Boundaries in driven systems

Gunter M. Schütz

Instituto Superior Técnico, University of Lisbon

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1. Introduction to the theme

Many-body systems out of equilibrium

• Mathematical modelling: infinite system or periodic boundary conditions

- translation invariance
- conservation laws
- symmetry and duality

★ Bulk behaviour unaffected

• Real physical systems: box, boundary fields and/or open b.c.

- No translation invariance
- Exchange of mass, energy and other conserved quantities
- bulk symmetries broken

★ Bulk behaviour depends on b.c.

One space dimension

• dramatic and unexpected effects

- non-equilibrium bulk phase transitions
- long-range correlations
- anomalous transport
- ...

★ Challenge:

- deal with absence of translation invariance, conservation laws, conventional symmetries
- understand emergence of new phenomena

Some questions of current interest (phenomena)

- Steady states with broken conservation law (microscopic)

- steady state selection in bulk and boundary-driven systems
- correlations in boundary-driven systems

- Hydrodynamics (macroscopic)

- boundary conditions in terms of pde
- microscopic structure of rarefaction waves and discontinuities
- solitons and other travelling waves
- spde's for fluctuation fields

- Large deviations (microscopic and macroscopic)

- additivity principle
- macroscopic fluctuation theory
- dynamical phase transitions

Some problems of current interest (models)

Traditional studies: short range interactions and short-range correlations in the absence of boundaries

- Long-range interactions

- long-range jumps
- local jumps with long-range rates
$\Rightarrow$ How do we define microscopic b.c.?

- Long-range correlations even without boundaries

$\Rightarrow$ Do such models exist in 1 dim?

- Many conservation laws

- Deterministic cellular automata

- ...

All seems somehow interconnected ...

$\Rightarrow$ Questions: Which feature is important for what on which level of description in the presence of boundaries? Are there any general answers? Universality?

- Some basic insights that have emerged:

– Boundary-driven: Current supported by long-range correlations

– Bulk and boundary driven: Travelling wave hits boundary

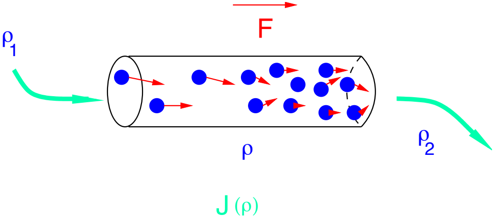
★ Ambitious. Today: discuss some recent developments in the study of steady states, hydrodynamics, and fluctuations in the presence of boundaries as well as related problems.

★ Attack the problem of general insights by studying concrete models

2. Boundary-induced phase transitions

Open driven diffusive systems

- bulk: (i) biased random motion, (ii) short range interaction, (iii) particle conservation
- boundaries: coupling to external reservoirs with fixed densities



$\Rightarrow$ stationary particle current $J(\rho)$

$\Rightarrow$ Steady-state selection (which density)?

Boundary-induced phase transitions [Krug (1991), Popkov, GMS (1999)]

- Extremal-current principle [Popkov, GMS (1999)]

$$J = \begin{cases} \max_{\rho \in [\rho^+, \rho^-]} J(\rho) & \rho^- > \rho^+ \\ \min_{\rho \in [\rho^-, \rho^+]} J(\rho) & \rho^- < \rho^+ \end{cases}$$

- Universal density profile $\rho_k = \sqrt{\frac{\kappa}{\pi k}}$ in extremal current phases

[Hager, Krug, Popkov, GMS (2001)]

- Derivations:

- regularization of hydrodynamic equation with Dirichlet boundary condition For $\rho^+ = 0$: [Krug (1991)

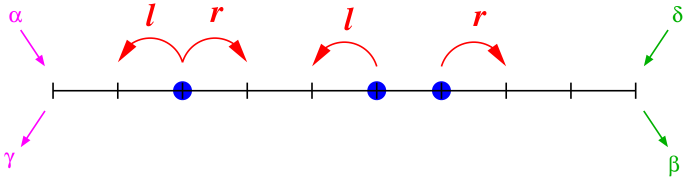
- flow of microscopic fluctuations [Popkov, GMS (1999)]

