Space-time structure of extreme current events in the ASEP

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joint work with V. Popkov, D. Simon

- Asymmetric Simple Exclusion Process conditioned on a large flux
- Invariant measure and spectral properties
- Time-dependent correlation functions
- Conclusions

1. Asymmetric Simple Exclusion Process conditioned on a large flux

Asymmetric Simple Exclusion Process (ASEP)



MacDonald, Gibbs, Pipkin (1968); Spitzer (1970)

- short range interaction (excluded volume, $n_x = 0,1$)
- diffusive motion (random walk with exponential waiting time)
- drift (asymmetric hopping rates due to external potential or self-propelled particles)
- periodic or open boundaries -> permanent nonequilibrium state (non-reversible stochastic dynamics)

Density $\rho_x(t) = \langle n_x(t) \rangle$ Current $j_x = p \langle n_x(1-n_{x+1}) \rangle - q \langle (1-n_x)n_{x+1} \rangle$ Integrated current $J_x(t)$ Continuity equation $\dot{\rho}_x(t) = j_{x-1}(t) - j_x(t)$ Law of large numbers $J_x(t)/t \sim j(\rho)$ for $t \rightarrow \infty$

Applications:

- molecular diffusion in zeolites
- colloidal particles in narrow channels
- ion channels
- molecular motors
- gel electrophoresis
- one-dimensional interface growth
- automobile traffic flow

Polysom, Spinndrüse einer Raupe 0.25 μm

Protein synthesis: Translation through several ribosomes. Polypeptide chains increase in length in direction of translation



Three phases of kinesin transport (Chowdhury et al.)

Traffic flow:



- Exactly solvable model
- "Ising model of non-equilibrium statistical mechanics"

Master equation for probability $P(\eta,t)$ of configuration η :

$$\frac{d}{dt} P(\eta,t) = \sum_{\eta' \neq \eta} [w(\eta',\eta) P(\eta',t) - w(\eta,\eta') P(\eta,t)] \qquad \eta \in \{0,1\}^{L}$$

Quantum Hamiltonian representation:

 $\eta \rightarrow \mid \eta \rangle \in C^{\otimes_{L}} P(\eta,t) = \langle \eta \mid P(t) \rangle$

Schrödinger equation in imaginary time

$$\frac{d}{dt} | P(t) \rangle = -H | P(t) \rangle$$

$$H = -\sum_{k} p \left[s_{k}^{+} s_{k+1}^{-} - n_{k}^{-} (1 - n_{k+1}^{-}) \right] n + q \left[s_{k}^{-} s_{k+1}^{+} - (1 - n_{k}^{-}) n_{k+1}^{-} \right]$$

Pauli matrices $s^{\pm} = (\sigma^{x} \pm \sigma^{y})/2$, $n = (1 - \sigma^{z})/2$ (Heisenberg ferromagnet \Leftrightarrow spinless fermions) Stochasticity: diagonal elements (exit rates) ≥ 0 , offdiagonal elements (neg. transition rates) ≤ 0 Probability conservation: $< s \mid H = 0$ with constant summation vector (1,1,1,...)

Stationary properties (periodic boundary conditions):

• Invariant measure = ground state | ρ > of H with eigenvalue 0: Bernoulli product measure with density ρ , current j*(ρ) = (p-q) $\rho(1-\rho)$ [Spitzer (1970)]

==> simple structure, no spatial correlations

• Dynamical structure function in thermodynamic limit L $\rightarrow \infty$

 $S(p,t) = -\sum_{x} e^{ipx} (< n_x(t) n_0(0) > - \rho^2)$

~ S(u) for $p \rightarrow 0, t \rightarrow \infty$

with scaling variable $u = p^{3/2}t$ [Prähofer, Spohn (2002)]

==> non-trivial spatio-temporal correlations

• Spectral gap of H = longest relaxation time in periodic system: $\epsilon \propto 1/L^{3/2}$ [Gwa, Spohn (1991)]

==> dynamical exponent z = 3/2 (KPZ universality class)

Large deviations:

Time-integrated total current J(t) and average current j = J/T

- ► Universal scaling limits of distribution of integrated current P(J,T) = Prob[J(T) = J][Praehofer. Spohn (2002)]
- > Large deviation principle $P(J,T) \propto e^{T f(j)}$ with large deviation function f(j)
- <u>Cumulant function μ(s) for current</u>

