Steady-state selection in multi-species driven diffusive systems

Ali Zahra

Joint work with Luigi Cantini

[Arxiv:2309.06231]

IRS 2024 Conference - Institut Henri Poincare

January 24, 2024

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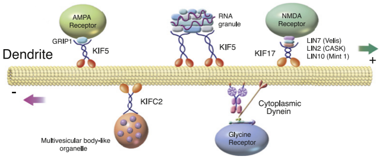
Driven Diffusive Systems

We consider classical many-body systems with short-range interaction and noisy dynamics in 1D. Assume the particles are subject an "external field", so that there is an average current even in a homogenous state. We call such systems **Driven Diffusive Systems**. We refer to the current expression in a homogenous state as **the hydrodynamic current $J(\rho)$**

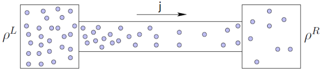


Molecular transport on an axon [Hirokawa 2010]

- Fundamental objects for out-of-equilibrium statistical physics
- Simplest example on the lattice: The Asymmetric simple exclusion process (ASEP) for which the hydrodynamic current is $J(\rho) = (p - q)\rho(1 - \rho)$

Max-Min Principle (Extremal Current Principle)

What happens if you couple a driven diffusive system to réservoirs?



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Extremal current principle: [Krug, Popkov, Schütz, Hager...]

$$j = \begin{cases} \max_{\rho\in[\rho^R,\rho^L]}(J(\rho)) & \text{if } \rho^L > \rho^R \\ \min_{\rho\in[\rho^L,\rho^R]}(J(\rho)) & \text{if } \rho^L < \rho^R \end{cases}$$

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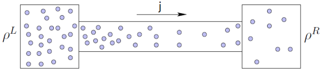

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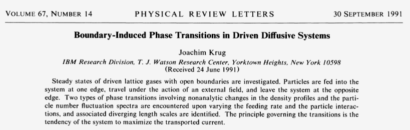
VOLUME 67, NUMBER 14 PHYSICAL REVIEW LETTERS 30 SEPTEMBER 1991

Boundary-Induced Phase Transitions in Driven Diffusive Systems

Joachim Krug

IBM Research Division, T. J. Watson Research Center, Yorktown Heights, New York 10598

(Received 24 June 1991)

Steady states of driven lattice gases with open boundaries are investigated. Particles are fed into the system at one edge, travel under the action of an external field, and leave the system at the opposite edge. Two types of phase transitions involving nonanalytic changes in the density profiles and the particle number fluctuation spectra are encountered upon varying the feeding rate and the particle interactions, and associated diverging length scales are identified. The principle governing the transitions is the tendency of the system to maximize the transported current.

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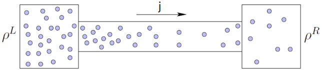

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Boundary-Induced Phase Transitions in Driven Diffusive Systems

EUROPHYSICS LETTERS

Europhys. Lett., **48** (3), pp. 257-263 (1999)

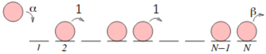
Steady-state selection in driven diffusive systems with open boundaries

V. Popkov[1,2] and G. M. Schütz[1]

[1] *Institut für Festkörperforschung, Forschungszentrum Jülich - 52425 Jülich, Germany*
[2] *Institute for Low Temperature Physics - 310164 Kharkov, Ukraine*

Example: TASEP with open boundaries

$\rho^L = \alpha$ $\qquad\qquad$ $\rho^R = 1 - \beta$



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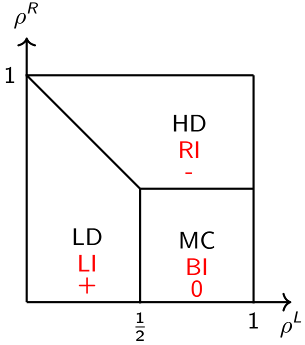

$$J(\rho) = \rho(1-\rho)$$
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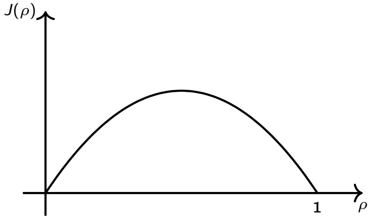

