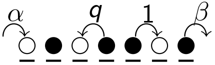
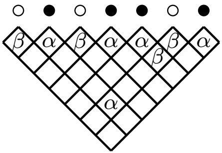
Combinatorics of hopping particles and positivity in Markov chains

Lauren K. Williams, Harvard





Overview of the talk

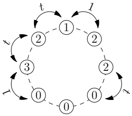
- A model for hopping particles: the asymmetric simple exclusion process
- Positivity in Markov chains; the Markov chain tree theorem
- Variations of the ASEP and special functions
- Summary and open problems

Many of the results I'll mention are based on joint works with

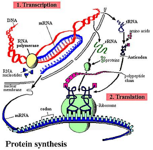
- Sylvie Corteel  Olya Mandelshtam 

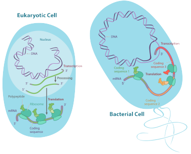
The asymmetric simple exclusion process (ASEP)

- Introduced by biologists (MacDonald, Gibbs, Pipkin) in 1968, and independently by a mathematician (Spitzer) in 1970.
- Particles hop on a 1D lattice; at most one particle per site. Particles may have different *weights*, which affect their hopping rate.
- Lattice could be a line with open boundaries or a *ring*...



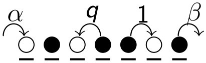
- Cited as a model for traffic flow and for translation in protein synthesis





- Over 1000 papers on the exclusion process on the arXiv: Liggett, Derrida, Evans, Hakim, Pasquier, Spohn, Sasamoto, Yau, Borodin, Corwin, Ferrari, Seppalainen, Tracy-Widom, ...

The ASEP with open boundaries



Fix a $1D$ lattice of n sites, which can be occupied by particles. Choose parameters q, α, β between 0 and 1.

• New particles can enter the lattice from the left at rate α, and particles can exit to the right at rate β.

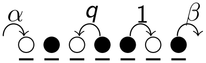
• A particle can hop right at rate 1 and left at rate q.
Model is *asymmetric*: we don't require $q = 1$.

• *Exclusion:* at most one particle on each site

Depict particles as • and "holes" as ∘.

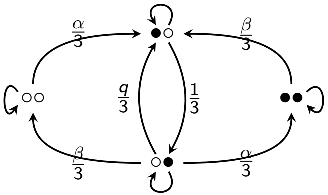
• Question: what happens as time $T \to \infty$?

The ASEP with open boundaries



- Let B_n be the set of all 2^n words of length n on letters $\{\circ, \bullet\}$.
- The ASEP is the Markov chain on B_n with transition probabilities:
  - If $X = A \bullet \circ B$ and $Y = A \circ \bullet B$ then $\mathrm{Pr}(X \to Y) = \frac{1}{n+1}$ and $\mathrm{Pr}(Y \to X) = \frac{q}{n+1}$.
  - If $X = \circ B$ and $Y = \bullet B$ then $\mathrm{Pr}(X \to Y) = \frac{\alpha}{n+1}$.
  - If $X = B \bullet$ and $Y = B \circ$ then $\mathrm{Pr}(X \to Y) = \frac{\beta}{n+1}$.
  - Otherwise $Pr(X \to Y) = 0$ for $Y \neq X$ and $\mathrm{Pr}(X \to X) = 1 - \sum_{X \neq Y} \mathrm{Pr}(X \to Y)$.

The ASEP with open boundaries



The stationary distribution π is unique: we can compute it by solving the *global balance* equations: for all states $\tau \in B_n$, we have

$$\pi(\tau)\sum_{\sigma\neq\tau}\mathrm{Pr}(\tau\to\sigma)=\sum_{\sigma\neq\tau}\pi(\sigma)\mathrm{Pr}(\sigma\to\tau),$$

where both sums are over all states $\sigma \neq \tau$.

start this example!

The ASEP with open boundaries

State τ	Stationary measure $\pi(\tau)$
●●	$\frac{\alpha^2}{Z}$
●○	$\frac{\alpha\beta(\alpha+\beta+q)}{Z}$
○●	$\frac{\alpha\beta}{Z}$
○○	$\frac{\beta^2}{Z}$

where

$$Z = \alpha^2 + \alpha\beta(\alpha+\beta+q) + \alpha\beta + \beta^2.$$

Since the sum of probabilities is 1, we prefer to ignore the denominator ...

