

Large deviations functions and dynamical phase transitions

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LPMA, Paris



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Outline

1 Motivations

2 Kinetically Constrained Models

Cécile Appert-Rolland¹, Estelle Pitard², Frédéric van Wijland³
Juan P. Garrahan⁴, Robert L. Jack⁵

¹LPT, Orsay ²LCVN, Montpellier ³MSC, Paris 7

⁴School of physics and astronomy, Nottingham ⁵Department of physics, Bath

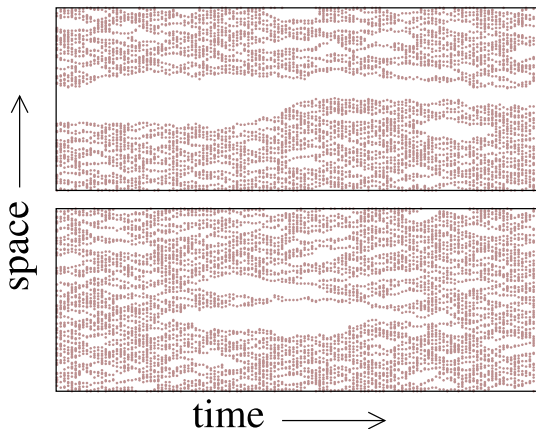
3 Transport models

Cécile Appert-Rolland¹, Thierry Bodineau², Bernard Derrida³,
Alberto Imparato⁴, Frédéric van Wijland⁵
Julien Tailleur⁶, Jorge Kurchan⁷

¹LPT, Orsay ²DMA, Paris ³LPS, Paris ⁴DPA, Aarhus

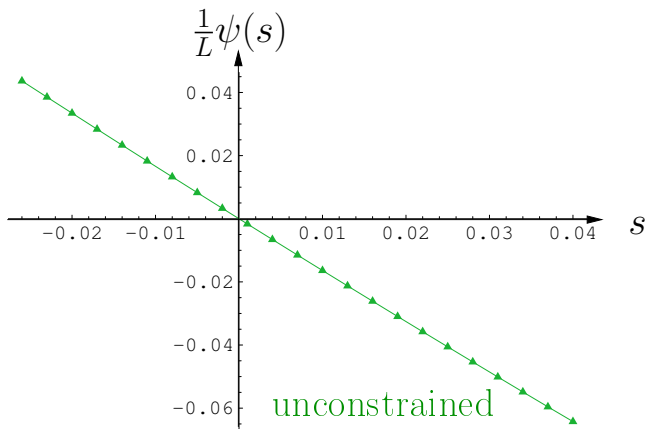
⁵MSC, Paris ⁶School of Physics, Edinburgh ⁷ESPCI, Paris

Space-time “bubbles” of inactivity

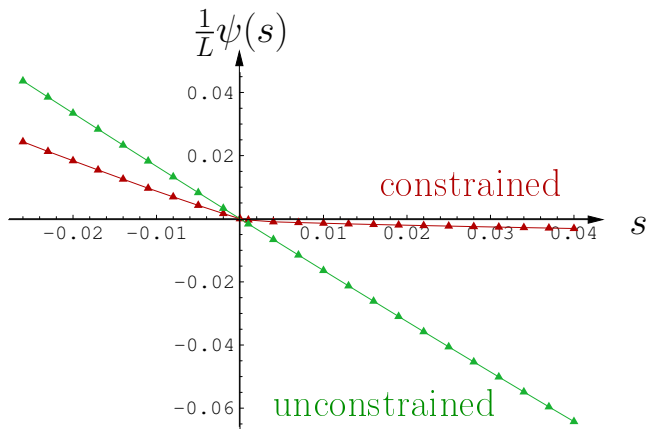


From: Merolle, Garrahan and Chandler, PNAS **102**, 10837 (2005)

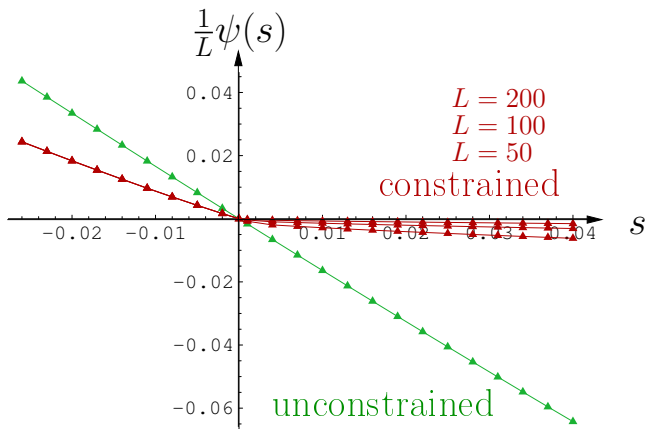
Dynamical phase transition: FA model (d=1)