- entropy solutions for hydrodynamic equations [Bahadoran [2010]

Open asymmetric simple exclusion process (ASEP)

- ASEP: At most one particle per site on integer lattice with L sites
$$\boldsymbol{\eta} = (\eta_1, \ldots, \eta_L),\ \eta_k \in \{0, 1\}$$

Process	Transition	Rate
Jump to the right	$10 \to 01$	r
Jump to the left	$01 \to 10$	ℓ
Deposition at site 1 (L)	$0 \to 1$	α (δ)
Annihilation at site 1 (L)	$1 \to 0$	γ (β)



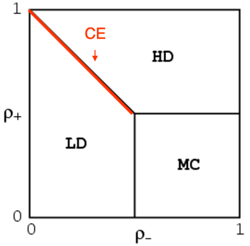
- Invariant measure for p.b.c.: Bernoulli product measure with density ρ (uncorrelated)

- Stationary current: $J(\rho) = (r - \ell)\rho(1-\rho)$

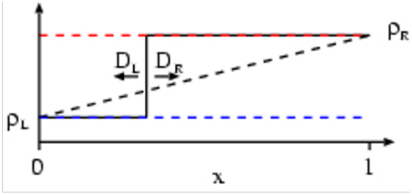
- Open: exact stationary distribution via matrix product ansatz [Derrida, Evans, Hakim, Pasquier (1993)] or recursive [Domany, GMS (1993)]

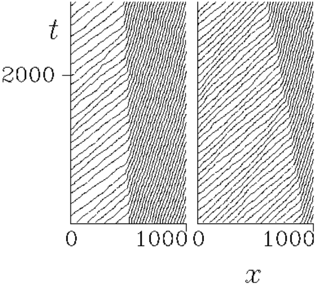
- Phase diagram:

- Low-density phase LD $\rho = \rho_-$
- coexistence line (first order transition)
- High-density phase HD $\rho = \rho_+$
- second order transition lines
- maximal-current phase $\rho = 1/2$



• First order transition: microscopic sharpness of macroscopic shock discontinuity





• Second order transition: confinement of rarefaction wave and nonlinear fluctuating hydrodynamics

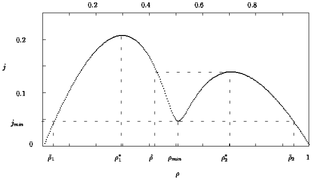
Open Katz-Lebowitz-Spohn model

- Exclusion process with next-nearest-neighbour interaction [Katz, Lebowitz, Spohn (1985)]
- TAKLZ: Bulk jump rates at bond $(k, k+1)$

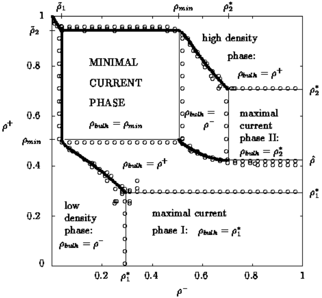
Transition	Rate
$0100 \to 0010$	$1+\delta$
$1100 \to 1010$	$1+\epsilon$
$0101 \to 0011$	$1-\epsilon$
$1101 \to 1011$	$1-\delta$

- Invariant measure for p.b.c.: Ising measure (short-range correlations)

Stationary current $J(\rho)$:



Phase diagram ($\delta > 0$, $\epsilon > 0$):



3. Reverse duality for the open ASEP

Duality

- Consider two Markov processes $\boldsymbol{\eta}(t)$ and $\mathrm{x}(t)$ with generally different countable state spaces

- Intensity matrices $W_{\boldsymbol{\eta}\boldsymbol{\eta}'} = w(\boldsymbol{\eta} \to \boldsymbol{\eta}')$, $Q_{\mathrm{x}\mathrm{x}'} = w(\mathrm{x} \to \mathrm{x}')$

- Quantum Hamiltonian formalism: $H = -W^T$, $G = -Q^T$

- Invariant measures $\mu^*_{\boldsymbol{\eta}}$, π^*_{x}

- Reverse processes for strictly positive invariant measures:

$$H_{rev} = \hat{\mu}^* H^T (\hat{\mu}^*)^{-1}, \quad G_{rev} = \hat{\pi}^* G^T (\hat{\pi}^*)^{-1}$$