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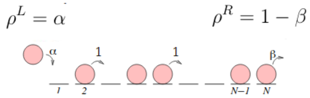

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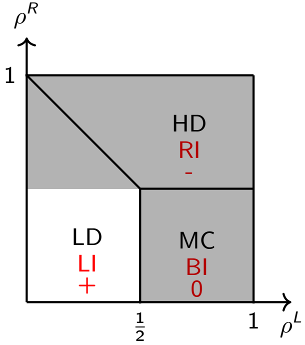

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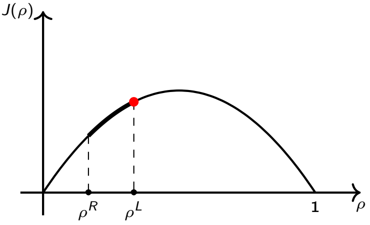

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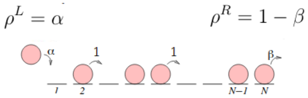

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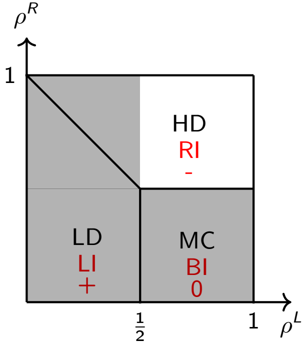

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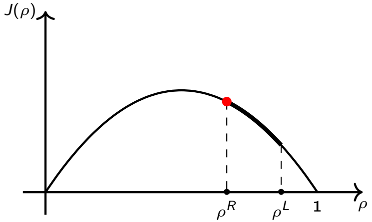

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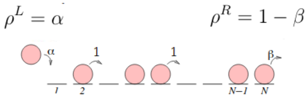

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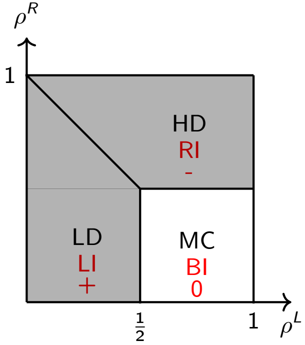

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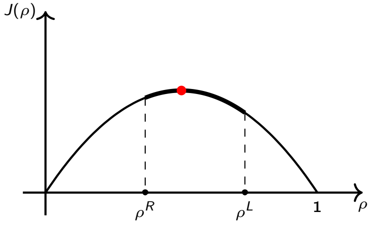

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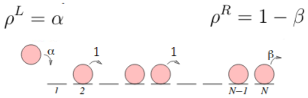

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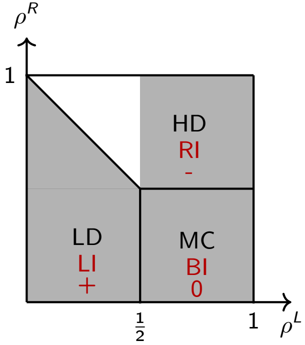

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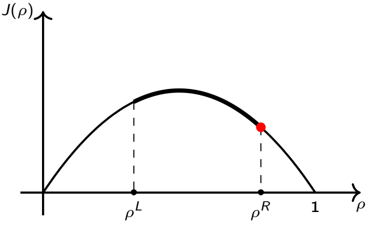

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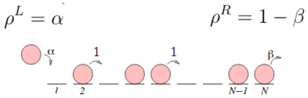

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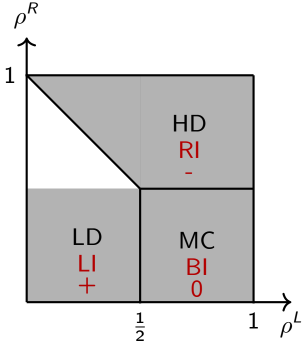