 $\lim_{T \to \infty} \ln \left[P(J,T) \ e^{sJ(T)} \right] / T = \lim_{T \to \infty} \ln < e^{sJ(T)} > /T =: \mu(s)$

• <u>Legrende transformation</u>: $s(j) = -f'(j), \quad j(s) = \mu'(s)$

==> $\mu(s) = \max_{j} [f(j) + sj]$

Universal properties of its cumulants in finite systems [Appert-Rolland, Derrida, Lecomte, van Wijland (2008)]

Extreme events:

What is the spatio-temporal structure of the system during prolonged events of untypical current? "Same" large-scale behaviour or "different" from typical dynamics?

- Consider quasi-stationary scenario:
- Fix density ρ and system size L
- Condition process on *nontypical* integrated current J(T) in large time interval [0,T]
- Work with ``grand canonical ensemble" v_s : J(T)/T fluctuates around mean $j_{cond}(s,\rho) \neq j^*(\rho)$
- Study behaviour in time window $[t_1, t_2]$ with t_1 and T- t_2 large



==> stationary effective process with J(T)/T as typical current

• Generator of effective process

$$\mathsf{H}_{\mathsf{eff}} = \Delta \mathsf{H}' \, \Delta^{-1} - \mu$$

where

$$H' = -\sum_{k} p \left[e^{s} s_{k}^{+} s_{k+1}^{-} - n_{k} (1 - n_{k+1}) \right] n + q \left[e^{-s} s_{k}^{-} s_{k+1}^{+} - (1 - n_{k}) n_{k+1} \right]$$

 μ : lowest eigenvalue of H'

 $\Delta = \Sigma_{\eta} \mu_{L}(\eta) |\eta \rangle \langle \eta |$ diagonal matrix with components $\mu_{L}(\eta) = \langle \mu | \eta \rangle$

 $<\!\!\mu$ I, I μ > lowest eigenvectors (left and right resp.)

• Interpretation

$$< A(t) >_{eff} = \lim_{t_1, T-t_2 \to \infty} < A(t) e^{sJ(T)} > / < e^{sJ(T)} >$$

for observable A(t), $t \in [t_1, t_2]$

- Transition rates $\eta \twoheadrightarrow \eta'$ of effective process

 $w_{\eta'\eta} = w'_{\eta'\eta} \ \mu_L(\eta') \ / \ \mu_L(\eta)$

- ==> Generally: same transitions, but different rates
- Invariant measure

 $\mathsf{P}^{*}(\eta) = \mu_{\mathsf{R}}(\eta) \ \mu_{\mathsf{L}}(\eta) \ / \ \mathsf{Z}$

normalization $Z = \Sigma_{\eta} \mu_{R}(\eta) \mu_{L}(\eta)$

==> quadratic in components of ground state vector (link to quantum expectations?)

solution of eigenvalue problem for lowest eigenvalue allows for construction of effective process for conditioned dynamics and computation of conditioned expectations

2. Invariant measure and spectral gap

(Trivial) Exercise: Single particle, jump rates p,q

==> effective process: biased random walk with hopping rates pes, qe-s

- invariant measure: uniform (effective interaction: external field)
- current $j(s) = (pe^s qe^{-s})/L$
- s > 0 corresponds to current enhancement (generelly j(s) monotone)

==> focus on large s (totally asymmetric random walk), rescale jump rates by 1/pe^s

Interacting case (ASEP) in this limit?

- TASEP

- no qualitative difference to s>0 finite expected

- hopping rates p,q irrelevant (including SEP p=q)

Main results:

1) Repulsive long-range interaction, hopping rate for particle k at site $n_k \prod_{l \neq k} \frac{\sin \pi \frac{n_k - n_l + 1}{L}}{\sin \pi \frac{n_k - n_l}{L}}$

