Computer algebra for the study of two-dimensional exclusion processes

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Outline

1. Two-dimensional disordered ASEP
2. Steady state and the partition function
3. Currents
4. Scott Russell phenomenon out of equilibrium

Motivation

- Exact solutions of nonequilibium statistical mechanical models have proven useful in developing fundamental laws.
- For example, the asymmetric simple exclusion process (ASEP) in one-dimension has had remarkable success.
- The stationary distribution of the open ASEP was determined exactly by Derrida, Evans, Hakim and Pasquier (J. Phys. A, 1993) using the matrix ansatz.
- The additivity principle of Bodineau and Derrida has come out of a thorough study of the ASEP.

Motivation

- Several generalisations of the ASEP have also been solved exactly.
- For example, the steady state of the TASEP on a ring (i.e. with periodic boundary conditions) with multiple species was determined by Ferrari and Martin (Ann. Prob.,2007).
- The steady state of a disordered zero range process (LREP) with multiple species on a ring was computed by A., Martin and Mandelshtam (`arXiv:2209.09859`).

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- However, all of these are one-dimensional models.
- Very few (if any) two-dimensional models have been solved exactly.
- Very few models with disorder have been solved exactly.

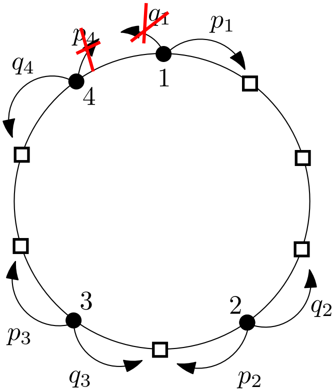
Disordered ASEP

- Evans (*Europhys. Lett.*, 1996) considered an ASEP on a ring where the hopping rates are disordered.
- Ring of size L with n particles.
- The k'th particle performs transitions

$$\bullet \; \square \to \square \; \bullet \quad \text{with rate } p_k,$$
$$\square \; \bullet \to \bullet \; \square \quad \text{with rate } q_k.$$

- Since particles cannot cross each other, we label the particles $\bullet_1, \dots, \bullet_n$.

Example



The configuration $\bullet_1\square\square\square\,\bullet_2\,\square\,\bullet_3\,\square\square\bullet_4$ for the system with $L = 10$ and $n = 4$.

Results

- Evans gave a formula for the steady state using the matrix ansatz.
- He also computed the nonequilibrium partition function and the current.

Show example in `Mathematica`

Formulas for $L = 4$, $n = 2$

Configuration	steady state weight
$(\bullet_2, \square, \square, \bullet_1)$	$(p_1 + q_2)^2$
$(\bullet_2, \square, \bullet_1, \square)$	$(p_2 + q_1)(p_1 + q_2)$
$(\bullet_2, \bullet_1, \square, \square)$	$(p_2 + q_1)^2$