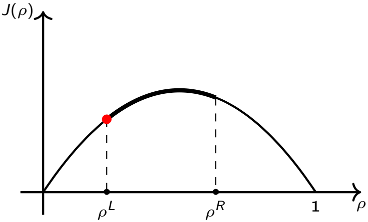

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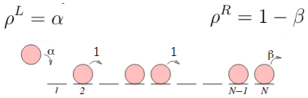

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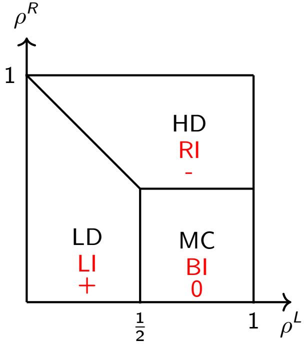

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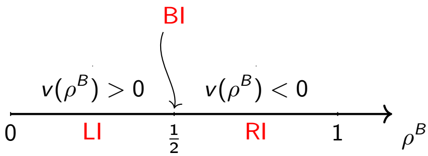

Phase Diagram in ρ^B

A principle for multi-component systems

How to generalize the Max-Min principle to multi-component systems?

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Reformulation [Cantini, Zahra, 2023]

Bulk density and current are derived from the solution at zero of the Riemann problem of the corresponding boundary densities.

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A principle for multi-components systems

Bulk densities and currents are derived from the solution at zero of the Riemann problem of the corresponding boundary densities.

How do you put it into practice?

Problem: In general, we don't know what are the boundary densities, for concrete applications. For lattice models with n species, we can fix the boundary rates:

$$j \xrightarrow{\nu^L_{i,j}} i \qquad i \xrightarrow{\nu^R_{i,j}} j$$

We can write the left and right current as a function of the left and right densities

$$J_i^L(\boldsymbol{\rho}^L) = \sum_{i=1}^{n} \rho_j \nu_{ji}^L - \rho_i \sum_{i=1}^{N} \nu_{ij}^L$$

$$J_i^R(\boldsymbol{\rho}^R) = \sum_{i=1}^{n} \rho_j \nu_{ji}^R - \rho_i \sum_{i=1}^{N} \nu_{ij}^R$$

In the steady state, we have

$$\left.\begin{array}{l} \boldsymbol{J}^L(\boldsymbol{\rho}^L) = \boldsymbol{J}(\boldsymbol{\rho}^B) = \boldsymbol{J}^R(\boldsymbol{\rho}^R) \\ (\boldsymbol{\rho}^L, \boldsymbol{\rho}^R) \xrightarrow{\mathrm{RP_0}} \boldsymbol{\rho}^B \end{array}\right\} \text{Iterative Scheme solution}$$

Can we speak about a phase diagram?

Toy model: The two-TASEP

$$\bullet * \xrightarrow{\beta} * \bullet \qquad * \circ \xrightarrow{\alpha} \circ * \qquad \bullet \circ \xrightarrow{1} \circ \bullet$$

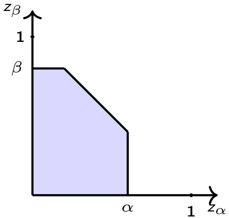
The hydrodynamic currents are found using the Nested Algebraic Bethe Ansatz(N-ABA) [Cantini '08]

$$J_0 = z_\alpha(z_\beta - 1) + \rho_\circ(z_\alpha - z_\beta)$$
$$J_\bullet = z_\beta(1 - z_\alpha) + \rho_\bullet(z_\alpha - z_\beta)$$

