

TASEP with long-range interaction

(= ASEP conditioned on enhanced flux)

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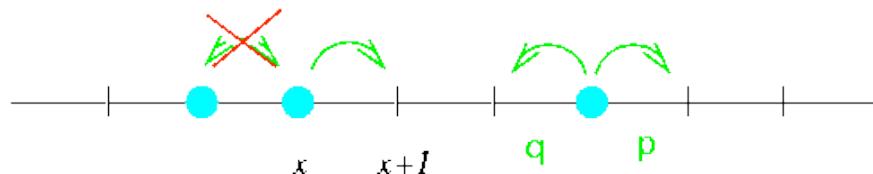
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joint work with V. Popkov, D. Simon

- TASEP with long-range interaction and ASEP conditioned on large flux
- Invariant measure and spectral properties
- Time-dependent correlation functions
- Conclusions

1. TASEP with long-range interaction and ASEP conditioned on large flux

Asymmetric Simple Exclusion Process (ASEP)



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

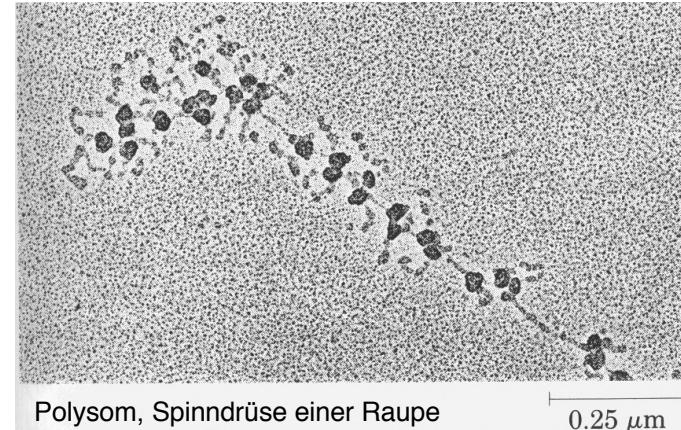
- short range interaction (excluded volume, $n_x = 0, 1$)
- diffusive motion (random walk with exponential waiting time)
- drift (asymmetric hopping rates due to external potential or self-propelled particles)
- periodic or open boundaries \rightarrow permanent nonequilibrium state (non-reversible stochastic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

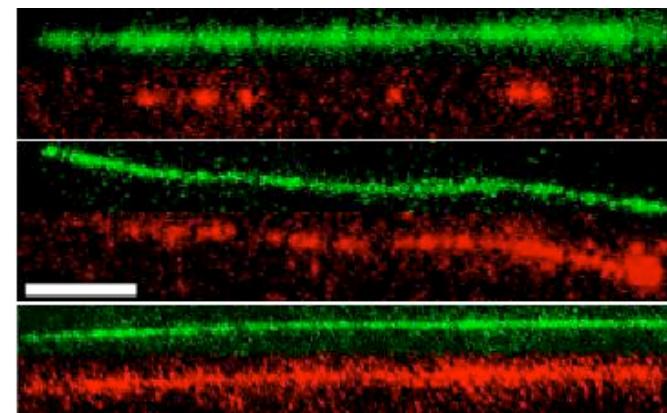
Continuity equation $\dot{\rho}_x(t) = j_{x-1}(t) - j_x(t)$ Law of large numbers $J_x(t)/t \sim j(\rho)$ for $t \rightarrow \infty$

Applications:

