The lifted TASEP, an integrable example of non-reversible Markov chains

Werner Krauth

Department of Physics, Ecole normale supérieure

Paris, France

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Institute for Applied Mathematics, Universität Bonn (Germany)

S. C. Kapfer, W. Krauth; PRL (2017)
'Irreversible Local Markov Chains with Rapid Convergence towards Equilibrium'

Z. Lei, W. Krauth, A. C. Maggs; PRE (2019)
'Event-chain Monte Carlo with factor fields'

F. Essler, W. Krauth; arxiv:2306.13059
'Lifted TASEP: a Bethe-ansatz integrable paradigm for non-reversible Markov chains'

X. Zhang, W. Krauth; arxiv:2311.17346
'Diameters of symmetric and lifted simple exclusion models'

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Markov chains

- Sample space Ω (e.g. point particles, water molecules)
- Markov chain $\leftarrow$ Sequence of random variables
  $(X_0 \sim \pi^{\{0\}}, X_1 \sim \pi^{\{1\}}, X_2 \sim \pi^{\{2\}} \dots)$
  X_{t+1} depends only on X_t, t is a 'time'
- Transition matrix P:
  - P_{ij}: conditional probability to move from i to j.
  - $\pi^{\{t+1\}} = \pi^{\{t\}} P$
- Equilibrium distribution π:
  - Satisfies global balance $\pi = \pi P$
  - Reversible algorithm (99.9%) satisfy detailed balance
    $\pi_i P_{ij} = \pi_j P_{ji}$

  NB: P irreducible $\implies$ π unique.
- Aperiodicity: Absence of cycles. P irreducible and aperiodic:

$$\pi^{\{t\}} \to \pi \quad \text{for } t \to \infty$$

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Conductance (bottleneck ratio)

$$\Phi \equiv \min_{S \subset \Omega, \pi_S \leq \frac{1}{2}} \frac{\mathcal{F}_{S \to \overline{S}}}{\pi_S} = \min_{S \subset \Omega, \pi_S \leq \frac{1}{2}} \frac{\sum_{i \in S, j \notin S} \pi_i P_{ij}}{\pi_S}.$$

- Reversible Markov chains:

$$\frac{1}{\Phi} \leq \tau_{\text{corr}} \leq \frac{8}{\Phi^2}$$

('$\leq$': Sinclair & Jerrum (1986), Lemma (3.3))

- Arbitrary Markov chain (see Chen et al. (1999)):

$$\frac{1}{4\Phi} \leq \mathcal{A} \leq \frac{20}{\Phi^2},$$

($\mathcal{A}$: set time: Expectation of $\max_S (t_S \times \pi_S)$ from equilibrium)

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Lifting (Chen et al. (1999))

- Markov chain Π (Ω, P, π) $\Leftrightarrow$ Lifted Markov chain $\hat{\Pi}$ $(\hat{\Omega}, \hat{P}, \hat{\pi})$
- Mapping f from $\hat{\Omega}$ to Ω.
- **Condition 1**: π is preserved

$$\pi_v = \hat{\pi}\left[f^{-1}(v)\right] = \sum_{i \in f^{-1}(v)} \hat{\pi}_i,$$

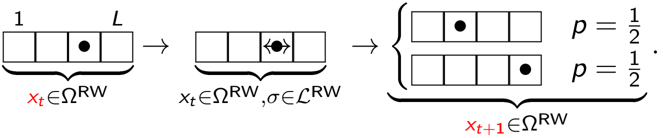
- **Condition 2**: flows are preserved

$$\underbrace{\pi_v P_{vu}}_{\text{collapsed flow}} = \sum_{i \in f^{-1}(v), j \in f^{-1}(u)} \overbrace{\hat{\pi}_i \hat{P}_{ij}}^{\text{lifted flow}} .$$

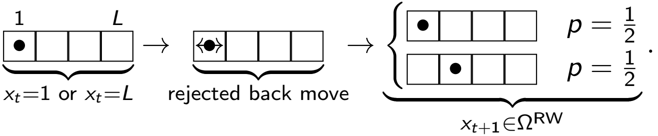
- $\hat{P}$ cannot have larger (better) conductance than P.