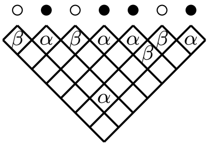
State τ	Unnormalized probability $\Psi(\tau)$
●●	α^2
●○	$\alpha\beta(\alpha+\beta+q)$
○●	$\alpha\beta$
○○	β^2

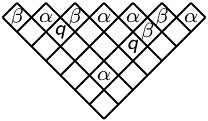
- The probabilities look "nice" – polynomials with positive coefficients, not too many terms. This remains true for larger n.
- Is there a *combinatorial formula*?

Definition (Corteel-W. 2011)

A **staircase tableau** T of size n is a Young diagram of shape $(n, \ldots, 2, 1)$ such that each box is either empty or contains an α or β, such that:

1. no box in the top row is empty
2. each box SE of a β and in the same diagonal as that β is empty.
3. each box SW of an α and in the same diagonal as that α is empty.



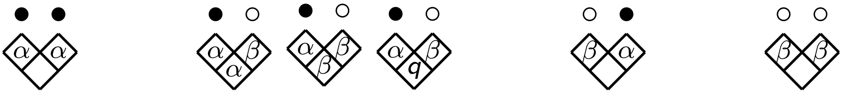


- Empty boxes either **restricted** or **unrestricted**. After placing a q in each unrestricted box, we define the *weight* $\mathrm{wt}(T)$ of T to be $\alpha^i \beta^j q^k$ where i, j and k are the numbers of α's, β's, and q's in T.
- The *type* of T is the word obtained by reading the letters in the top row of T and replacing each α by $\bullet$ and β by $\circ$.
- Rk: there are $(n+1)!$ staircase tableaux of size n.

The ASEP with open boundaries

Theorem (Corteel-W.)

Consider the ASEP with open boundaries on a lattice of n sites. Let $\tau = (\tau_1, \ldots, \tau_n) \in \{\bullet, \circ\}^n$ be a state. Then the unnormalized steady state probability $\Psi(\tau)$ is equal to $\sum_T \mathrm{wt}(T)$, where the sum is over the staircase tableaux of type τ.



Tableaux above allow us to compute the unnormalized probabilities:

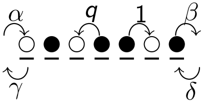
State τ	Unnormalized probability $\Psi(\tau)$
$\bullet\bullet$	α^2
$\bullet\circ$	$\alpha\beta(\alpha+\beta+q)$
$\circ\bullet$	$\alpha\beta$
$\circ\circ$	β^2

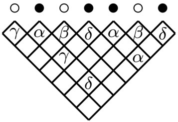
The ASEP with open boundaries

Theorem (Corteel-W.)

Consider the ASEP with open boundaries on a lattice of n sites. Let $\tau = (\tau_1, \ldots, \tau_n) \in \{\bullet, \circ\}^n$ be a state. Then the unnormalized steady state probability $\Psi(\tau)$ is equal to $\sum_T \mathrm{wt}(T)$, where the sum is over the staircase tableaux of type τ.

- Two proofs of this result: (1) by constructing a Markov chain on tableaux that projects or "lumps" to the ASEP.
  (2) by using the *Matrix Ansatz* of Derrida-Evans-Hakim-Pasquier.
- Theorem generalizes to five-parameter open boundary ASEP (C-W).



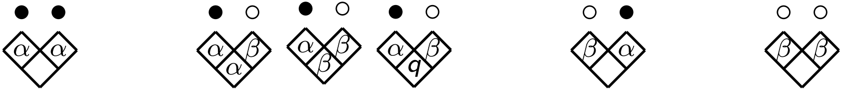


- Specializations of the generating function for these staircase tableaux give rise to the numbers: $4^n n!$, $(2n+1)!!$, $(n+1)!$, Catalan numbers, Eulerian numbers, Fibonacci numbers, etc (C-Stanley-Stanton-W)

The ASEP with open boundaries

Theorem (Corteel-W.)

Consider the ASEP with open boundaries on a lattice of n sites. Let $\tau = (\tau_1, \ldots, \tau_n) \in \{\bullet, \circ\}^n$ be a state. Then the unnormalized steady state probability $\Psi(\tau)$ is equal to $\sum_T \mathrm{wt}(T)$, where the sum is over the staircase tableaux of type τ.