2) Invariant measure:
$$P_{12...N}^{\text{eff}} = \frac{1}{K_{N,L}} \prod_{\substack{l,k\\1 \le l < k \le N}} \sin^2 \pi \frac{n_k - n_l}{L}$$

where

$$K_{N,L} = 2^{-N(N-1)} L^N$$

3) Current:
$$J(\rho) = \frac{\sin(\pi\rho)}{\sin(\pi/L)}$$

4) Correlation function (L $\rightarrow \infty$): $\langle \hat{n}_k \hat{n}_{k+m} \rangle^{\text{eff}} = \rho^2 - \frac{1}{\pi^2} \frac{\sin^2 m \pi \rho}{m^2}$ [Lieb, Schultz, Mattis (1961)]

5) Spectral gap: $\epsilon = 2 \sin(\pi \rho) \sin(\pi/L)$

Proofs:

1) Bethe ansatz for eigenvectors with eigenfunctions $Y_{z1,...,zN}(n_1,...,n_N)$

$$|\varphi\rangle = \sum_{1 \le n_1 < n_2 < n_3 \le L} \sum_{\sigma \in S_N} A_{\sigma} z_{\sigma(1)}^{n_1} z_{\sigma(2)}^{n_2} \cdots z_{\sigma(N)}^{n_N} |n_1 n_2 \cdots n_N\rangle$$

$$\frac{A_{\ldots\sigma(ij)\ldots}}{A_{\ldots ij\ldots}} = -\frac{\alpha_{ji}}{\alpha_{ij}} = -\frac{pe^s + qe^{-s}z_iz_j - z_j}{pe^s + qe^{-s}z_iz_j - z_i}$$

2) Periodic boundary conditions

$$\prod_{i=1,i\neq k}^{N} (-1)\frac{\alpha_{ki}}{\alpha_{ik}} = z_k^L = (-1)^{N-1} \prod_{i=1}^{N} \frac{p e^s + q e^{-s} z_i z_k - z_k}{p e^s + q e^{-s} z_i z_k - z_i}$$

3) s $\rightarrow \infty$ (proof of completeness easy) $z_k = \exp(i\gamma_k)$

with quantized pseudomomentum $\,\gamma_k\,{\in}\,2\pi$ (j_k - (N+1)/2) / L

Wave function = Slater determinant

$$Y_{12\dots N} = \det \begin{vmatrix} z_1^{n_1} & z_1^{n_2} & \dots & z_1^{n_N} \\ z_2^{n_1} & z_2^{n_2} & \dots & z_2^{n_N} \\ \dots & \dots & \dots & \dots \\ z_N^{n_1} & z_N^{n_2} & \dots & z_N^{n_N} \end{vmatrix}$$

Effective hopping rates [cf. Spohn (1999) for symmetric hopping]

$$W_{C'C}^{\text{eff}} = \frac{Y'_{12...N}}{Y_{12...N}} = \prod_{l \neq k} \frac{\sin \pi ((n_k - n_l + 1)/L)}{\sin \pi ((n_k - n_l)/L)}$$

Long range interaction potential (x = n/L)

$$U(x_1, x_2, \dots, x_N) = -2 \sum_{\substack{l,k \\ l \neq k}} \log |\sin \pi (x_l - x_k)|$$

Force on particle k: $-2\pi \Sigma_{l\neq k} \cot (\pi(x_l - x_k))$

Invariant measure: Ground state of H where $\gamma_k = \frac{2(k - (N + 1/2))\pi}{L}$, k = 1, 2, ..., N

$$P_{12...N}^{\text{eff}} = \frac{1}{K_{N,L}} \prod_{\substack{l,k\\1 \le l < k \le N}} \sin^2 \pi \frac{n_k - n_l}{L}$$

$$K_{N,L} = 2^{-N(N-1)} L^N$$

Some properties:

1) Ordering: (x=n/L)

(A) max
$$Y_{12...N}$$
 is reached for $|x_{k+1} - x_k| = \frac{1}{N}$ for all k
(B) $Y_{12...N} = 0$ for $\prod_{k=1}^{N} (x_{k+1} - x_k) = 0.$

(of order 1/L^q for q short distance particle pairs)

==> repulsive ("antiferromagnetic") ordering

2) <u>Stationary current</u> = - ground state energy of H = sum of single-particle modes - $e^{-i\gamma k}$

$$J = \sum_{k=1}^{N} \cos \frac{2(k - ((N+1)/2))\pi}{L} = \frac{\sin \pi \rho}{\sin(\pi/L)}$$

Finite-size corrections for large L:

 $J = L \sin(\pi \rho) [1/\pi + \pi c/(6L^2) + ...]$ with c=1 ==> Link to conformal invariance

3) Density correlation function: (m>0) [Lieb, Schultz, Mattis (1961)]

$$\langle \hat{n}_k \hat{n}_{k+m} \rangle^{\text{eff}} = \rho^2 - \frac{1}{\pi^2} \frac{\sin^2 m \pi \rho}{m^2}$$

$$\rho = 1/2: = \begin{cases} 1/4 \text{ (no correlation)} & \text{m even} \\ 1/4 - 1/\pi^2 \text{m}^2 \text{ (long range anti-correlation)} & \text{m odd} \end{cases}$$

4) Circular unitary ensemble:

- Haar measure (uniform) on unitary group U(N) (complex NxN matrices, $U^{\dagger}U = 1$)

- Probability density of eigenvalues $e^{-i\theta k}$

$$P_{\text{CUE}}(\theta_1,\ldots,\theta_N) = \frac{1}{Z_N} \prod_{1 \le k < l \le N} \left| e^{i\theta_k} - e^{i\theta_j} \right|^2 = \frac{1}{Z'_N} \prod_{1 \le k < l \le N} \sin^2 \left(\frac{\theta_k - \theta_l}{2} \right)$$

- Dyson's Brownian motion $U_t = \exp(iH_t)$ with H_t Hermitian random matrix with Brownian elements and induced effective interacting motion on eigenvalues of U_t

$$\mathrm{d}\theta_k = \sum_{l \neq k} \cot\left(\frac{\theta_l - \theta_k}{2}\right) \,\mathrm{d}t + \mathrm{d}B_t^{(k)}$$

5) <u>Spectral gap:</u> Replace edge Fourier mode N by N+1 (k=1,2,...N-1,N+1)

 $\epsilon = 2 \sin(\pi \rho) \sin(\pi/L)$

Large L behaviour:

 $\epsilon \sim \sin(\pi \rho) 2\pi \times L^{-1} => z=1$, universal "critical exponent" x=1

3. Time-dependent correlation functions

Consider time-dependent properties of observables under evolution with H_{eff} = Δ H' Δ^{-1} – μ

Theorem: For observables G,F (functions of occupation numbers)

 $\langle G(t) F(0) \rangle_{eff} = \langle \mu | G'(t) F(0) | \mu \rangle$

where $G'(t) = e^{H't} G e^{-H't}$

- *Proof:* Observe that observables G,F are represented by diagonal matrices and by definition $\langle G(t) F(0) \rangle_{eff} = \langle s | G e^{-Heff t} F | P^* \rangle$ is the time-dependent correlation function. Then:
- $\succ \quad [\Delta, F] = 0 \qquad (since \Delta is also diagonal)$

Main results:

1) Transition probability
$$P_L(\eta, t; \eta_0, 0) = e^{E_0 t} \sqrt{\frac{\langle \eta \rangle_{eff}}{\langle \eta_0 \rangle_{eff}}} \det[g_L(m_j - n_i, t)]$$

where
$$g_L(d,t) = \sum_{\kappa=0}^{\infty} \left[(-1)^{\kappa} sign(d) \right]^{N+1} \frac{t^{d_L+\kappa L}}{(d_L+\kappa L)!},$$
$$d \in \{-L+1,...,L-1\}, d_L = d_L \}$$

for d > 0, $d_L = d + L$ for $d \le 0$

2) Dynamic structure factor in thermodynamic limit (scaling form u = pt)

$$\hat{S}(u) = \frac{|u|}{2\pi t} e^{-iu\cos\rho\pi - |u|\sin\rho\pi}$$

with collective velocity v_c = j'($\rho)$ = cos $\pi\rho$

Proofs:

Definition
$$P_L(\eta, t; \eta_0, 0) = \frac{\langle \hat{\eta}(t) \hat{\eta}_0 \rangle_{eff}}{\langle \hat{\eta}_0 \rangle_{eff}}$$

Normalized eigenvectors $|\mu_{\{k\}} >$ with pseudomomenta $\{k\}$:

$$\chi_{m_1 m_2 \cdots m_N}(\{k\}) = \frac{1}{N! L^{N/2}} T_{\{m\}} \sum_{Q} (-1)^Q \mathrm{e}^{i \sum_{j=1}^N m_{Q_j} \alpha_{k_j}}$$