Random walk (RW) on the one-dimensional lattice

- In the bulk:

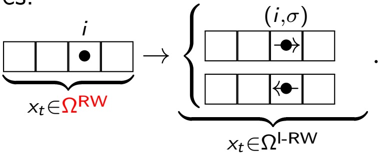


- At the boundary:

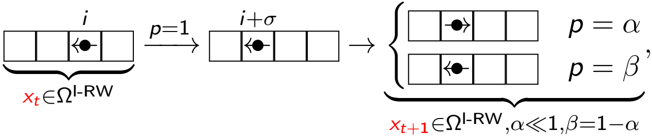


Lifted random walk (l-RW)

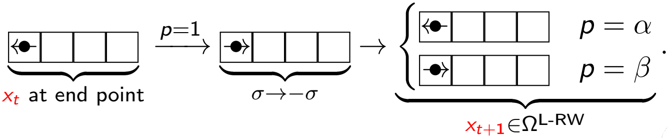
- Lifting of samples:



- In the bulk:



- At the boundary (a miracle takes place):



Diaconis, Holmes, Neal (2000)

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Random walk, lifted random walk (examples)

- 1 ≡ [•][ ][ ][ ]   2 ≡ [ ][•][ ][ ]   3 ≡ [ ][ ][•][ ]   4 ≡ [ ][ ][ ][•]

$$P^{RW}_{\text{walls}} = \frac{1}{2}\begin{bmatrix} 1 & 1 & \cdot & \cdot \\ 1 & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & 1 \\ \cdot & \cdot & 1 & 1 \end{bmatrix}$$

- Lifted random walk (NB: $\alpha + \beta = 1, \quad \alpha \sim 1/L$)

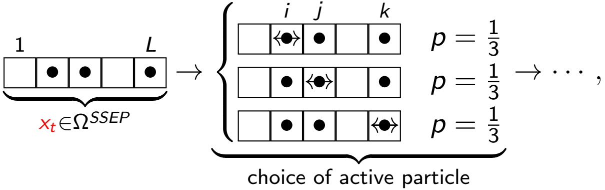
1 ≡ [•→][ ][ ][ ]   3 ≡ [ ][•→][ ][ ]   5 ≡ [ ][ ][•→][ ]   7 ≡ [ ][ ][ ][•→]

2 ≡ [←•][ ][ ][ ]   4 ≡ [ ][←•][ ][ ]   6 ≡ [ ][ ][←•][ ]   8 ≡ [ ][ ][ ][←•]

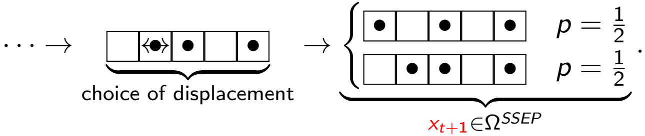
$$P^{\text{lRW}}_{\text{walls}} = \begin{bmatrix} \cdot & \cdot & \beta & \alpha & \cdot & \cdot & \cdot & \cdot \\ \beta & \alpha & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \beta & \alpha & \cdot & \cdot \\ \alpha & \beta & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \beta & \alpha \\ \cdot & \cdot & \alpha & \beta & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \alpha & \beta \\ \cdot & \cdot & \cdot & \cdot & \alpha & \beta & \cdot & \cdot \end{bmatrix},$$

Symmetric simple exclusion process (SSEP)

- Move (first part ...)



- Move (... second part)



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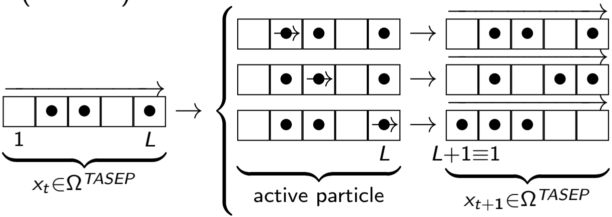
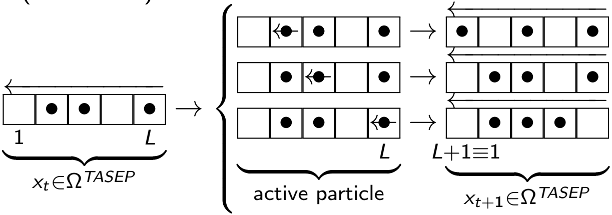
Totally asymmetric simple exclusion process (TASEP)

- Move (forward)



- Move (backward)



- forward–backward coupling (ad-hoc, or boundary conditions).

NB: Non-reversible, i.e. non-equilibrium, but samples equilibrium Boltzmann distribution.