– Diagonal matrices: $\hat{\mu}^*$, $\hat{\pi}^*$ with $\mu^*_{\boldsymbol{\eta}}$, π^*_{x} on the diagonal

• (Conventional) Duality: Relationship between two processes that yields time-dependent expectations of one process in terms of the dual in terms of a duality function $D(\mathrm{x}, \boldsymbol{\eta})$ [Liggett, 1985]

• Paradigmatic example: Symmetric simple exclusion process (SSEP) where hard-core particles perform lattice random walk

– Expectation of local density at time t for many-particle initial state given in terms of transition probability for just one particle

– Joint expectation for N particles at times $t_1, \ldots, t_N$ given in terms of transition probability for N particles

– Origin: $SU(2)$ symmetry of generator (apparent through relationship to quantum XXX Heisenberg spin chain [GMS and Sandow, 1994])

- Duality at the level of generators: $DH = G^T D$

- Duality matrix $D_{\mathrm{x}\boldsymbol{\eta}} = D(\mathrm{x}, \boldsymbol{\eta})$

- Expectation $\langle\, D(\mathrm{x}, \boldsymbol{\eta}(t))\,\rangle_{\boldsymbol{\eta}} = \langle\, D(\mathrm{x}(t), \boldsymbol{\eta})\,\rangle_{\mathrm{x}}$

- For family of functions $f^{\mathrm{x}}(\boldsymbol{\eta}) := D(\mathrm{x}, \boldsymbol{\eta})$:

$$\langle\, f^{\mathrm{x}}(t)\,\rangle_{\mu} = \sum_{\mathrm{y}} P(\mathrm{x}, t|\mathrm{y}, 0)\langle\, f^{\mathrm{y}}(0)\,\rangle_{\mu}$$

with transition probability $P(\mathrm{x}, t|\mathrm{y}, 0)$ of dual process

- Useful information about expectations if dual process has simple properties

- Reversible process $H = G^T$: Duality = Symmetry

• Reverse duality: $HR = RG^T$

with reverse duality matrix R and duality function $R_{\boldsymbol{\eta}\mathrm{x}} = R(\boldsymbol{\eta}, \mathrm{x})$

• Useful information about measures if reverse dual process has simple properties

- For family of measures $\mu_{\boldsymbol{\eta}}^{\mathrm{x}}(t) := R(\boldsymbol{\eta}, \mathrm{x})$:

$$\mu_{\boldsymbol{\eta}}^{\mathrm{x}}(t) = \sum_{\mathrm{y}} P(\mathrm{x}, t|\mathrm{y}, 0)\mu_{\boldsymbol{\eta}}^{\mathrm{y}}(0)$$

- Duality function can take negative values (corresponding to signed measures)

• Reversible process $H = G^T$: Reverse duality = Symmetry

★ BUT: open boundary breaks symmetry

Open ASEP

- Hopping asymmetry and time scale $q := \sqrt{\frac{r}{\ell}}, \quad w := \sqrt{r\ell}$
- Boundary densities $\rho_\pm$ and boundary jump barriers $\omega_\pm$

$$\alpha = (r+\omega_-)\rho_-, \quad \gamma = (\ell+\omega_-)(1-\rho_-)$$
$$\beta = (r+\omega_+)(1-\rho_+), \quad \delta = (\ell+\omega_+)\rho_+$$

- Fugacities:

$$z_\sharp \equiv z(\rho_\sharp) = \frac{\rho_\sharp}{1-\rho_\sharp}$$

- Sandow function [Sandow, 1994]

$$\kappa_\pm(x,y) := \frac{1}{2x}(y-x+r-\ell \pm \sqrt{(y-x+r-\ell))^2+4xy})$$

$$\kappa_+(\alpha,\gamma) = z_-^{-1}, \quad \kappa_+(\beta,\delta) = z_+$$

$$\kappa_-(\alpha,\gamma) = -\frac{\ell+\omega_-}{r+\omega_-}, \quad \kappa_-(\beta,\delta) = -\frac{\ell+\omega_+}{r+\omega_+}$$