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

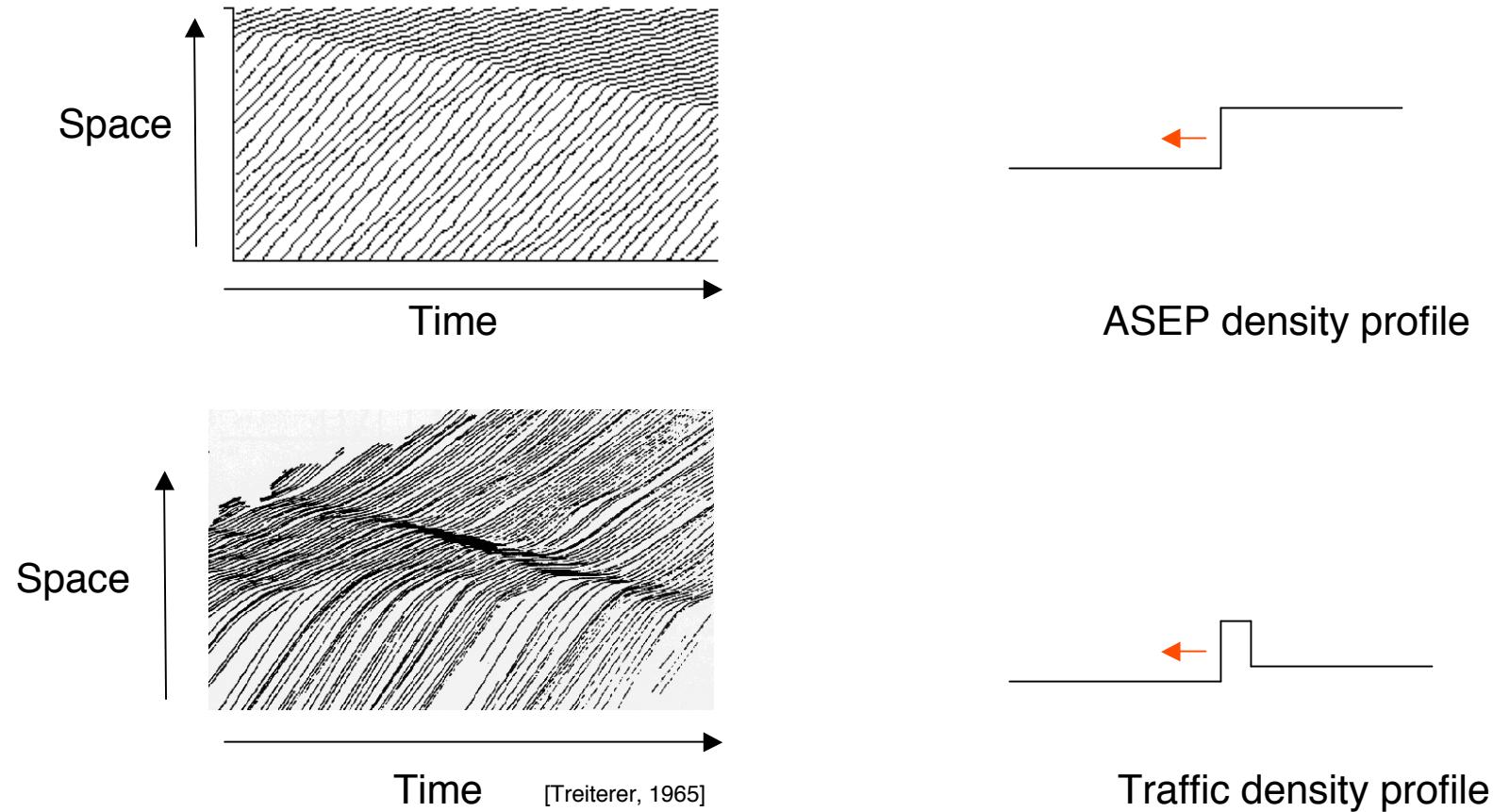


Protein synthesis: Translation through several ribosomes. Polypeptide chains increase in length in direction of translation



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 :

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

Quantum Hamiltonian representation:

$$\eta \rightarrow |\eta\rangle \in C^{\otimes L} \quad P(\eta, t) = \langle \eta | P(t) \rangle$$

Schrödinger equation
in imaginary time

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

$$H = - \sum_k p [s_k^+ s_{k+1}^- - n_k (1-n_{k+1})] n + q [s_k^- s_{k+1}^+ - (1-n_k)n_{k+1}]$$

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: $\langle s | H = 0$ with constant summation vector $(1, 1, 1, \dots)$