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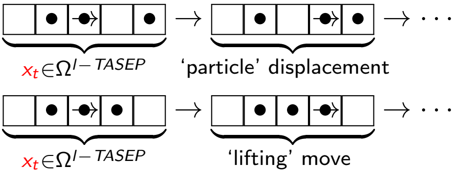
Lifted TASEP (definition)

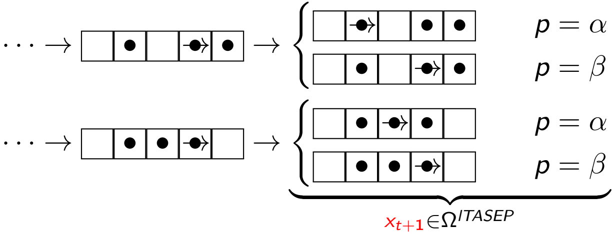
- $\Omega^{l-TASEP} = \Omega^{SSEP} \times \{-1, +1\} \times \{1, \dots, N\}$, $\mathcal{L} = \emptyset$
- Move (first part ...)



(1)

(2)

- Move (second part ...)



(1b)

(2b)

Essler & Krauth (2023)

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TASEP (example)

NB: Consider only the forward-moving sector (pbc):

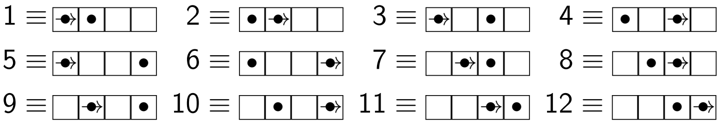
$$1 \equiv \overrightarrow{\begin{array}{|c|c|c|c|}\hline \bullet & \bullet & & \\ \hline\end{array}} \quad 2 \equiv \overrightarrow{\begin{array}{|c|c|c|c|}\hline \bullet & & \bullet & \\ \hline\end{array}} \quad 3 \equiv \overrightarrow{\begin{array}{|c|c|c|c|}\hline \bullet & & & \bullet \\ \hline\end{array}}$$

$$4 \equiv \overrightarrow{\begin{array}{|c|c|c|c|}\hline & \bullet & \bullet & \\ \hline\end{array}} \quad 5 \equiv \overrightarrow{\begin{array}{|c|c|c|c|}\hline & \bullet & & \bullet \\ \hline\end{array}} \quad 6 \equiv \overrightarrow{\begin{array}{|c|c|c|c|}\hline & & \bullet & \bullet \\ \hline\end{array}}$$

$$P^{TASEP} = \frac{1}{2}\begin{bmatrix} 1 & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & 1 & 1 & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & 1 & \cdot & \cdot & \cdot & 1 \end{bmatrix} \, .$$

Lifted TASEP (example 1)

NB: Consider only the forward-moving sector (pbc):



$$P = \begin{bmatrix}
\alpha & \beta & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \alpha & \beta & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \beta & \alpha & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \alpha & \beta & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \beta & \alpha & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \beta & \alpha & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \alpha & \beta & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \alpha & \beta & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \beta & \alpha \\
\beta & \alpha & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \alpha & \beta \\
\cdot & \cdot & \beta & \alpha & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot
\end{bmatrix}$$

Lifted TASEP (example 2)

L-TASEP with $N = 3$, $L = 5$, $\alpha = 0.5$, in 'cyclic' representation.