• Invariant matrix product measure (MPM) with generally infinite-dimensional matrices [Derrida et al., 1993]

• Special manifolds

$$\mathcal{B}_N := \{\alpha, \beta, \gamma, \delta \in \mathbb{R}^+ : \kappa_+(\alpha,\gamma)\kappa_+(\beta,\delta) = q^{2N}\}$$

$$\mathcal{B}_N^M := \{\alpha, \beta, \gamma, \delta \in \mathcal{B}_N : \kappa_-(\alpha,\gamma)\kappa_-(\beta,\delta) = q^{-2M}\}, \quad 1 \leq M \leq N$$

⋆ No MPM on $\mathcal{B}_N^M$ for $L \leq N - M + 1$ [Essler and Rittenberg, 1996]

⋆ $(N+1)$-dimensional matrices on manifold $\mathcal{B}_N \setminus \mathcal{B}_N^M$ for any L and on $\mathcal{B}_N^M$ for $L > N - M + 1$ [Mallick and Sandow, 1997]

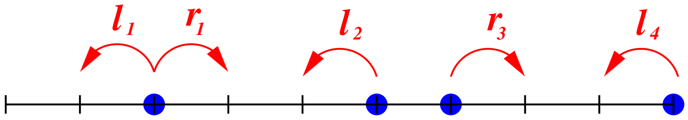
⋆ $M = 1$, $L = N$: Finite blocking measure with strictly increasing marginal fugacities $z_k \propto q^{2k}$ [Bryc and Swieca, 2019]

Shock ASEP

- At most one particle per site on integer lattice with L sites, N particles, single-file jumps, reflecting boundaries

$\mathrm{x} = (x_1, \ldots, x_N)$, $1 \le x_1 < \cdots < x_i < x_{i+1} < \cdots < x_N \le L$

Process	Transition	Rate
Jump of particle i to the right	$x_i \to x_i + 1$	r_i
Jump of particle i to the left	$x_i \to x_i - 1$	ℓ_i



$$r_i = (r - \ell)\frac{\rho_i(1-\rho_i)}{\rho_i - \rho_{i-1}}, \quad \ell_i = (r - \ell)\frac{\rho_{i-1}(1-\rho_{i-1})}{\rho_i - \rho_{i-1}}$$

with pairwise unequal parameters $\rho_i \in (0, 1)$

Proposition (Reversibility of shock ASEP)

The N-particle shock exclusion process with reflecting boundaries is reversible w.r.t. the unnormalized product measure

$$\pi_x^* = \prod_{i=1}^{N} d_i^{2x_i}$$

where

$$d_i := \sqrt{\frac{r_i}{\ell_i}}$$

is the hopping asymmetry of particle i.

Proof: (i) The definition of the shock ASEP implies

$$z_i = q^2 z_{i-1} \qquad (\star)$$

(ii) Straightforward computation shows $G^{rev} = \hat{\pi}^* G^T (\hat{\pi}^*)^{-1} = G$.

□

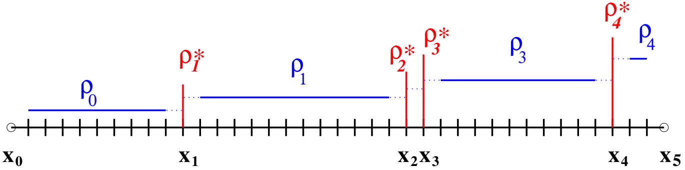
Definition (Bernoulli shock measures)

With auxiliary boundary reservoir sites $x_0 := 0$ *and* $x_{N+1} := L+1$ *the product measure* $\mu_{\boldsymbol{\eta}}^{x} = \prod_{k=1}^{L} p_{\eta_k}^{x}$ *with marginals*

$$p_{\eta_k}^{x} = \begin{cases} (1-\rho_i^\star)(1-\eta_k) + \rho_i^\star \eta_k & k = x_i, \quad 1 \leq i \leq N \\ (1-\rho_i)(1-\eta_k) + \rho_i \eta_k & x_i < k < x_{i+1}, \quad 0 \leq i \leq N \end{cases}$$

is called a Bernoulli shock measure with N *microscopic shocks at positions* $x_i \in \{1, \ldots, L\}$ *and bulk densities* ρ_i *for* $0 \leq i \leq N$*, and shock densities* $\rho_i^\star$ *for* $1 \leq i \leq N$.