Where the z variables are solution of a saddle-point equation:

$$\frac{\rho_\circ}{z_\alpha} + \frac{\rho_\bullet}{z_\alpha - 1} + \frac{1 - \rho_\circ - \rho_\bullet}{z_\alpha - \alpha} = 0$$
$$\frac{\rho_\bullet}{z_\beta} + \frac{\rho_\circ}{z_\beta - 1} + \frac{1 - \rho_\circ - \rho_\bullet}{z_\beta - \beta} = 0$$

$z_\alpha \in [0, min(1, \alpha)]$ and $z_\beta \in [0, min(1, \beta)]$



Hyperbolic System of Coupled Conservation Laws

We assume the hydrodynamic hypothesis and we define coarse grained densities $\rho_\circ(x,t)$ and $\rho_\bullet(x,t)$. We have a System of coupled conservation equations:

$$\partial_t \rho_\circ + \partial_x J_\circ = 0$$
$$\partial_t \rho_\bullet + \partial_x J_\bullet = 0$$

The $z's$ variables happen to be the Riemann variables that "diagonalize" the system: [Cantini Zahra '22]

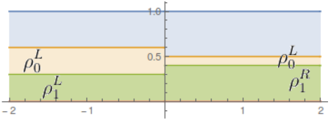
$$\left(\frac{\rho_\circ}{z_\alpha^2} + \frac{\rho_\bullet}{(z_\alpha-1)^2} + \frac{1-\rho_\circ-\rho_\bullet}{(z_\alpha-\alpha)^2}\right)\partial_t z_\alpha + \left(\frac{J_0}{z_\alpha^2} + \frac{J_\bullet}{(z_\alpha-1)^2} - \frac{J_0+J_\bullet}{(z_\alpha-\alpha)^2}\right)\partial_x z_\alpha = 0$$
$$\left(\frac{\rho_\bullet}{z_\beta^2} + \frac{\rho_\circ}{(z_\beta-1)^2} + \frac{1-\rho_\circ-\rho_\bullet}{(z_\beta-\beta)^2}\right)\partial_t z_\beta + \left(\frac{J_\bullet}{z_\beta^2} + \frac{J_0}{(z_\beta-1)^2} - \frac{J_0+J_\bullet}{(z_\beta-\beta)^2}\right)\partial_x z_\beta = 0$$

They can be written in a compact form:

$$\partial_t z_\alpha + v_\alpha(z_\alpha, z_\beta)\partial_x z_\alpha = 0$$
$$\partial_t z_\beta + v_\beta(z_\alpha, z_\beta)\partial_x z_\beta = 0$$

The rarefaction fans

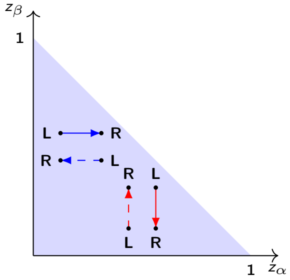
Riemann problem: uniform initial profile with a discontinuity at the origin.



Special solutions (elementary solutions) best characterised by in the z-plane:

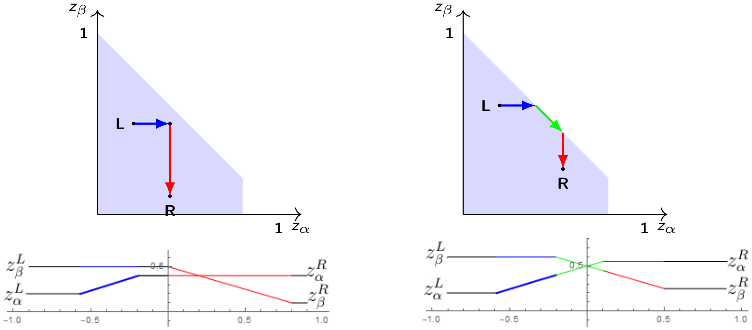
- **Rarafaction fans**: two types α and β +TASEP-like fan
- **Shock solutions** two types α, and β