$$P^{l-T}_{3-5} = \frac{1}{2} \left(\begin{array}{cccccc|cccccc|cccccc|cccccc|cccccc}
1&0&0&0&0&0 & 0&0&1&0&0&0 & 0&0&0&0&0&0 & 0&0&0&0&0&0 & 0&0&0&0&0&0 \\
0&1&0&0&0&0 & 0&0&0&0&1&0 & 0&0&0&0&0&0 & 0&0&0&0&0&0 & 0&0&0&0&0&0 \\
0&0&1&0&0&0 & 0&0&0&0&0&1 & 0&0&0&0&0&0 & 0&0&0&0&0&0 & 0&0&0&0&0&0 \\
0&0&0&0&0&0 & 1&0&0&0&0&0 & 0&0&0&0&0&0 & 0&0&0&0&0&1 & 0&0&0&0&0&0 \\
0&0&0&0&0&0 & 0&1&0&0&0&0 & 0&0&0&0&0&0 & 0&0&0&0&0&0 & 0&0&0&1&0&0 \\
0&0&0&0&0&0 & 0&0&0&1&0&0 & 0&0&0&0&0&0 & 0&0&0&0&0&0 & 0&0&0&0&1&0 \\
\hline
0&0&0&0&0&0 & 1&0&0&0&0&0 & 0&0&1&0&0&0 & 0&0&0&0&0&0 & 0&0&0&0&0&0 \\
0&0&0&0&0&0 & 0&1&0&0&0&0 & 0&0&0&0&1&0 & 0&0&0&0&0&0 & 0&0&0&0&0&0 \\
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0&0&0&0&0&0 & 0&0&0&0&0&0 & 1&0&0&0&0&0 & 0&0&0&0&0&0 & 0&0&0&0&0&1 \\
0&0&0&1&0&0 & 0&0&0&0&0&0 & 0&1&0&0&0&0 & 0&0&0&0&0&0 & 0&0&0&0&0&0 \\
0&0&0&0&1&0 & 0&0&0&0&0&0 & 0&0&0&1&0&0 & 0&0&0&0&0&0 & 0&0&0&0&0&0 \\
\hline
0&0&0&0&0&0 & 0&0&0&0&0&0 & 1&0&0&0&0&0 & 0&0&1&0&0&0 & 0&0&0&0&0&0 \\
0&0&0&0&0&0 & 0&0&0&0&0&0 & 0&1&0&0&0&0 & 0&0&0&0&1&0 & 0&0&0&0&0&0 \\
0&0&0&0&0&0 & 0&0&0&0&0&0 & 0&0&1&0&0&0 & 0&0&0&0&0&1 & 0&0&0&0&0&0 \\
0&0&0&0&0&1 & 0&0&0&0&0&0 & 0&0&0&0&0&0 & 1&0&0&0&0&0 & 0&0&0&0&0&0 \\
0&0&0&0&0&0 & 0&0&0&1&0&0 & 0&0&0&0&0&0 & 0&1&0&0&0&0 & 0&0&0&0&0&0 \\
0&0&0&0&0&0 & 0&0&0&0&1&0 & 0&0&0&0&0&0 & 0&0&0&1&0&0 & 0&0&0&0&0&0 \\
\hline
0&0&0&0&0&0 & 0&0&0&0&0&0 & 0&0&0&0&0&0 & 1&0&0&0&0&0 & 0&0&1&0&0&0 \\
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0&0&0&0&0&0 & 0&0&0&0&0&1 & 0&0&0&0&0&0 & 0&0&0&0&0&0 & 1&0&0&0&0&0 \\
0&0&0&0&0&0 & 0&0&0&0&0&0 & 0&0&0&1&0&0 & 0&0&0&0&0&0 & 0&1&0&0&0&0 \\
0&0&0&0&0&0 & 0&0&0&0&0&0 & 0&0&0&0&1&0 & 0&0&0&0&0&0 & 0&0&0&1&0&0 \\
\hline
0&0&1&0&0&0 & 0&0&0&0&0&0 & 0&0&0&0&0&0 & 0&0&0&0&0&0 & 1&0&0&0&0&0 \\
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0&0&0&0&0&1 & 0&0&0&0&0&0 & 0&0&0&0&0&0 & 0&0&0&0&0&0 & 0&0&1&0&0&0 \\
1&0&0&0&0&0 & 0&0&0&0&0&0 & 0&0&0&0&0&1 & 0&0&0&0&0&0 & 0&0&0&0&0&0 \\
0&1&0&0&0&0 & 0&0&0&0&0&0 & 0&0&0&0&0&0 & 0&0&0&1&0&0 & 0&0&0&0&0&0 \\
0&0&0&1&0&0 & 0&0&0&0&0&0 & 0&0&0&0&0&0 & 0&0&0&0&1&0 & 0&0&0&0&0&0
\end{array} \right)$$

Hard facts for L-TASEP

- P^{l-T} is irreducible, aperiodic ($0 < \alpha < 1$).
- P^{l-T} is doubly stochastic: $\pi = \text{const.}$
- $|\Omega^{l-T}| = N\binom{L}{N}$
- diameters (Zhang & Krauth 2023)

$$d_{N,L}^{l-T} \begin{cases} = N(L-N) + 2N - 3 & \text{conj.} \\ \leq N(2L-N) + \mathcal{O}(L) & \text{proven} \end{cases}$$

$$d_{N,L}^{SSEP} = \begin{cases} N(L-N) & \text{hard-wall bc.} \\ \left\lceil \frac{N(L-N)}{2} \right\rceil & \text{periodic bc.} \end{cases}$$

