle = |n\rangle + |n-1\rangle$

Non-Service Time: $E|n\rangle = |n\rangle + |n+1\rangle$

This queueing process can be generalized to the N-TASEP. *The matrices act on the queue at each time step:* they are constructed by inspection of the different possible arrivals at a given time.

2. Current Fluctuations in the open ASEP

Total Current in the ASEP with Open Boundaries



The observable Y_t counts the total number of particles exchanged between the system and the left reservoir between times 0 and t. Hence, $Y_{t+dt} = Y_t + y$ with

- $y = +1$ if a particle enters at site 1 (at rate α),
- $y = -1$ if a particle exits from 1 (at rate γ)
- $y = 0$ if no particle exchange with the left reservoir has occurred during dt.

These three mutually exclusive types of transitions lead to a three parts decomposition of the Markov Matrix: $M = M_+ + M_- + M_0$.

Current Statistics as an eigenvalue

The statistics of Y_T can be probed by the cumulant-generating function $E(\mu)$ when $t \to \infty$:

$$\langle e^{\mu Y_t} \rangle \simeq e^{E(\mu) t}$$

$E(\mu)$ is shown to be the dominant eigenvalue of the deformed matrix

$$\boxed{M(\mu) = M_0 + e^{\mu} M_+ + e^{-\mu} M_-}$$

Expanding, one has: $E(\mu) = 0 + J\mu + \Delta \frac{\mu^2}{2} + C_3 \frac{\mu^3}{3!} \dots$

- Average current J: obtained by the DEHP Matrix Ansatz (1993).
- Variance Δ: calculated by a tensor product of three DEHP algebras (B. Derrida, M. R. Evans, KM, 1995).

For the k-th term in the expansion of $E(\gamma)$, we built a Matrix Ansatz at order k, by making $(2k-1)$ Tensor Products of Quadratic Algebras.

Mimics the construction used for the multispecies exclusion process.

Generalized Matrix Ansatz

We have proved that the dominant eigenvector of the deformed matrix $M(\mu)$ is given by the following matrix product representation:

$$F_\mu(\mathcal{C}) = \frac{1}{Z_L^{(k)}} \langle W_k | \prod_{i=1}^{L} (\tau_i D_k + (1-\tau_i) E_k) | V_k \rangle + \mathcal{O}\left(\mu^{k+1}\right)$$

The matrices D_k and E_k are the same as above

$$\begin{aligned} D_{k+1} &= (1 \otimes 1 + d \otimes e) \otimes D_k + (1 \otimes d + d \otimes 1) \otimes E_k \\ E_{k+1} &= (1 \otimes 1 + e \otimes d) \otimes E_k + (e \otimes 1 + 1 \otimes e) \otimes D_k \end{aligned}$$

The boundary vectors $\langle W_k|$ and $|V_k\rangle$ are constructed recursively:

$$|V_k\rangle = |\beta\rangle |\tilde{V}\rangle |V_{k-1}\rangle \quad \text{and} \quad \langle W_k| = \langle W^\mu | \langle \tilde{W}^\mu | \langle W_{k-1}|$$

$$[\beta(1-d) - \delta(1-e)] \, |\tilde{V}\rangle = 0$$

$$\langle W^\mu | [\alpha(1 + \mathrm{e}^{\mu}\, e) - \gamma(1 + \mathrm{e}^{-\mu}\, d)] = (1-q) \langle W^\mu |$$

$$\langle \tilde{W}^\mu | [\alpha(1 - \mathrm{e}^{\mu}\, e) - \gamma(1 - \mathrm{e}^{-\mu}\, d)] = 0$$

Asymptotic behaviour in the Phase Diagram

- Maximal Current Phase:

$$\mu = -\frac{L^{-1/2}}{2\sqrt{\pi}} \sum_{k=1}^{\infty} \frac{(2k)!}{k!k^{(k+3/2)}} B^k$$

$$\mathcal{E} - \frac{1-q}{4}\mu = -\frac{(1-q)L^{-3/2}}{16\sqrt{\pi}} \sum_{k=1}^{\infty} \frac{(2k)!}{k!k^{(k+5/2)}} B^k$$

- Low Density (and High Density) Phases:
  Dominant singularity at a_+: $\phi_k(z) \sim F^k(z)$. By Lagrange Inversion:

$$E(\mu) = (1-q)(1-\rho_a)\frac{\mathrm{e}^{\mu}-1}{\mathrm{e}^{\mu}+(1-\rho_a)/\rho_a}$$

(cf de Gier and Essler, 2011).

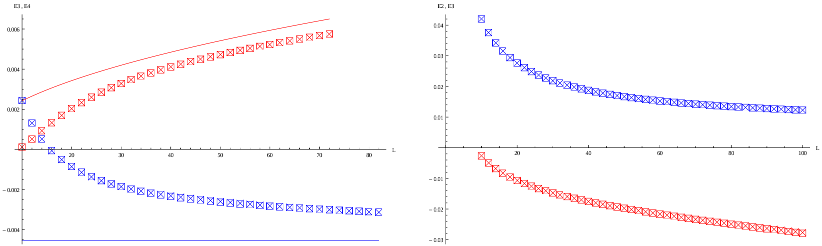
Current Large Deviation Function:

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

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

Matches the predictions of Macroscopic Fluctuation Theory in the Weak Asymmetry Limit, as observed by T. Bodineau and B. Derrida.

Numerical results (DMRG)



Left: **Max. Current** ($q = 0.5$, $a_+ = b_+ = 0.65$, $a_- = b_- = 0.6$), Third and Fourth cumulant.

Right: **High Density** ($q = 0.5$, $a_+ = 0.28$, $b_+ = 1.15$, $a_- = -0.48$ and $b_- = -0.27$), Second and Third cumulant.

A. Lazarescu and K. Mallick, J. Phys. A 44, 315001 2011).
M. Gorissen, A. Lazarescu, K.M., C. Vanderzande, PRL **109** 170601 (2012).

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: $E_3 \to \frac{2187-1280\sqrt{3}}{10368} \pi \sim -0.0090978...$

General 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:

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

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.

General 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

$$X[W_B](z_1) = \oint_{\mathcal{C}} \frac{dz_2}{\imath 2\pi\, z_2} W_B(z_2) K\left(\frac{z_1}{z_2}\right)$$

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

- The complex contour $\mathcal{C}$ encircles 0, q^ka_+, q^ka_-, q^kb_+, q^kb_- for $k \geq 0$.

Conclusion

Systems out of equilibrium are ubiquitous in nature. They break time reversal invariance. Often, they are characterized by non-vanishing stationary currents. In general, the steady-state measures are not given by the Boltzmann-Gibbs Law.

Exact solutions have been obtained for one-dimensional processes, thanks to various techniques: Bethe Ansatz, Determinantal Processes and Matrix Product Representations.

Tensor Products of Matrix Product States have allowed us to study multispecies generalizations of the exclusion process as well as current fluctuations in the open ASEP.

Many partially solved/open questions: multispecies processes with open boundaries? Systematic construction of the Matrix Ansatz and relation to integrability (cf E. Ragoucy's talk). Applications to other single-file models and queueing processes.