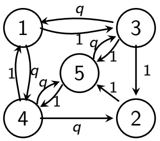


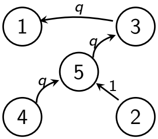
Questions:

- How unusual is it that we can write the unnormalized steady state probabilities as polys in the parameters with positive coefficients?
- or that we can give combinatorial formulas for them?
- Can we always do this for finite Markov chains?
- In some sense, the answer is yes ...

The Markov chain tree theorem

Let G be the *state diagram* of a finite-state irreducible Markov chain whose set of states is V. Each directed edge (i, j) is labeled by $\Pr(i \to j)$.





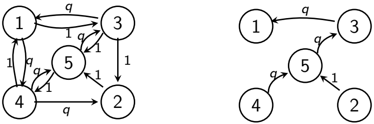
An acyclic connected subgraph T is a **spanning tree** rooted at r if T includes each vertex of V and all edges of T point towards the root r. Define *weight* of T as $\text{wt}(T) := \prod_{e \in T} \Pr(e)$.

Theorem (Markov Chain Tree Theorem (Hill, Leighton-Rivest))

The stationary distribution is proportional to the measure that assigns to state τ the "unnormalized probability"

$$\Psi(\tau) := \sum_{root(T)=\tau} wt(T).$$ *example!*

The Markov chain tree theorem



Theorem (Markov Chain Tree Theorem (Hill, Leighton-Rivest))

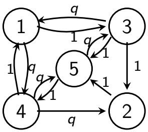
The steady state prob of state τ is proportional to the measure $\Psi(\tau) := \sum_{root(T)=\tau} wt(T)$.

That is, the steady state prob equals $\pi(\tau) = \frac{\Psi(\tau)}{Z}$, *where* $Z = \sum_{\tau} \Psi(\tau)$.

- This does give a positive combinatorial formula for the stationary distribution of any finite irreducible Markov chain.
- However, there is often a common factor in all of the $\Psi(\tau)$.
- In general, if one divides by common factor, resulting polynomials may contain negative coefficients.

The Markov chain tree theorem

State τ	Unnormalized probability $\Psi(\tau)$
1	$2q^3 + q^2 + q + 2$
2	$q^4 + 3q^3 + 4q^2 + 3q + 1$
3	$2q^3 + 2q^2 + q + 1$
4	$q^3 + q^2 + 2q + 2$
5	$2q^3 + 4q^2 + 4q + 2$



The unnormalized probabilities above share a common factor of $(q+1)$. Dividing by this common factor gives the (more compact) unnormalized probabilities $\overline{\Psi}(\tau)$ shown below.

State τ	Unnormalized probability $\overline{\Psi}(\tau)$
1	$2q^2 - q + 2$
2	$q^3 + 2q^2 + 2q + 1$
3	$2q^2 + 1$
4	$q^2 + 2$
5	$2q^2 + 2q + 2$

Positivity in Markov chains

This example motivates the following definitions.

Consider an unnormalized measure $(\Psi_1, \ldots, \Psi_n)$ on the set $\{1, 2, \ldots, n\}$ in which each component $\Psi_i(q_1, \ldots, q_N)$ is a polynomial in $\mathbb{Z}[q_1, \ldots, q_N]$.[a] We say that $(\Psi_1, \ldots, \Psi_n)$ is *manifestly positive* if the coefficients of Ψ_i are positive for all i. We say that $(\Psi_1, \ldots, \Psi_n)$ is *compact* if there is no polynomial $\phi(q_1, \ldots, q_N) \neq 1$ which divides all the components Ψ_i.

[a] We don't require that $\sum_i \Psi_i = 1$; to obtain a probability distribution we can just divide each term by $Z := \sum_i \Psi_i$.

Question

Consider a Markov chain whose transition probabilities are auxiliary parameters $q_1, \ldots, q_N$. When should we expect such a Markov chain to have a compact, manifestly positive formula for the stationary distribution?

