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 nonequilibrium 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.
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.
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
  
  $\bullet \square \rightarrow \square \bullet$ with rate $p_k$,
  $\square \bullet \rightarrow \bullet \square$ with rate $q_k$.

- Since particles cannot cross each other, we label the particles $\bullet_1, \ldots, \bullet_n$. 
The configuration $\bullet_1 \Box \Box \bullet_2 \Box \bullet_3 \Box \Box \bullet_4$ 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 $L = 4, n = 2$

<table>
<thead>
<tr>
<th>Configuration</th>
<th>steady state weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(\bullet_2, \square, \square, \bullet_1)$</td>
<td>$(p_1 + q_2)^2$</td>
</tr>
<tr>
<td>$(\bullet_2, \square, \bullet_1, \square)$</td>
<td>$(p_2 + q_1)(p_1 + q_2)$</td>
</tr>
<tr>
<td>$(\bullet_2, \bullet_1, \square, \square)$</td>
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</tr>
</tbody>
</table>

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.
- $|\hat{\Omega}_{L,n}| = n \binom{L}{n} n^{L-n}$. 

}|\hat{\Omega}_{L,n}| = n \binom{L}{n} n^{L-n}.
Illustration
Forward transitions: • in row $k$, column $j$

\[
\begin{align*}
\text{in row } k, \text{ column } j: & \\
& k' \\
& k \\
& j, j + 1 \\
\end{align*}
\]

\[
\begin{align*}
\text{in row } k, \text{ column } j: & \\
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\text{in row } k, \text{ column } j: & \\
& k' \\
& k \\
& j, j + 1 \\
\end{align*}
\]
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 $\omega$ 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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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 $\omega$ 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 \(k\):

\[
\begin{pmatrix}
p_1 \\
\vdots \\
p_{i-1} \\
\square \\
q_{i+1} \\
\vdots \\
q_k \\
p_{k+1} \\
\vdots \\
p_n
\end{pmatrix}
\quad \text{or} \quad
\begin{pmatrix}
q_1 \\
\vdots \\
q_k \\
p_{k+1} \\
\vdots \\
q_{i+1} \\
\vdots \\
q_n
\end{pmatrix}
\]

\(i \leq k\) \quad \text{or} \quad \(i > k\)
Weights of configurations

- The weight associated to this $\square$ is

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

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

$$\text{wt}(\omega) = \prod_{k=1}^{n} \prod_{(i,j) \in C_k} w_{\square}(i, k).$$
The weight of the configuration in the above figure is

\[
(q_4 q_1 p_2)^2 (q_1 p_2 p_3) (p_3 p_4 p_1) (p_4 p_1 p_2) (q_2 q_3 q_4) = p_1^2 p_2^4 p_3^2 p_4^2 q_1^3 q_2 q_3 q_4^3.
\]
Let the **steady state probabilities** in $\hat{\Omega}_{L,n}$ be denoted by $\hat{\pi}$.


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

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

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

  $$Z_{L,n} = \sum_{\omega \in \hat{\Omega}_{L,n}} \text{wt}(\omega).$$

**Idea of proof:** Verify the master equation.
Restricted partition function

Set

\[ W(k) = \sum_{j=1}^{n} w(j, k). \]

Corollary

The restricted partition function \( Z_{L,n} \) is given by:

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

\[
Z_{L,n} = \binom{L-1}{n-1} [n]_{p,q}^{L-n}.
\]
Recall that the elementary symmetric polynomial \( e_k(x_1, \ldots, x_j) \), for \( 1 \leq k \leq j \), is given by

\[
e_k(x_1, \ldots, x_j) = \sum_{1 \leq i_1 < i_2 < \cdots < i_k \leq j} x_{i_1}x_{i_2} \cdots x_{i_k}.
\]

(1)

Corollary

If \( q_i = p_i \) for all \( i \), then

\[
Z_{L,n} = \binom{L-1}{n-1} e_{n-1}(p_1, \ldots, p_n)^{L-n}.
\]

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!
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


For \( 1 \leq i \leq n \), we have

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

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 $J^h(\square)(j)$ denote the horizontal current of □’s crossing columns $j$ and $j+1$.


*For any $j \in [L]$,*

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


We have

\[
J_{□}^{i+} = p_1 \cdots p_n \frac{Z_{L-1,n}}{LZ_{L,N}}, \quad J_{□}^{i-} = q_1 \cdots q_n \frac{Z_{L-1,n}}{LZ_{L,N}},
\]

**Corollary**

The vertical current of □’s between rows \(i\) and \(i + 1\) is the same as the horizontal current of 1’s, i.e.

\[
J_{□}^{i} = J_{•}.
\]
Scott Russell linkage
In our 2D ASEP, horizontal motion of ●’s gives rise to vertical motion of □’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 . . .
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
A natural question is whether the Scott Russell phenomenon holds only in steady state or out of it.

It trivially holds when all $q_i = 0$ because each • jump causes a □ jump.
A natural question is whether the Scott Russell phenomenon holds only in steady state or out of it. It trivially holds when all $q_i = 0$ because each ● jump causes a □ jump.

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 $e^{\lambda}$.

- 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 \( \lambda_i \) 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 \( \lambda_1, \ldots, \lambda_n \).

Theorem (A., 2023+)

*There exists a diagonal matrix \( I \) such that \( IM_1 = M_2 I \).*