$N = 4$



Theorem (One-particle reverse duality)

Let H be the generator of the open ASEP and for parameters ρ_0 and ρ_1 let G be the generator of a simple biased random walk with jump rates r_1, ℓ_1 and reflecting boundaries. Further, let $\mu_{\boldsymbol{\eta}}^{x}$ be the BSM with left bulk density $\rho_0 = \rho_-$ and shock density

$$\rho_1^\star = \frac{\alpha}{\alpha + \gamma}.$$

The generators H and G satisfy the reverse-duality relation

$$HR = RG^T$$

w.r.t. the duality matrix R with matrix elements $R_{\boldsymbol{\eta}x} = d_1^{2x} \mu_{\boldsymbol{\eta}}^{x}$ if and only if the following two conditions are satisfied:
(i) The shock stability condition $(\star)$ is satisfied for $i = 1$,
(ii) The boundary rates are on the manifold $\mathcal{B}_1^1$.

Corollary (Shock random walk)

Denote by $\mu_{\boldsymbol{\eta}}^{x}(t)$ the distribution at time t of the open ASEP, and let Conditions (i) - (ii) of the previous Theorem be satisfied. Then, for any $x \in \{1, \dots, L\}$

$$\mu_{\boldsymbol{\eta}}^{x}(t) = \sum_{y=1}^{L} P(y, t|x, 0)\, \mu_{\boldsymbol{\eta}}^{y}(0)$$

where

$$P(y, t|x, 0) = \frac{d_1^2 - 1}{d_1^{2L} - 1} d_1^{2(y-1)} + \frac{2}{L} \sum_{p=1}^{L-1} d_1^{y-x} \psi_p(x) \psi_p(y) \frac{w}{\epsilon_p} \mathrm{e}^{-\epsilon_p t}$$

with $\epsilon_p = w \left[d_1 + d_1^{-1} - 2\cos\left(\frac{\pi p}{L}\right)\right]$ *and* $\psi_p(y) := d_1 \sin\left(\frac{\pi p y}{L}\right) - \sin\left(\frac{\pi p (y-1)}{L}\right)$ *is the transition probability of the biased random walk starting at time $t = 0$ from x. The limit $\mu_{\boldsymbol{\eta}}^{*} := \lim_{t\to\infty} \mu_{\boldsymbol{\eta}}^{x}(t)$ is the unique invariant measure and is given by the convex combination*

$$\mu_{\boldsymbol{\eta}}^{*} = \frac{d_1^2 - 1}{d_1^{2L} - 1} \sum_{y=1}^{L} d_1^{2(y-1)} \mu_{\boldsymbol{\eta}}^{y}$$

of shock measures $\mu_{\boldsymbol{\eta}}^{y}$.

Remarks

(1) On large scales the drift velocity and diffusion coefficient are given by the rates of the shock exclusion process even if $(\star)$ *is not satisfied* [Ferrari and Fontes (1994)]

(2) The invariant measure of the open ASEP can be expressed by the two-dimensional representation of the stationary matrix product algebra. [Mallick and Sandow, 1997)]

(3) The spectrum of the generator G *given by the eigenvalues* ϵ_p *yields a subset of eigenvalues of the generator* H *of the open ASEP and is in agreement with the picture of spectral properties arising from a shock random walk off the manifold* $\mathcal{B}_1^1$.

[GMS and Domany (1993), Dudziński and GMS (2000); Santen and Appert (2002); de Gier and Essler (2006)]

Theorem (N-particle reverse duality)

Let H be the generator of the open ASEP and for parameters $\rho_0, \ldots, \rho_N$ let G be the generator of the N-particle shock exclusion process. Further, let $\mu_{\boldsymbol{\eta}}^{x}$ be the BSM with left boundary density $\rho_0 = \rho_-$ and shock fugacities

$$z_i^\star = \frac{\alpha}{\gamma} q^{2(i-1)}$$

for $1 \leq i \leq N \leq L$. The reverse-duality relation

$$HR = RG^T$$

w.r.t. the duality matrix R with matrix elements $R_{\boldsymbol{\eta} x} = \pi(x)\mu_{\boldsymbol{\eta}}^{x}$ holds if and only if the following two conditions are satisfied:
(i) The microscopic shock stability condition ($\star$) is satisfied for all $i \in \{1, \ldots, N\}$,
(ii) The boundary rates are on the manifold $\mathcal{B}_N^1$.