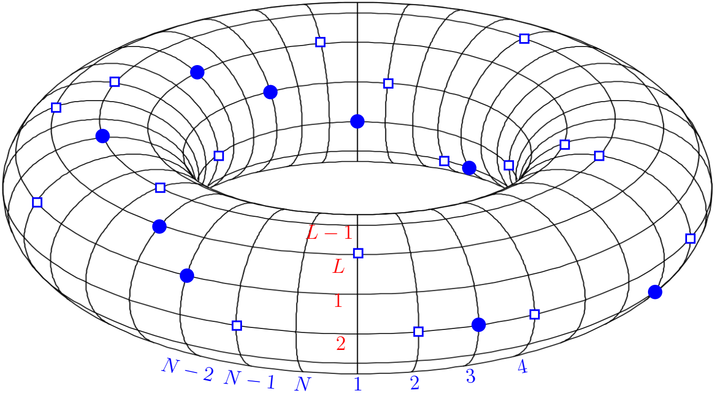
The partition function is

$$4\left((p_1 + q_2)^2 + (p_2 + q_1)(p_1 + q_2) + (p_2 + q_1)^2\right).$$

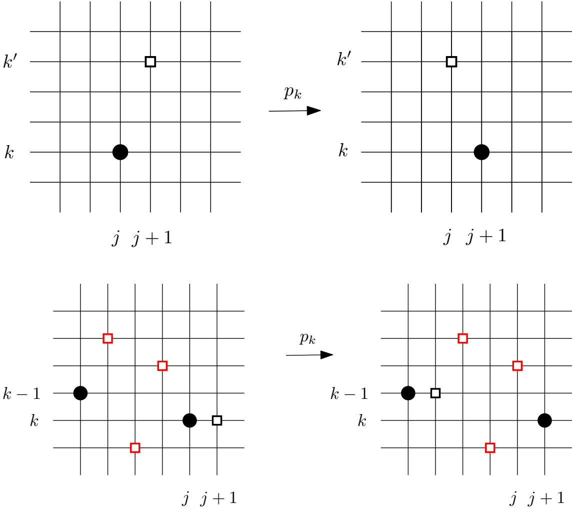
The two-dimensional exclusion process

- Discrete $L \times n$ torus with two kinds of particles and vacancies.
- Denote first class particles by $\bullet$, second class particles by $\square$ and vacancies by 0.
- Let $\hat{\Omega}_{L,n}$ consist of configurations such that:
  - Each row contains exactly one $\bullet$.
  - Each column contains exactly one particle (either $\bullet$ or $\square$).
  - The columns indices of $\bullet$'s read from left to right form a cyclically increasing sequence.
- Thus, we have n $\bullet$'s and $L - n$ $\square$'s.
- $|\hat{\Omega}_{L,n}| = n\binom{L}{n} n^{L-n}$.

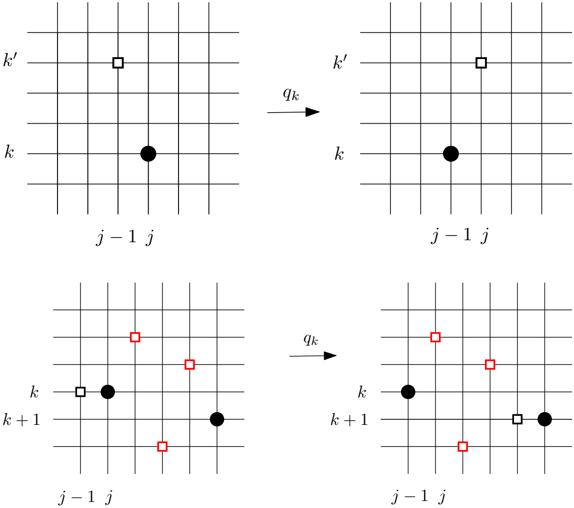
Illustration



Forward transitions: • in row k, column j



Backward transitions: • in row k, column j



Translation invariance

Show simulations in `Python`, Credit: K. Ayyer

Translation invariance

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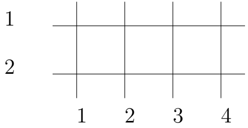
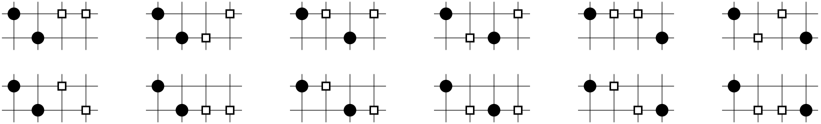
- The transitions are such that the process is invariant under horizontal translations.
- Therefore, it is enough to focus on $\omega \in \hat{\Omega}_{L,n}$ with $\omega_{1,1} = \bullet$.
- We call such configurations restricted configurations.
- For restricted configurations, the column indices of $\bullet$'s in ω must be a strictly increasing sequence.

Example: $L = 4, n = 2$





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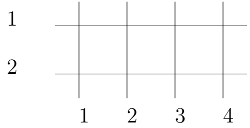

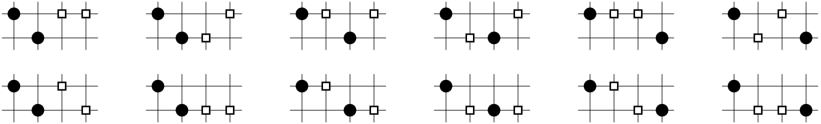

Show example in SageMath and Mathematica, Credit: P. Nadeau

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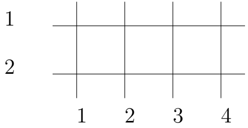

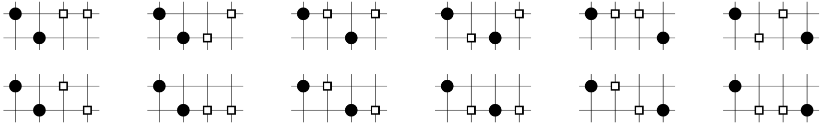

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Can this be made faster in SageMath?

Irreducibility

Lemma

Let $L \geq 1$ and $1 \leq n < L$. If all parameters $p_k, q_k > 0$, the exclusion process on $\hat{\Omega}_{L,n}$ is irreducible.