What if we apply the Markov chain tree theorem to ASEP

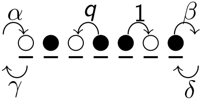
Theorem (Markov Chain Tree Theorem (Hill, Leighton-Rivest))

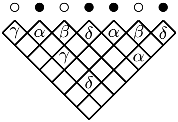
The steady state prob of state τ is proportional to the measure $\Psi(\tau) := \sum_{root(T)=\tau} wt(T)$.

- The MCTT gives a positive combinatorial formula for the stationary distribution of any finite irreducible Markov chain on n states, but it has $O(n^{n-2})$ terms!
- In the case of the ASEP, it gives the staircase tableaux formula *multiplied by a polynomial $Q_n(\alpha, \beta, q)$ whose number of terms grows exponentially with n*:

n	$Q_n(1,1,1)$
2	1
3	4
4	840
5	2285015040
6	11335132600511975880768000

The ASEP, tableaux, and orthogonal polynomials

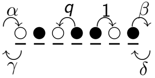




- We've see so far that we can use staircase tableaux to compute the stationary distribution for the ASEP.
- Uchiyama-Sasamoto-Wadati (2005) showed that there is a close relation between the ASEP with open boundaries and *Askey-Wilson polynomials* $P_n(x; a, b, c, d; q)$, orthogonal polynomials which sit at the top of the hierarchy of the classical orthogonal polynomials.
- Combining this work with our staircase tableaux formulas for ASEP gives rise to combinatorial formulas for the *moments* of Askey-Wilson polynomials (Corteel-W, Corteel-Stanley-Stanton-W).
- There are many variations of the ASEP which also admit beautiful combinatorial formulas and connections to special functions.

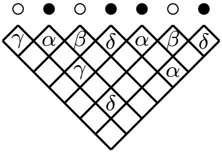
Recall: the open boundary ASEP

Prob/ Stat mech: the open boundary ASEP



Combinatorics:

staircase tableaux



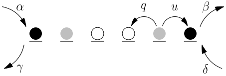
Combinatorial polynomials:

Askey-Wilson

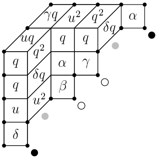
Note: Askey-Wilson polynomials are the one-variable case of the multivariate *Koornwinder polynomials*. Can we generalize this picture so as to replace Askey-Wilson polynomials by Koornwinder polynomials?

The open boundary multispecies ASEP

Prob/ Stat mech: open-boundary multispecies ASEP



Combinatorics:
rhombic staircase tableaux

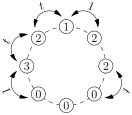


Combinatorial polynomials:
Koornwinder polynomials

- Macdonald-Koornwinder moments and the two-species exclusion process (Corteel–W., arXiv: May 4, 2015.)
- Asymmetric simple exclusion process with open boundaries and Koornwinder polynomials (Cantini, arXiv: May 31 2015)
- Combinatorics of the two-species ASEP and Koornwinder moments (Corteel–Mandelshtam–W, arXiv: Oct 2015).

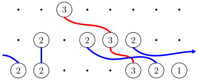
Note: Koornwinder polynomials are the Macdonald polynomials attached to the non-reduced affine root system of type $(C_n^\vee, C_n)$. Can we modify this picture so as to replace Koornwinder polynomials by (type A) Macdonald polynomials?

Prob/ Stat mech: multispecies ASEP



Combinatorics:

Multiline queues, tableaux



Combinatorial polynomials:

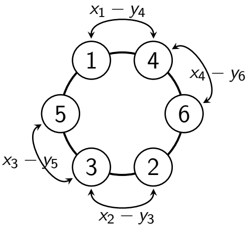
Macdonald polynomials

- Matrix product formula for Macdonald polynomials (Cantini–deGier–Wheeler 2015.)
- Stationary distributions of the multi-type ASEPs (Martin 2018).
- From multiline queues to Macdonald polynomials via the exclusion process (Corteel–Mandelshtam–W. 2018).
- Compact formulas for Macdonald polynomials and quasisymmetric Macdonald polynomials (Corteel–Haglund–Mason–Mandelshtam–W. 2019).

We've seen variations of ASEP that are connected to Askey-Wilson, Koornwinder, and Macdonald polynomials. What other special functions can we see?