Stationary properties (periodic boundary conditions):

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

==> simple structure, no spatial correlations

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

$$S(p,t) \equiv - \sum_x e^{ipx} (\langle n_x(t) n_0(0) \rangle - \rho^2)$$

$\sim S(u)$ 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: $\varepsilon \propto 1/L^{3/2}$ [Gwa, Spohn (1991)]

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

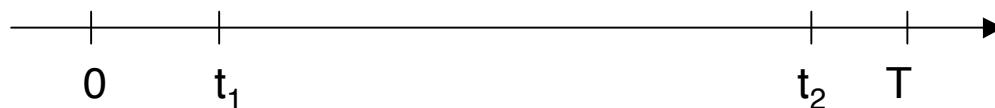
Extreme events:

- Time-integrated total current $J(t)$ of finite periodic system has non-trivial distribution with universal properties of its moments [Appert-Rolland, Derrida, Lecomte, van Wijland (2008)]

==> What is the spatio-temporal structure of the system during prolonged events of untypical current?

- 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 $j_{\text{cond}}(s, \rho) \neq j^*(\rho)$
- Study behaviour in large interval $[t_1, t_2]$ with $t_1 > 0$, $T - t_2 > 0$



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

- Generator of effective process [Simon (2009)]

$$H_{\text{eff}} = \Delta H' \Delta^{-1} - \mu$$

where

$$H' = - \sum_k e^s p [s_k^+ s_{k+1}^- - n_k (1-n_{k+1})] n + q e^{-s} [s_k^- s_{k+1}^+ - (1-n_k) n_{k+1}]$$

μ : lowest eigenvalue of H'

$\Delta = \sum_\eta \mu_L(\eta) |\eta\rangle\langle\eta|$ diagonal matrix with components $\mu_L(\eta) = \langle\mu|\eta\rangle$

$\langle\mu l, l\mu\rangle$ lowest eigenvectors (left and right resp.)

- Interpretation

$$\langle A(t) \rangle_{\text{eff}} = \lim_{T \rightarrow \infty} \langle A(t) e^{sJ(T)} \rangle / \langle e^{sJ(T)} \rangle$$

for observable $A(t) = A(\eta_t)$

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

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

\Rightarrow Generically: same transitions, but long-range interactions

- Invariant measure

$$P^*(\eta) = \mu_R(\eta) \mu_L(\eta) / Z$$

$$\text{normalization } Z = \sum_{\eta} \mu_R(\eta) \mu_L(\eta)$$

\Rightarrow 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

- Large deviation function $f(j)$ for integrated current $P(J) = \text{Prob}[J(T) = J]$:

$$P(J) \propto e^{T f(j)} \text{ for large } T$$

with average current $j = J/T$

- Cumulant function for current

$$\lim_{T \rightarrow \infty} \ln [P(J) e^{sJ(T)}] / T = \lim_{T \rightarrow \infty} \ln \langle e^{sJ(T)} \rangle / T = \mu(s)$$

- Legrende transformation

$$\mu(s) = \max_j [f(j) + sj]$$

$$j(s) = \mu'(s) \quad s(j) = -f''(j)$$

❖ general approach for any counting variable, not restricted to conditioning on total current

2. Invariant measure and spectral gap

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

\Rightarrow effective process: biased random walk with hopping rates pe^s, qe^{-s}

- invariant measure: uniform (effective interaction: external field)

- current $j(s) = (pe^s - qe^{-s})/L$

- $s > 0$ corresponds to current enhancement (generally $j(s)$ monotone)

\Rightarrow focus on large s (totally asymmetric random walk), rescale jump rates by $1/pe^s$

Interacting case (ASEP) in this limit?