Rarefaction curves coincide with shock curves: Temple class model



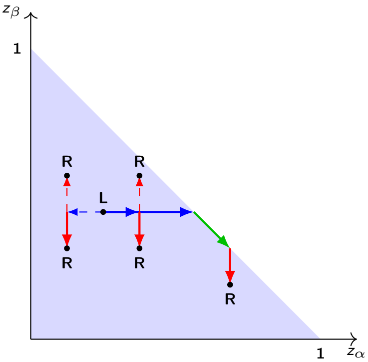
General solutions for the Riemann problem

The arrows allows to navigate in the z space.
Solutions behave according to the relative positions of the points (z_α^L, z_β^L) and (z_α^R, z_β^R)



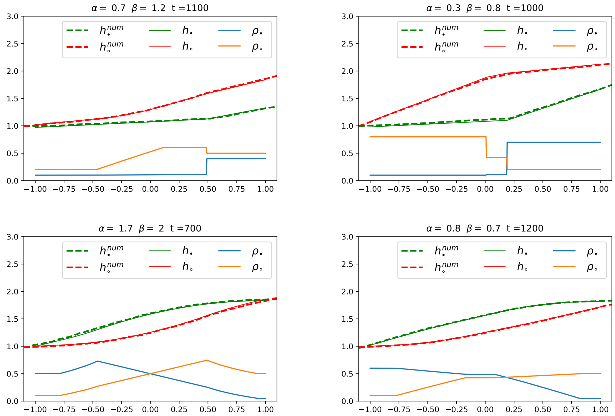
The General solutions

Combining the elementary solutions, we can "navigate" between any two point of the z plane.



Solutions for the density

Some simulations of the integral of the density(h):



Application: Two-Species TASEP with open boundaries

Three exchange rates on each boundary:

$$\boldsymbol{\nu}^L = (\nu^L_{\bullet\circ}, \nu^L_{\bullet *}, \nu^L_{*\circ})$$
$$\boldsymbol{\nu}^R = (\nu^R_{\bullet\circ}, \nu^R_{\bullet *}, \nu^R_{*\circ})$$

Problem: Determining the densities on the boundaries and on the bulk from the rates.

The average currents on the boundaries:

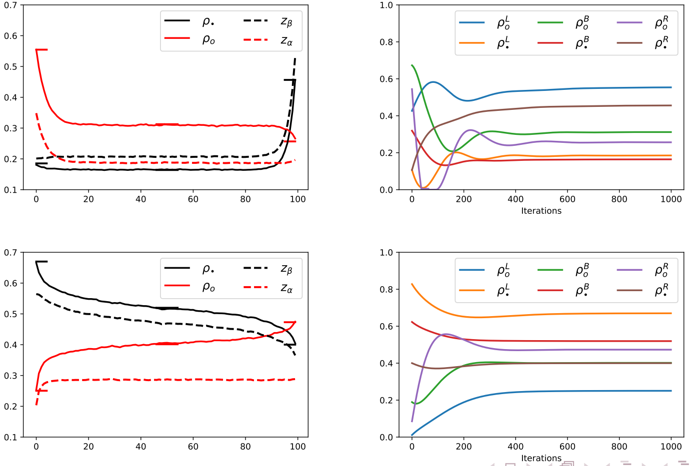
$$J^L_\bullet = \nu^L_{\bullet\circ}\rho^L_\circ + \nu^L_{\bullet *}(1 - \rho^L_\circ - \rho^L_\bullet)$$
$$J^L_\circ = -(\nu^L_{\bullet\circ} + \nu^L_{*\circ})\rho^L_\circ$$
$$J^R_\circ = -\nu^R_{\bullet\circ}\rho^R_\bullet - \nu^R_{*\circ}(1 - \rho^R_\circ - \rho^R_\bullet)$$
$$J^R_\bullet = (\nu^R_{\bullet\circ} + \nu^R_{\bullet *})\rho^R_\bullet$$