The inhomogeneous multispecies TASEP on a ring

Prob/ Stat mech: inhomogeneous multispecies TASEP



Combinatorics:

Multiline queues

Evil-avoiding permutations

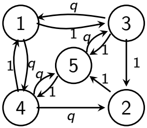
Combinatorial polys:

(double) Schubert polynomials

- A Markov chain on the symmetric group which is Schubert positive? (Lam–W., 2012)
- Matrix product solution of an inhomogeneous multispecies TASEP (Arita–Mallick, 2013)
- Inhomogeneous multispecies TASEP on a ring with spectral parameters (Cantini, 2016).
- Schubert polynomials and the inhomogeneous TASEP on a ring (Kim–W.,2021).

Open problems

Recall that the stationary distribution of a Markov chain (whose transition probabilities are auxiliary parameters $q_1, \ldots, q_N$), when written in its *compact form* ("lowest terms"), could consist of polynomials with negative coefficients.



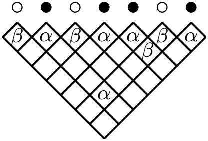
State τ	Unnormalized probability $\overline{\Psi}(\tau)$
1	$2q^2 - q + 2$
2	$q^3 + 2q^2 + 2q + 1$
3	$2q^2 + 1$
4	$q^2 + 2$
5	$2q^2 + 2q + 2$

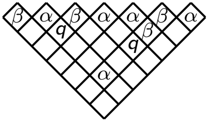
Question

When should we expect such a Markov chain to have a compact, manifestly positive formula for the stationary distribution?

Open problems

Recall that there are $(n+1)!$ staircase tableaux of size n, and that they encode the stationary distribution of the open-boundary ASEP.



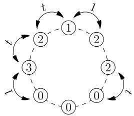
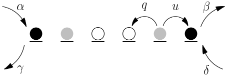


Question

What does a "typical" staircase tableaux look like when $n \to \infty$?
What about when $\alpha \gg \beta$ (high density of particles)?
Or $\beta \gg \alpha$ (low density of particles)?

Open problems

There is a family of Macdonald polys associated to each affine root system.

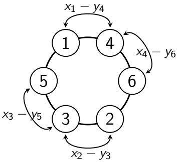
- The "usual" Macdonald polynomials are those associated to $\tilde{A}$; related to multispecies ASEP on a ring. 
- The Koornwinder polynomials are the Macdonald polynoimals associated to the non-reduced affine root system $(C_n^\vee, C_n)$; these are related to the open-boundary multispecies ASEP. 

Question

What about Macdonald polynomials associated to another affine root system? Are they related to the ASEP on some other lattice?

Open problems

Inhomogeneous multispecies TASEP



- We know that many steady state probabilities of the inhomogeneous multispecies TASEP are proportional to products of (double) Schubert polynomials (Cantini, Kim-W).
- **Conjecture:** In the case $y_i = 0$, each steady state probability can be written as a positive sum of Schubert polynomials (2012 Lam-W.). Is there a geometric interpretation for these probabilities?
- When $y_i = 0$, there is a multiline queue formula for the steady state probabilities (Arita-Mallick).
  Open problem: Extend this formula to the case of general y_i.

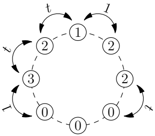
Open problems

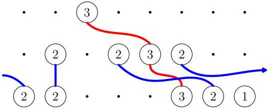
- We've seen that Askey-Wilson polynomials, Koornwinder polynomials, Macdonald polynomials, and Schubert polynomials are all related to variations of the ASEP.
- To give one more example, work in progress of Ayyer–Mandelshtam–Martin relates the *modified Macdonald polynomials* to the multispecies totally asymmetric zero-range process on a ring.

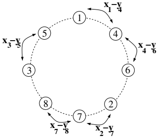
Question

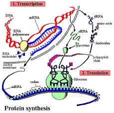
Choose your favorite family of special functions or orthogonal polynomials. Can they (or their moments) be realized as partition functions of a nice Markov chain?

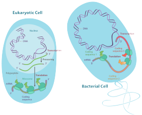
Thank you for listening!











- Combinatorics of hopping particles and positivity in Markov chains (W.), London Math Society Newsletter, 500th Anniversary Issue, May 2022.
- From multiline queues to Macdonald polynomials (Corteel–Mandelshtam–W.), to appear in Amer. J. Math.
- Schubert polynomials and the inhomogeneous TASEP on a ring (Kim–W.), to appear in IMRN.