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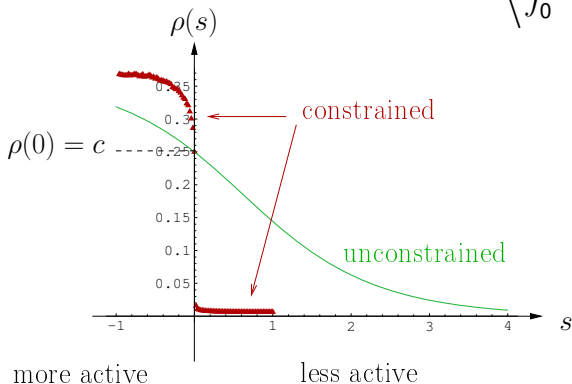
Comparison between **constrained** and **unconstrained** dynamics

Dynamical phase transition: FA model ($d=1$)

Comparison between **constrained** and **unconstrained** dynamics

Dynamical phase transition: FA model (d=1)

$$\rho(s) = \left\langle \int_0^t d\tau \frac{1}{L} \sum_i n_i \right\rangle_s$$



Comparison between **constrained** and **unconstrained** dynamics

Dynamical Landau free energy $\mathcal{F}(\rho, s)$

Probability, in the s -state, to measure
a **time-averaged density** ρ btw. 0 and t $\left| \sim e^{-tL\mathcal{F}(\rho,s)} \right.$

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Extremalization procedure

$$\psi(\mathbf{s}) = - \min_{\rho} \mathcal{F}(\rho, \mathbf{s})$$

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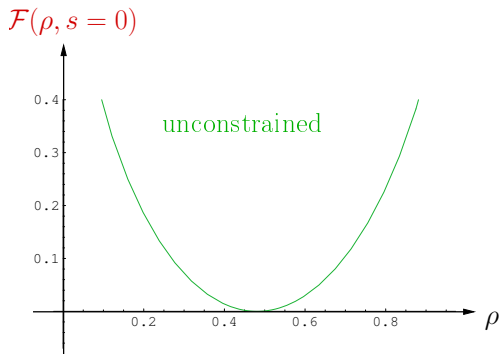
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Minimum reached at $\rho = \rho(\mathbf{s})$:

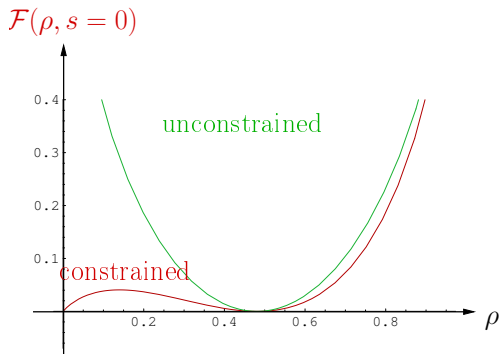
$$\psi(\mathbf{s}) = \mathcal{F}(\rho(\mathbf{s}), \mathbf{s})$$

Dynamical Landau free-energy landscape



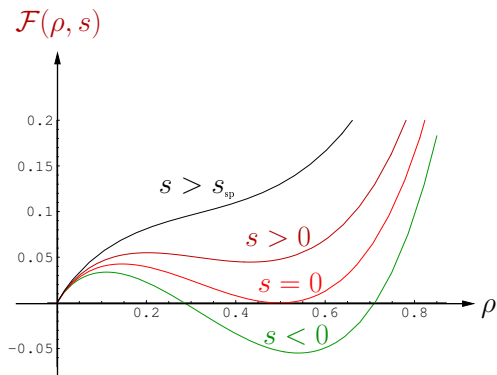
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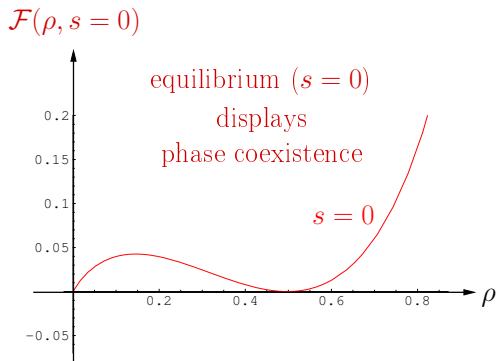
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Dynamical Landau free-energy landscape



$$\psi(s) = - \min_{\rho} \mathcal{F}(\rho, s) = -\mathcal{F}(\rho(s), s)$$

Dynamical Landau free-energy landscape

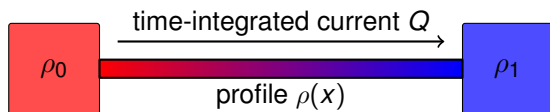


$$\text{Prob}_{[0,t]}(\rho) \sim e^{-tL\mathcal{F}(\rho,s)}$$

Open questions

- Finite-size scaling
- Results in finite dimension
- Measurable ($s = 0$) consequences of the transition, at finite time