As a consequence, the steady state is unique.

Weights of configurations

- Let $\omega \in \hat{\Omega}_{L,n}$ be a restricted configuration.
- Let the locations of the 1's in ω by $((1, a_1), \ldots, (n, a_n))$, where $1 = a_1 < \cdots < a_n$.
- Let $C_k \equiv C_k(\omega)$ be the set of those positions (i, j) with $a_k < j < a_{k+1}$ such that $\omega(i, j) = \square$.
- We will assign a weight to every 0 lying in such a column.
- This weight will either be p_j or q_j if the 0 is in row j.

Weights of configurations

- Suppose $(i, j) \in C_k$.
- Two possibilities, depending on the relative order of i with respect to k:

$$\underset{i \le k}{\begin{pmatrix} p_1 \\ \vdots \\ p_{i-1} \\ \square \\ q_{i+1} \\ \vdots \\ q_k \\ p_{k+1} \\ \vdots \\ p_n \end{pmatrix}} \quad \text{or} \quad \underset{i > k}{\begin{pmatrix} q_1 \\ \vdots \\ q_k \\ p_{k+1} \\ \vdots \\ p_{i-1} \\ \square \\ q_{i+1} \\ \vdots \\ q_n \end{pmatrix}}$$

Weights of configurations

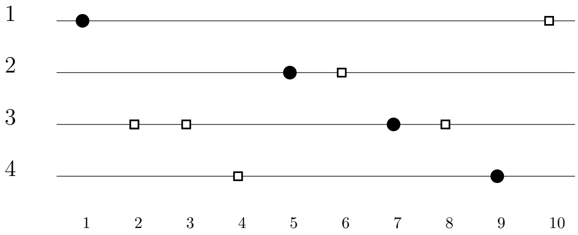
- The weight associated to this $\square$ is

$$w_{\square}(i,k) = \begin{cases} p_1 \dots p_{i-1} q_{i+1} \dots q_k p_{k+1} \dots p_n & 1 \le i \le k, \\ q_1 \dots q_k p_{k+1} \dots p_{i-1} q_{i+1} \dots q_n & k < i \le n. \end{cases}$$

- The weight $\mathrm{wt}(\omega)$ of $\omega \in \hat{\Omega}_{L,n}$ is

$$\mathrm{wt}(\omega) = \prod_{k=1}^{n} \prod_{(i,j)\in C_k} w_{\square}(i,k).$$

Example



- The weight of the configuration in the above figure is

$$\underbrace{(q_4 q_1 p_2)^2 (q_1 p_2 p_3)}_{C_1} \underbrace{(p_3 p_4 p_1)}_{C_2} \underbrace{(p_4 p_1 p_2)}_{C_3} \underbrace{(q_2 q_3 q_4)}_{C_4}$$

$$= p_1^2 p_2^4 p_3^2 p_4^2 q_1^3 q_2 q_3 q_4^3.$$

Steady state

Let the steady state probabilities in $\hat{\Omega}_{L,n}$ be denoted by $\hat{\pi}$.

Theorem (A. & P. Nadeau, *Europ. J. Comb.*, 2022)

- *Suppose* $p_k, q_k > 0$ *for* $1 \leq k \leq n$.
- *Then the stationary probability of the configuration* ω *for the exclusion process on* $\hat{\Omega}_{L,n}$ *given by*

$$\hat{\pi}(\omega) = \frac{\mathrm{wt}(\omega)}{L\, Z_{L,n}}.$$

- *Here* $Z_{L,n}$ *is the restricted (nonequilibrium) partition function,*

$$Z_{L,n} = \sum_{\substack{\omega \in \hat{\Omega}_{L,n} \\ \omega_{1,1}=1}} \mathrm{wt}(\omega).$$

Idea of proof: Verify the master equation.

Restricted partition function

Set

$$W_{\square}(k) = \sum_{j=1}^{n} w_{\square}(j,k).$$

Corollary

The restricted partition function $Z_{L,n}$ is given by:

$$Z_{L,n} = [x^{L-n}] \prod_{k=1}^{n} \frac{1}{1 - W_{\square}(k)x}.$$

Special cases

Define the (p, q)-analogue of an integer $n \in \mathbb{N}$ as

$$[n]_{p,q} = p^{n-1} + p^{n-2}q + \cdots + q^{n-1}.$$

Corollary

If $p_i = p$ and $q_i = q$ for all i, then

$$Z_{L,n} = \binom{L-1}{n-1} [n]_{p,q}^{L-n}.$$

Special cases

Recall that the elementary symmetric polynomial $e_k(x_1, \dots, x_j)$, for $1 \leq k \leq j$, is given by

$$e_k(x_1, \dots, x_j) = \sum_{1 \leq i_1 < i_2 < \cdots < i_k \leq j} x_{i_1} x_{i_2} \dots x_{i_k}. \tag{1}$$

Corollary

If $q_i = p_i$ for all i, then

$$Z_{L,n} = \binom{L-1}{n-1} e_{n-1}(p_1, \dots, p_n)^{L-n}.$$

Extra symmetry!