Corollaries

(1) The evolution of the open ASEP with an initial BSM with N shocks is given by the transition probabilities of the conservative N-particle shock exclusion process.
(2) The shock ASEP is also intertwining dual of the open ASEP.

Remarks

(1) Spectral properties of the generator H have been obtained from the Bethe ansatz
[Nepomechie (2004); De Gier and Essler (2005); Simon (2009); Crampé et al. (2010)]

(2) The conservative reflective boundaries of the reverse dual are in contrast to the conventional duality for the open SSEP which is dual to the SSEP with nonconservative absorbing boundaries.
[Spohn (1983); Carinci et al. (2013); Frassek et al. (2020)]

(3) A reverse dual with absorbing boundaries exists. *[GMS (2022)]*

Outline of proofs

- To prove reverse duality notice:

(a) Columns of duality matrix R are the BSM probability vectors $|\,\mu^{\mathrm{x}}\,\rangle$

(b) Duality implies invariant subspace spanned by the BSM probability vectors: $H|\,\mu^{\mathrm{x}}\,\rangle \in \mathrm{span}\{|\,\mu^{\mathrm{y}}\,\rangle\}$

$\Rightarrow$ Step 1: Use local transitions to prove that $H|\,\mu^{\mathrm{x}}\,\rangle = \sum_{\mathrm{y}} G_{\mathrm{xy}}|\,\mu^{\mathrm{y}}\,\rangle\}$

$\Rightarrow$ Step 2: Prove by computation that coefficients G_{xy} are nonpositive for $\mathrm{x} \neq \mathrm{y}$ and conserve probability, i.e., $G_{\mathrm{xx}} = -\sum_{\mathrm{x}\neq\mathrm{y}} G_{\mathrm{xy}}$

- To prove explicit time-dependent transition probability for one shock notice that G is a tridiagonal Toeplitz matrix

4. Outlook

• Reverse duality yields detailed microscopic structure of shocks under certain conditions

- microscopically sharp
- random walk of a single shock
- coalescence (bound state) of multiple shocks

$\Rightarrow$ Generalization to $\mathcal{B}_N^M$?

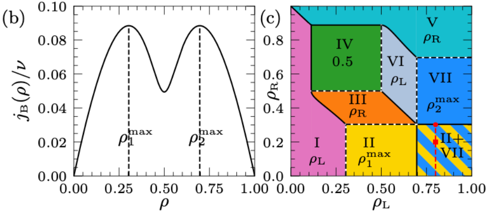
$\Rightarrow$ Underlying symmetry?

• Similar results for ASEP conditioned on atypical current [Belitsky, GMS (2015)]

$\Rightarrow$ Connection to dynamical phase transition, travelling waves, ?

• (reverse) duality in other models with open boundaries?

• Open KLS model ($\delta = 0$, $\epsilon > 0$): Symmetric current-density relation, coexistence in maximal current phase



– Maximal-current coexistence phase

– Downward contact discontinuity

– New phenomenon: Weak pinning $w(t, L) = L^{\alpha} f(t/L^{z})$ with unexpected exponents $\alpha \approx 3/4$, $z \approx 9/4$ [Schweers, Locher, GMS, Maass (2023)]

$\Rightarrow$ Microscopic structure and fluctuations of contact discontinuity?

• Multiple conservation laws?

• ...

This meeting:

Boundary driven systems:

- Hydrodynamic description of open boundaries

- Long-range correlations via duality

- Large deviation theory

Role of conservation laws and travelling waves:

- Microscopic shocks for one conservation law via duality

- Boundary-induced phase transitions for bulk-driven systems with two conservation laws

- Universal features of travelling waves in the absence of a conservation law