Questions



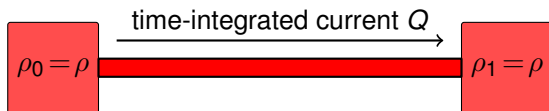
- Non-equilibrium steady-state

$$\text{Prob}[\rho(x)]$$

- (Non-)equilibrium fluctuations of dynamical observables

$$\text{Prob}[Q]$$

Questions



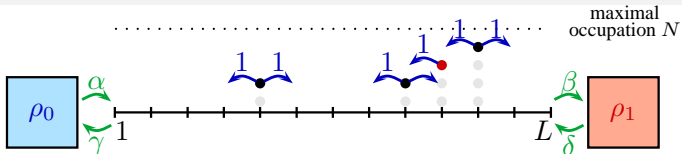
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Exclusion Processes



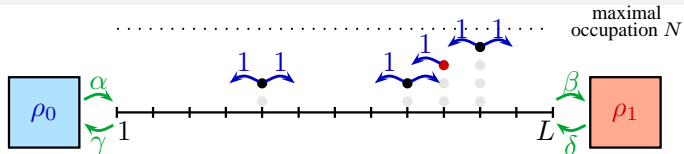
- Configurations: occupation numbers $\{n_i\}$
- Exclusion rule: $0 \leq n_i \leq N$
- Markov evolution

$$\partial_t P(\{n_i\}) = \sum_{n'_i} [W(n'_i \rightarrow n_i) P(\{n'_i\}) - W(n_i \rightarrow n'_i) P(\{n_i\})]$$

- Large deviation function of the time-integrated current Q

$$\langle e^{-sQ} \rangle \sim e^{t\psi(s)} \quad (\Leftrightarrow \text{determining } P(Q))$$

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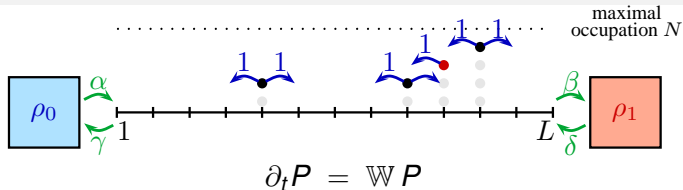
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Operator representation

[Schütz & Sandow PRE 49 2726]



$$\mathbb{W} = \sum_{1 \leq k \leq L-1} [S_k^+ S_{k+1}^- + S_k^- S_{k+1}^+ - \hat{n}_k (1 - \hat{n}_{k+1}) - \hat{n}_{k+1} (1 - \hat{n}_k)]$$

$$+ \alpha [S_1^+ - (1 - \hat{n}_1)] + \gamma [S_1^- - \hat{n}_1]$$

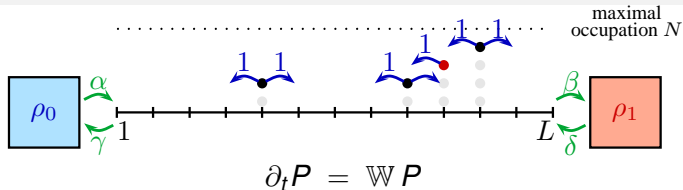
$$+ \delta [S_L^+ - (1 - \hat{n}_L)] + \beta [S_L^- - \hat{n}_L]$$

S^\pm and **creation and annihilation operators:**

$$S^+ |n\rangle = (N - n) |n + 1\rangle \quad S^- |n\rangle = n |n - 1\rangle$$

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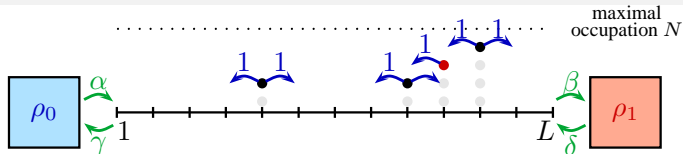
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S^\pm and **creation and annihilation operators:**

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S^\pm and $S^z = \hat{n} - \frac{N}{2}$ are **spin operators** (with $j = \frac{N}{2}$)

Operator representation



$$\langle e^{-sQ} \rangle \sim e^{t\psi(s)} \quad \text{with} \quad \psi(s) = \max \text{Sp } \mathbb{W}(s)$$

$$\begin{aligned} \mathbb{W}(s) = & \sum_{1 \leq k \leq L-1} [S_k^+ S_{k+1}^- + S_k^- S_{k+1}^+ - \hat{n}_k(1 - \hat{n}_{k+1}) - \hat{n}_{k+1}(1 - \hat{n}_k)] \\ & + \alpha [S_1^+ - (1 - \hat{n}_1)] + \gamma [S_1^- - \hat{n}_1] \\ & + \delta [S_L^+ e^s - (1 - \hat{n}_L)] + \beta [S_L^- e^{-s} - \hat{n}_L] \end{aligned}$$