- Activity drift

$$\left\langle \boxed{\cdots}\underset{x^a_{t+1}}{\boxed{-\!\bullet\!\!\to}}\boxed{\cdots} - \boxed{\cdots}\underset{x^a_t}{\boxed{-\!\bullet\!\!\to}}\boxed{\cdots} \right\rangle = \begin{cases} 1 & \beta \text{ move} \\ -(L-N)/N & \alpha \text{ move} \end{cases} = -\alpha\frac{L}{N}+1$$

- Critical pullback $\alpha_{\text{crit}} = N/L$: drift velocitiy $\langle \ldots \rangle = 0$.

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Integrability, spectrum of $P_{N,L}^{I-T}$. Ex: $(N=3)$

- Eqs for left eigenvector ψ, complex eigenvalue λ:

$$\begin{aligned}
\lambda\psi_{\{\vec{j},k,l\}} &= \beta\psi_{\{\overrightarrow{j-1},k,l\}} + \alpha\psi_{\{j,\overrightarrow{k-1},l\}}, \quad j<k-1 \\
\lambda\psi_{\{j,\vec{k},l\}} &= \beta\psi_{\{j,\overrightarrow{k-1},l\}} + \alpha\psi_{\{j,k,\overrightarrow{l-1}\}}, \quad j<k-1 \\
\lambda\psi_{\{j,k,\vec{l}\}} &= \beta\psi_{\{j,k,\overrightarrow{l-1}\}} + \alpha\psi_{\{\overrightarrow{j-1},k,l\}}, \quad j<k-1
\end{aligned}$$

  and similar equations for $j=k-1$...

- Bethe ansatz:

$$\begin{aligned}
\psi_{\{\vec{j},k,l\}} &= A_{\vec{\bullet}\circ\circ} z_1^j z_2^k z_3^l + B_{\vec{\bullet}\circ\circ} z_1^j z_2^l z_3^k + \ldots + F_{\vec{\bullet}\circ\circ} z_1^l z_2^k z_3^j \\
\psi_{\{j,\vec{k},l\}} &= A_{\circ\vec{\bullet}\circ} z_1^j z_2^k z_3^l + B_{\circ\vec{\bullet}\circ} z_1^j z_2^l z_3^k + \ldots + F_{\circ\vec{\bullet}\circ} z_1^l z_2^k z_3^j \\
\psi_{\{j,k,\vec{l}\}} &= A_{\circ\circ\vec{\bullet}} z_1^j z_2^k z_3^l + B_{\circ\circ\vec{\bullet}} z_1^j z_2^l z_3^k + \ldots + F_{\circ\circ\vec{\bullet}} z_1^l z_2^k z_3^j
\end{aligned}$$

Integrability, Bethe-ansatz equations ($N = 3$)

- Comparing coefficients:

$$\prod_{a=1}^{3} \left(\lambda - \frac{\beta}{z_a} \right) = \frac{\alpha^3}{z_1 z_2 z_3}, \tag{3}$$

- Periodic boundary conditions:

$$z_a^{L-1} = \left(\frac{\lambda - \beta / z_a}{\alpha} \right) \prod_{b \neq a = 1}^{3} T(z_a, z_b), \quad a = 1, 2, 3. \tag{4}$$

with

$$T(z_a, z_b) = \frac{\lambda - \alpha - \beta / z_b}{\lambda - \alpha - \beta / z_a}.$$

- Numerical solutions of eqs (3) and (4) agree with complete (complex) spectrum of $P_{3,L}^{l-T}$.
- Essler & Krauth (2023).

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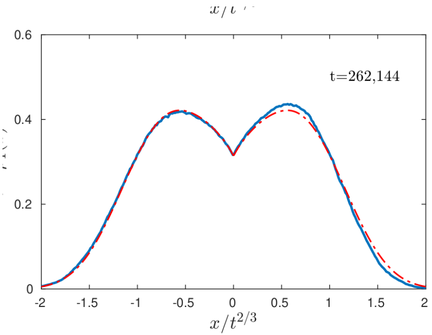
Synopsis of mixing and relaxation times

Algorithm	mixing	inv. gap	
SSEP	$N^3 \log N$	N^3	Lacoin (2016,17) | Aldous
TASEP	$N^{5/2}$	$N^{5/2}$	Dhar (1987) | Baik & Liu (2016
L-TASEP (α_{crit})	N^2	N^2	Essler & Krauth (2023)
L-TASEP ($\not\alpha_{\text{crit}}$)	?	$N^{5/2}$	

- In the L-TASEP, many indications of $L^{3/2}$ inverse-gap scaling, but L^2 inverse-gap is solid.