- unit operator 1 = (N!)⁻¹ $\Sigma_{\{k\}} \mid \mu_{\{k\}} > < \mu_{\{k\}} \mid$ (completeness)

$$=> \langle \hat{\eta}(t)\hat{\eta}_0 \rangle_{eff} = (N!)^3 \chi_{\eta}^*(\{k\}_0) \chi_{\eta_0}(\{k\}_0) e^{Et} \sum_{\{k\}} e^{-E_{\{k\}}t} \chi_{\eta_0}^*(\{k\}) \chi_{\eta}(\{k\})$$

- sum over {k}:
$$\frac{L^{-N}}{(N!)^2} \sum_{\{k\}} \sum_{Q,Q'} (-1)^{Q+Q'} e^{i\sum_{j=1}^N (m_{Q_j} - n_{Q'_j})\alpha_{k_j} - t\sum_{j=1}^N \varepsilon(\alpha_{k_j})}$$

 $\epsilon(\alpha_k) = - \exp(-i\alpha_k), \qquad \alpha_k = 2\pi(k - (N+1)/2)/L \quad (\text{ground state modes})$

- Antisymmetry:

$$\frac{L^{-N}}{(N!)^2} \sum_{\{k\}} \sum_{Q,Q'} (-1)^{Q+Q'} e^{i\sum_{j=1}^N (m_{Q_j} - n_{Q'_j})\alpha_{k_j} - t\sum_{j=1}^N \varepsilon(\alpha_{k_j})}$$
$$= \frac{L^{-N}}{N!} \sum_{\{k\}} \sum_Q (-1)^Q e^{i\sum_{j=1}^N (m_{Q_j} - n_j)\alpha_{k_j} - t\sum_{j=1}^N \varepsilon(\alpha_{k_j})}$$

- Define signed transition probability of random walk on torus Z/L, winding number κ

$$g_L(d,t) = \sum_{\kappa=0}^{\infty} \left[(-1)^{\kappa} \operatorname{sign}(d) \right]^{N+1} \frac{t^{d_L+\kappa L}}{(d_L+\kappa L)!}$$

- With Taylor expansion of exp(-t α_k) and exp(i α_k L) = (-1)^{N+1}

$$\frac{L^{-N}L^{N}}{N!N!} \sum_{Q} (-1)^{Q} \prod_{k=1}^{N} g_{L}(m_{Q_{k}} - n_{k}, t) = \frac{1}{(N!)^{2}} \det[g_{L}(m_{j} - n_{i}, t)]$$

Dynamic structure function:

Definition Stationary density-density correlation function:

 $S_{L}(n,t) = E_{L}^{*}[\eta_{x+n}(t)\eta_{x}(0)] - \rho^{2} = \langle \mu | \sigma^{z}_{x+n} e^{-Ht} \sigma^{z}_{x} | \mu \rangle - (1-\rho)^{2}/4$

Use free fermion property of H [LSM, 1961]

- Jordan Wigner transformation from Pauli matrices to free fermion annihilation/creation operators

- Fouriertransformation

- Solution of equations of motion $d/dt S_L(n,t)$ using anti-commutators

$$S_L(n,t) = \frac{1}{L^2} \sum_{k=1}^{N} e^{-i\alpha_k n + \varepsilon(\alpha_k)t} \sum_{l=1}^{L} e^{i\alpha_l n - \varepsilon(\alpha_l)t} - \frac{1}{L^2} \sum_{k=1}^{N} e^{i\alpha_k n - \varepsilon(\alpha_k)t} \sum_{l=1}^{N} e^{-i\alpha_l n + \varepsilon(\alpha_l)t}$$

Discrete FT: Dynamical structure function ($p \in \{1,...,L\}$):

$$\hat{S}_L(p,t) = \sum_{n=1}^{L} e^{-2\pi i p n/L} S_L(n,t)$$

periodic in L, vanishes for p = kL

$$\hat{S}_L(p,t) = \frac{1}{L} \sum_{k=1}^N \left[e^{(\varepsilon(\alpha_k) - \varepsilon(\alpha_{k+p}))t} - e^{-(\varepsilon(\alpha_k) - \varepsilon(\alpha_{k-p}))t} \right]$$
$$+ \frac{1}{L} \sum_{k=1}^N \sum_{l=N+1}^L e^{-(\varepsilon(\alpha_k) - \varepsilon(\alpha_l))t} \delta_{p,k-l}$$
$$:= \hat{S}_L^{(1)}(p,t) + \hat{S}_L^{(2)}(p,t)$$