- simpler algebra

- no qualitative difference to $s>0$ finite expected

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

Main results:

1) Invariant measure:

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

where

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

2) Current:

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

3) 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)]

4) Spectral gap:

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

Proofs:

1) Bethe ansatz for eigenvectors with eigenfunctions $Y_{z_1, \dots, z_N}(n_1, \dots, n_N)$

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

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

2) Periodic boundary conditions

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

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]

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

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 : $-2\pi \sum_{l \neq k} \cot(\pi(x_l - x_k))$

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

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

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

Some properties:

1) Ordering: ($x=n/L$)

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

(B) $Y_{12\dots N} = 0$ for $\prod_{k=1}^N (x_{k+1} - x_k) = 0$.

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

\Rightarrow repulsive (“antiferromagnetic”) ordering

2) Stationary current = - 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 :

$$J = L \sin(\pi\rho) [1/\pi + \pi c/(6L^2) + \dots] \quad \text{with } c=1 \implies \text{Link to conformal invariance}$$

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

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

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

4) Circular unitary ensemble:

- Haar measure (uniform) on unitary group $U(N)$ (complex $N \times N$ matrices, $U^\dagger U = 1$)
- Probability density of eigenvalues $e^{-i\theta_k}$

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

- 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

$$d\theta_k = \sum_{l \neq k} \cot \left(\frac{\theta_l - \theta_k}{2} \right) dt + dB_t^{(k)}$$

5) Spectral gap: Replace edge Fourier mode N by $N+1$ ($k=1, 2, \dots, N-1, N+1$)

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

Large L behaviour:

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

3. Time-dependent correlation functions

Consider time-dependent properties of observables under evolution with
 $H_{\text{eff}} = \Delta H' \Delta^{-1} - \mu$

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

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

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

Proof: Observe that observables G,F are represented by diagonal matrices and by definition $\langle G(t) F(0) \rangle_{\text{eff}} = \langle s | G e^{-H_{\text{eff}} t} F | P^* \rangle$ is the time-dependent correlation function. Then:

- $[\Delta, F] = 0$ (since Δ is also diagonal)
 - $|P^* \rangle = \Delta |\mu \rangle$
 - $\langle \mu | = \langle s | \Delta$
 - $e^{-H_{\text{eff}} t} \Delta = \Delta e^{-(H' - \mu) t}$
- } (consequences of transformation)

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

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

$$d \in \{-L+1, \dots, L-1\}, d_L = d$$

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

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 $|\mu_{\{k\}}\rangle$ with pseudomomenta $\{k\}$:

- wave function $|\mu_{\{k\}}\rangle = \sum_{\{\eta\}} \chi_{\eta}(\{k\}) |\eta\rangle$

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

- unit operator $1 = (N!)^{-1} \sum_{\{k\}} |\mu_{\{k\}}\rangle \langle \mu_{\{k\}}|$ (completeness)

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

- sum over $\{k\}$: $\frac{L^{-N}}{(N!)^2} \sum_{\{k\}} \sum_{Q, Q'} (-1)^{Q+Q'} e^{i \sum_{j=1}^N (m_Q - n_{Q'_j}) \alpha_{k_j} - i \sum_{j=1}^N \varepsilon(\alpha_{k_j})}$

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

- Antisymmetry:

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

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

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

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

$$\frac{L^{-N} L^N}{N! N!} \sum_Q (-1)^Q \prod_{k=1}^N g_L(m_{Q_k} - n_k, t) = \frac{1}{(N!)^2} \det[g_L(m_j - n_i, t)]$$

□

Dynamic structure function:

Definition Stationary density-density correlation function:

$$S_L(n,t) = E_L^*[\eta_{x+n}(t)\eta_x(0)] - \rho^2 = \langle \mu | \sigma_{x+n}^z e^{-Ht} \sigma_x^z | \mu \rangle - (1-\rho)^2/4$$

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 ($p \in \{1, \dots, L\}$):

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

periodic in L , vanishes for $p = kL$

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

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

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

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

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

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

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

\Rightarrow 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) Relation to quantum free fermions and Dyson's Brownian motion
- 3) Link of large deviation behaviour to conformal invariance?
- 4) Dynamical exponent $z=1$ (change of universality class)
- 5) Extensions to activity, non-conservative reaction-diffusion processes