Observations in the L-TASEP

At α_{crit}, there is no drift, but the motion is super-diffusive:



- Figure from Maggs (2023), for the lifted TASEP
- Analytics from Dumaz & Tóth (2013), for the 'true' self-repellent motion.
- NB: $L/t(L)^{2/3} = 1 \equiv t(L) = L^{3/2}$

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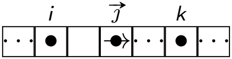
Generalized lifted(GL)-TASEP

- GL-TASEP, with configurations and stationary weights ...



$$\pi_{\{\dots,i,j,k,\dots\}} = \cdots \pi_{j-i}\pi_{k-j} \cdots .$$

- instead of the Metropolis et al. (1953) filter:

$$p^{\text{fact}}(j \to j+1) = \min\left[1, \frac{\pi_{j+1-i}\pi_{k-(j+1)}}{\pi_{j-i}\pi_{k-j}}\right]$$

- we use the factorized Metropolis filter (Michel et al. 2014):

$$p^{\text{fact}}(j \to j+1) = \min\left[1, \frac{\pi_{j+1-i}}{\pi_{j-i}}\right] \min\left[1, \frac{\pi_{k-(j+1)}}{\pi_{k-j}}\right].$$

- For repulsive interactions: $\pi_k \geq \pi_l$ for $k > l$, we have:

$$p^{\text{fact}}(j \to j+1) = \frac{\pi_{k-(j+1)}}{\pi_{k-j}}.$$

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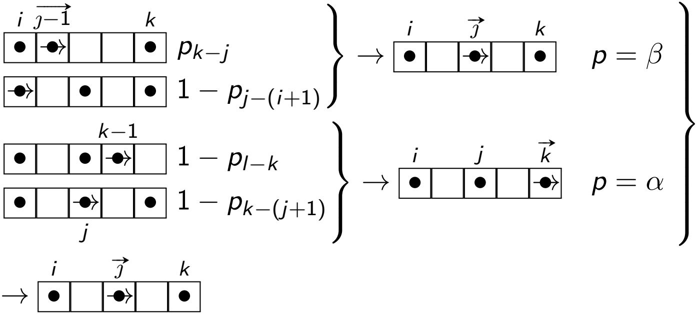
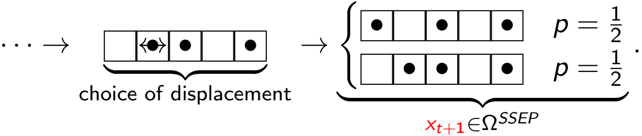
- Checking the global-balance condition $\sum_{x'} \pi_{x'} P(x', x) = \pi_x \ldots$



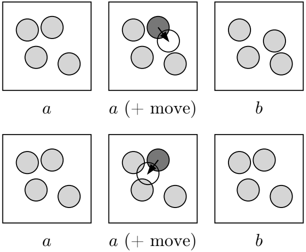
- … opens into a new world of MCMC algorithms…

The SSEP and the Metropolis algorithm

1. SSEP:



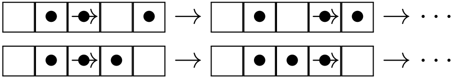
2. Metropolis (1953) algorithm:



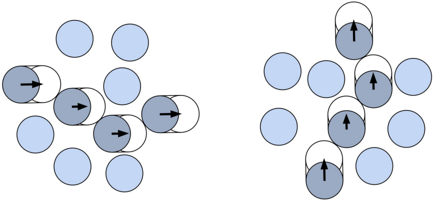
The Metropolis algorithm is reversible.

The lifted TASEP and event-chain Monte Carlo

1. Lifted TASEP:



2. Event-chain Monte Carlo algorithm (Bernard, Krauth, Wilson 2009):



Non-reversible, unchanged stationary distribution, orders of magnitude faster than Metropolis.

Département de Physique
École normale supérieure

Conclusion

- A second revolution in Markov-chain Monte Carlo underway.
- Non-reversible MCMC is what comes after the revolution.
- Lifting a practical method to create non-reversible algorithms.
- Lifted TASEP is an integrable model close to applications.
- Many open questions.