In the steady state:

$$\text{The Scheme} \begin{cases} \boldsymbol{J}^L(\boldsymbol{\rho}^L) = \boldsymbol{J}(\boldsymbol{\rho}^B) = \boldsymbol{J}^R(\boldsymbol{\rho}^R) \\ (\boldsymbol{\rho}^L, \boldsymbol{\rho}^R) \xrightarrow{\text{RP}_0} \boldsymbol{\rho}^B \end{cases}$$

Application: Two-species TASEP with open boundaries

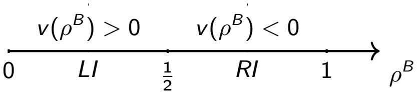
We have 6 equations with 6 variables that we can solve iteratively.



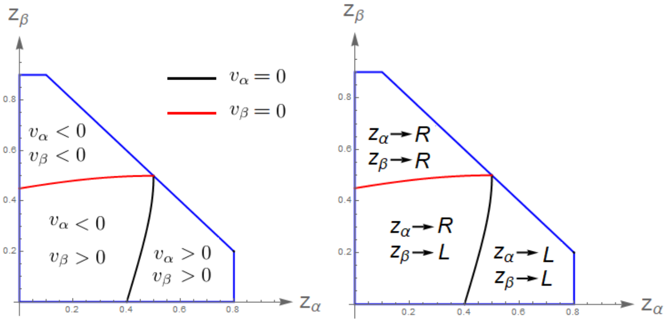
Boundary-induced phase diagram for Two-Species TASEP

The phase diagram is conveniently parameterized by the Riemann variables in the bulk:

- For single-species TASEP:



- For two-species TASEP:

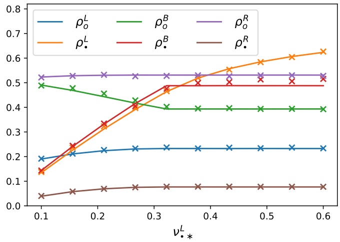


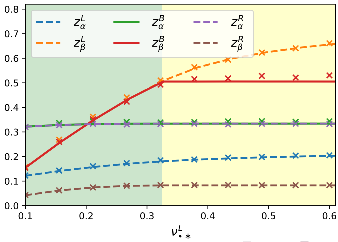
Phase diagram

Hyperbolicity of the conservation laws implies that some **Forbidden Phases**

	$v_\alpha < 0$	$v_\alpha = 0$	$v_\alpha > 0$
$v_\beta < 0$	RR	BR	LR
$v_\beta = 0$	$\times$	BB	LB
$v_\beta > 0$	$\times$	$\times$	LL

Numerical simulations varying $\nu^L_{\bullet *}$. For the green shaded region $v_\beta > 0$, while for the yellow shaded section $v_\beta = 0$. $v_\alpha < 0$ for both regions





Vanishing viscosity approach

We add an infinitesimal diffusion component to the current:

$$\boldsymbol{J}^{total} = \boldsymbol{J}(\boldsymbol{\rho}) - \epsilon D(\boldsymbol{\rho})\frac{\partial \boldsymbol{\rho}}{\partial x}$$

We can derive an ODE for the Riemann variables

$$\frac{\partial \boldsymbol{z}}{\partial x} = \epsilon^{-1} M^{-1} D^{-1}(J(\boldsymbol{z}) - J^{total}) := F(\boldsymbol{z})$$

Where $M_{ij} = \frac{\partial \rho_i}{\partial \xi_j}$. Obviously: $F(\boldsymbol{z}^{\boldsymbol{B}}) = 0$ We linearize the ODE in the neighborhood of the stationary point:

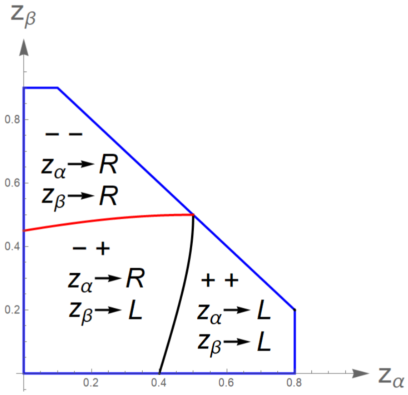
$$\frac{\partial F_i}{\partial \xi_j}(\boldsymbol{\xi}^B) = \epsilon^{-1} d_i^{-1} v_i \delta_{ij}$$