A useful lemma

Lemma

The weights associated to □'s satisfy

$$p_k w_\square(i,k) - q_k w_\square(i,k-1) = \begin{cases} 0 & i \neq k, \\ p_1 \cdots p_n - q_1 \cdots q_n & i = k. \end{cases}$$

Easily verified!

Current of •'s

- Since particles of type • only travel horizontally, we can only talk about horizontal currents for these.
- Let $J_\bullet$ denote the current for the particle of type • on the i'th row in the steady state.
- By particle conservation, this is independent of the choice of edge.
- Since •'s in successive rows cannot overtake each other, $J_\bullet$ is independent of i.

Current of $\bullet$'s

Theorem (Evans 1995, A. & P. Nadeau, *Europ. J. Comb.*, 2022)

For $1 \leq i \leq n$, we have

$$J_\bullet = (p_1 \dots p_n - q_1 \dots q_n) \frac{Z_{L-1,n}}{LZ_{L,n}}.$$

Evans gave the same formula for the 1D ASEP (in slightly different language).

Horizontal current of □'s

- The □'s travel both horizontally and vertically.
- So we can talk about two kinds of currents.
- In the horizontal direction, their motion can be both local and nonlocal.
- Let $J^{\mathrm{h}}_{\square}(j)$ denote the horizontal current of □'s crossing columns j and $j+1$.

Theorem (A. & P. Nadeau, *Europ. J. Comb.*, 2022)

For any $j \in [L]$,

$$J^{h}_{\square}(j) = -n(p_1 \cdots p_n - q_1 \cdots q_n)\frac{Z_{L-1,n}}{L Z_{L,n}}.$$

Vertical current of □'s

- In the vertical direction, the motion of □'s is always nonlocal.
- So, we cannot talk about the current across any one vertical edge.
- We will instead define the upward current $J_{\square}^{i+}$ between rows i and $i-1$, which occurs only with a forward transition of a • to its left in the same row.
- Similarly, the downward current $J_{\square}^{i-}$ between rows i and $i+1$ only occurs with a reverse transition of a • to its right in the same row.
- The net vertical current between rows i and $i+1$ is $J_{\square}^{i} = J_{\square}^{i+} - J_{\square}^{(i+1)-}$.

Vertical current of $\square$'s

Theorem (A. & P. Nadeau, *Europ. J. Comb.*, 2022)

We have

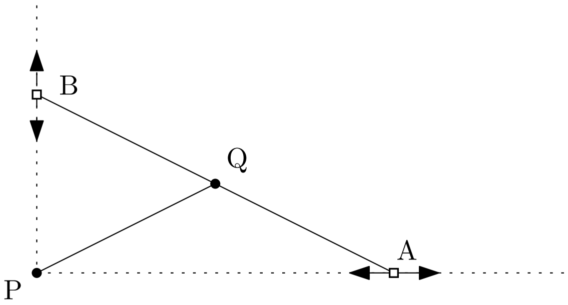
$$J_{\square}^{i+} = p_1 \dots p_n \frac{Z_{L-1,n}}{L Z_{L,N}}, \quad J_{\square}^{i-} = q_1 \dots q_n \frac{Z_{L-1,n}}{L Z_{L,N}},$$

Corollary

The vertical current of $\square$'s between rows i and $i+1$ is the same as the horizontal current of 1's, i.e.