With
$$t_k = (1 - e^{2\pi i k/L})t$$

$$\hat{S}_{L}^{(2)}(p,t) = \begin{cases} \frac{1}{L} \sum_{k=1}^{p} e^{t_{p}e^{-i\alpha_{k}}} & p = 1, \dots, N-1 \\ \frac{1}{L} \sum_{k=1}^{N} e^{t_{p}e^{-i\alpha_{k}}} & p = N, \dots, L-N \\ \frac{1}{L} \sum_{k=N+1-L+p}^{N} e^{t_{p}e^{-i\alpha_{k}}} & p = L-N+1, \dots, L-1 \end{cases}$$

Thermodynamic limit L $\rightarrow \infty t_p = (1-e^{ip})t$

$$\hat{S}^{(1)}(p,t) = \frac{1}{2\pi} \int_{-\rho\pi}^{\rho\pi} dx \left[e^{-e^{-ix}t_{-p}} - e^{e^{-ix}t_{p}} \right]$$

$$\hat{S}^{(2)}(p,t) = \begin{cases} \frac{1}{2\pi} \int_{-\rho\pi}^{-\rho\pi+p} dx \, \mathrm{e}^{t_p \mathrm{e}^{-ix}} & p \in [0, 2\rho\pi] \\ \frac{1}{2\pi} \int_{-\rho\pi}^{\rho\pi} dx \, \mathrm{e}^{t_p \mathrm{e}^{-ix}} & p \in [-\pi, \dots, -2\rho\pi] \cup [2\rho\pi, \dots, \pi] \\ \frac{1}{2\pi} \int_{\rho\pi+p}^{\rho\pi} dx \, \mathrm{e}^{t_p \mathrm{e}^{-ix}} & p \in [-2\rho\pi, 0] \end{cases}$$

$$=> \qquad \hat{S}(p,t) = \begin{cases} \frac{1}{2\pi} \int_{\rho\pi}^{\rho\pi+p} dx \, \mathrm{e}^{t_p \mathrm{e}^{-ix}} & p \in [0, 2\rho\pi] \\ \frac{1}{2\pi} \int_{-\rho\pi+p}^{\rho\pi+p} dx \, \mathrm{e}^{t_p \mathrm{e}^{-ix}} & p \in [-\pi, \dots, -2\rho\pi] \cup [2\rho\pi, \dots, \pi] \\ \frac{1}{2\pi} \int_{-\rho\pi+p}^{-\rho\pi} dx \, \mathrm{e}^{t_p \mathrm{e}^{-ix}} & p \in [-2\rho\pi, 0] \end{cases}$$

Particle-hole symmetry
$$\hat{S}(1-\rho, p, t) = \hat{S}(\rho, -p, t)$$

Stationary case:
$$\hat{S}(p,0) = \begin{cases} \frac{|p|}{2\pi} & p \in [-2\rho\pi, 2\rho\pi] \\ \rho & p \in [-\pi, \dots, -2\rho\pi] \cup [2\rho\pi, \dots, \pi] \end{cases}$$

==> Scaling limit for $p \rightarrow 0, t \rightarrow \infty, u$ =pt fixed

$$\hat{S}(u) = \frac{|u|}{2\pi t} e^{-iu\cos\rho\pi - |u|\sin\rho\pi}$$

4. Conclusions

- 1) ASEP in high current regime described by effective TASEP with long range interaction
- 2) Dynamical exponent z=1 (change of universality class)
- 3) Qualitative change of spatio-temporal patterns during extreme current events
- 4) Equal spacing most likely configuration for maximal current
- 5) Relation to quantum free fermions and Dyson's Brownian motion

Open questions:

- 1) Behaviour during precursor $[0,t_1]$ and aftermath $[T-t_2]$ periods?
- 2) Link of large deviation behaviour to conformal invariance?