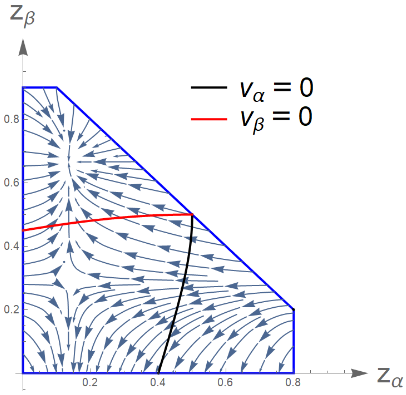
So the phase diagram is again governed by the set $\{v_i\}$:

- **A Sink** $v_i < 0$ for all i, this means that the bulk is driven from right
- **A Source** $v_i > 0$ for all i,this means that the bulk is driven from left.
- **A Saddle Point** $v_i \neq 0$ but have different signs. each z_i will be driven according to the sign of the corresponding v_i
- **Second Order Singularity** if some v_i are zero. The bulk will belong to the intersection of the manifolds $v_i = 0$

Vanishing viscosity approach

Illustration for 2-TASEP for $\alpha = 0.8, \beta = 0.9$





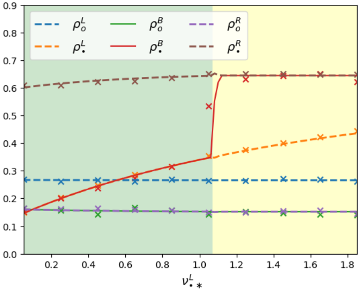
Two-ASEP

$$\nu_{ij} = \begin{cases} 1 & \text{if} \quad i > j \\ q & \text{if} \quad i < j \end{cases}$$

where we have chosen the following order on the species: $\bullet > * > \circ$.

$$J_\bullet = (1-q)\rho_\bullet(1-\rho_\bullet)$$
$$J_\circ = (q-1)\rho_\circ(1-\rho_\circ).$$

- Numerical simulations varying $\nu^L_{\bullet *}$.
- For the green shaded region $v_\bullet > 0$
- For the yellow shaded section $v_\bullet < 0$
- For both regions $v_\circ < 0$

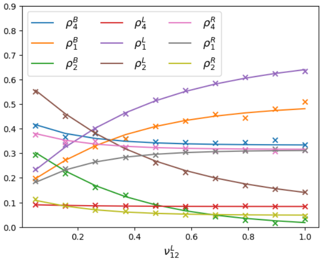


Three-TASEP

The last model we have considered, a 3-species TASEP, contains particles with labels $(1,2,3,4)$, where the type 4 can be seen as empty sites, and bulk hopping rates:

$$ij \xrightarrow{\nu_{ij}} ji \qquad \nu_{ij} = \begin{cases} 0 & \text{if} \quad i > j \\ \nu_{12} & \text{if} \quad (i,j) = (1,2) \\ \nu_{34} & \text{if} \quad (i,j) = (3,4) \\ 1 & \text{otherwise} \end{cases}$$

$$J_1 = J_\bullet(1-\rho_1-\rho_2, \rho_1, 1, \nu_{12})$$
$$J_2 = J_\bullet(\rho_4, \rho_1+\rho_2, \nu_{34}, 1) - J_1$$
$$J_4 = J_\circ(\rho_4, \rho_1+\rho_2, \nu_{34}, 1).$$



Perspective

- Investigating how rigorous the method is
- Relation to integrable boundaries
- Testing on more models with number of species $n > 2$
- Models which are not Temple class?
- Models that do not have convex currents

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