$$J_{\square}^{i} = J_{\bullet}.$$

Scott Russell linkage



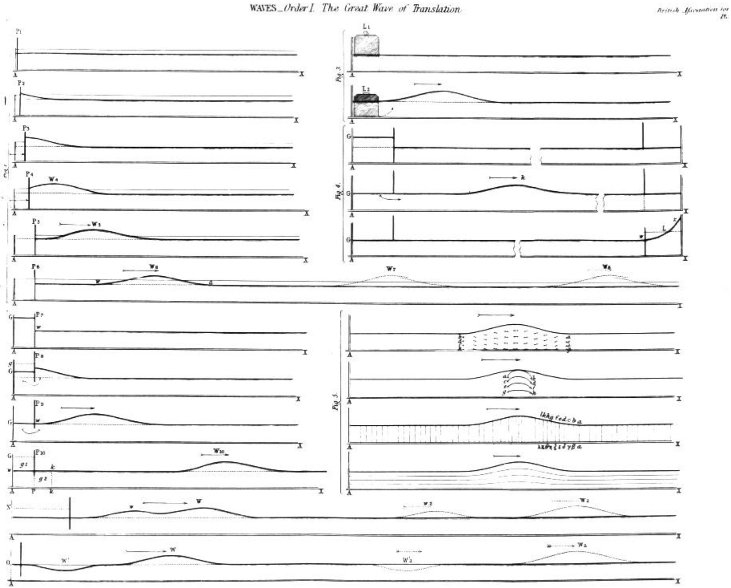
Scott Russell phenomenon

- In our 2D ASEP, horizontal motion of $\bullet$'s gives rise to vertical motion of $\square$'s.
- We call this the microscopic Scott Russell (linkage) phenomenon.
- This is a manifestly two-dimensional phenomenon.
- A Scott Russell linkage is a mechanism for transferring linear motion in one direction to a perpendicular direction.
- It is named after John Scott Russell, a Scottish civil engineer.
- It is a standard piece of equipment in most cars today.
- His other claim to fame is . . .

Report on Waves, Sep. 1844

I was observing the motion of a boat which was rapidly drawn along a narrow channel by a pair of horses, when the boat suddenly stopped - not so the mass of water in the channel which it had put in motion; it accumulated round the prow of the vessel in a state of violent agitation, then suddenly leaving it behind, rolled forward with great velocity, assuming the form of a large solitary elevation, a rounded, smooth and well-defined heap of water, which continued its course along the channel apparently without change of form or diminution of speed. I followed it on horseback, and overtook it still rolling on at a rate of some eight or nine miles an hour, preserving its original figure some thirty feet long and a foot to a foot and a half in height. Its height gradually diminished, and after a chase of one or two miles I lost it in the windings of the channel. Such, in the month of August 1834, was my first chance interview with that singular and beautiful phenomenon which I have called the Wave of Translation.

Image of a solitary wave



Out of equilibrium

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Show simulations in Python

Large deviation function

- We want to show that the large deviation functions (LDFs) of both $J_\bullet$ and $J_\square$ are the same.
- We can study these with the help of the Gärtner–Ellis theorem.
- Construct the tilted generators by multiplying the transitions which correspond to the observable by e^λ.
- By the Perron–Frobenius theorem, the largest eigenvalue is unique.
- The Legendre transform of the logarithm of this eigenvalue gives the LDF.

Tilted generators

- In general, it is difficult to show that two matrices have the same largest eigenvalues

Tilted generators

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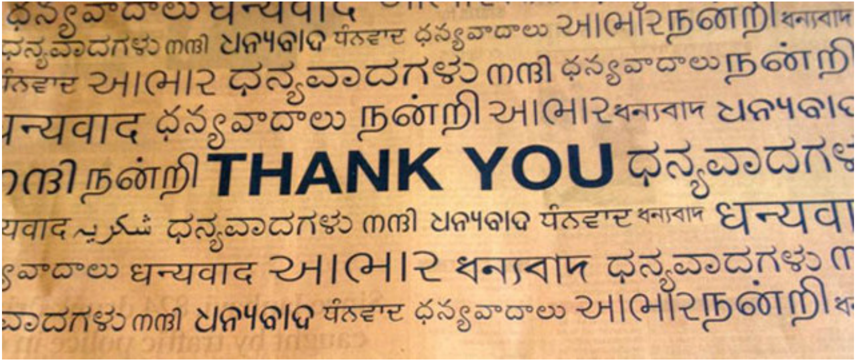
Show examples in SageMath

Intertwiner

- Fix L and n as before.
- For $1 \leq i \leq n$, let λ_i record the transitions for the horizontal (resp. vertical) current of $\bullet$'s (resp. $\square$'s) in row i (resp. between rows i and $i+1$).
- Let $M_\bullet$ and $M_\square$ be the tilted generators for the currents $J_\bullet$ and $J_\square$ respectively depending on parameters $\lambda_1, \dots, \lambda_n$.

Theorem (A., 2023+)

There exists a diagonal matrix I such that $IM_1 = M_2 I$.


THANK YOU