Bethe Ansatz method [\[Appert, Derrida, VL, van Wijland, PRE 78 021122\]](#)

SSEP: maximal occupation $N = 1$
Periodic boundary conditions

Bethe Ansatz method [Appert, Derrida, VL, van Wijland, PRE **78** 021122]

SSEP: maximal occupation $N = 1$

Periodic boundary conditions

Bethe Ansatz:

- eigenvector of components

$$\sum_{\mathcal{P}} \mathcal{A}(\mathcal{P}) \prod_{i=1}^{\mathcal{N}} [\zeta_{\mathcal{P}(i)}]^{x_i}$$

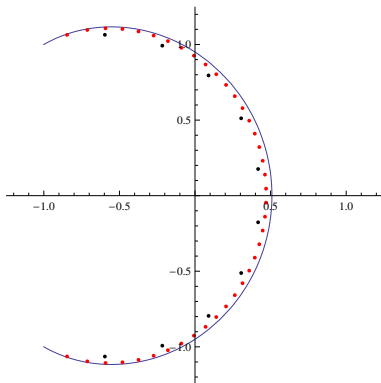
- eigenvalue

$$\psi(\mathbf{s}) = -2\mathcal{N} + \mathbf{e}^{-\mathbf{s}} [\zeta_1 + \dots + \zeta_{\mathcal{N}}] - \mathbf{e}^{\mathbf{s}} \left[\frac{1}{\zeta_1} + \dots + \frac{1}{\zeta_{\mathcal{N}}} \right]$$

- Bethe equations

$$\zeta_i^L = \prod_{\substack{j=1 \\ j \neq i}}^{\mathcal{N}} \left[-\frac{1 - 2\mathbf{e}^{-\mathbf{s}} \zeta_i + \mathbf{e}^{-2\mathbf{s}} \zeta_i \zeta_j}{1 - 2\mathbf{e}^{-\mathbf{s}} \zeta_j + \mathbf{e}^{-2\mathbf{s}} \zeta_i \zeta_j} \right]$$

Bethe Ansatz method [Appert, Derrida, VL, van Wijland, PRE **78** 021122]



Repartition of Bethe roots in the complex plane

Finite-size effects

[Appert, Derrida, VL, van Wijland, PRE **78** 021122]

- large deviation function

$$\psi(\mathbf{s}) = \underbrace{\frac{1}{L}\rho(1-\rho)\mathbf{s}^2}_{\text{order 0}} + \underbrace{L^{-2}\mathcal{F}(u)}_{\text{finite-size}} \quad \text{with} \quad u = -\frac{1}{2}\rho(1-\rho)\mathbf{s}^2$$

- universal function

$$\mathcal{F}(u) = \sum_{k \geq 2} \frac{(-2u)^k B_{2k-2}}{\Gamma(k)\Gamma(k+1)}$$

- scaling of cumulants for the total current

$$\begin{aligned} \frac{1}{t} \langle Q^2 \rangle &\sim L \\ \frac{1}{t} \langle Q^{2k} \rangle &\sim L^{2k-2} \quad (k \geq 2) \end{aligned}$$

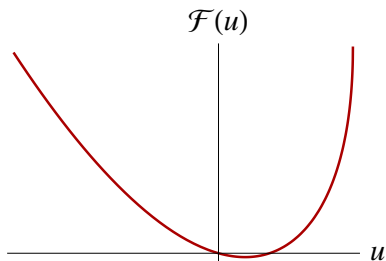
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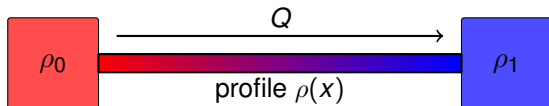
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Macroscopic limit

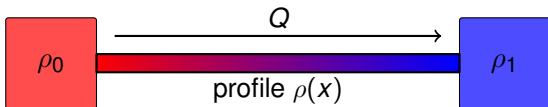
[Tailleur, Kurchan, VL, JPA 41 505001]

Using $SU(2)$ coherent states:

$$\langle \rho_f | e^{t\mathbb{W}} | \rho_i \rangle = \int_{\rho(0)=\rho_i}^{\rho(t)=\rho_f} \mathcal{D}\rho \mathcal{D}\hat{\rho} \exp\{L \underbrace{\mathcal{S}[\hat{\rho}, \rho]}_{\text{action}}\}$$

Macroscopic limit

[Tailleur, Kurchan, VL, JPA 41 505001]

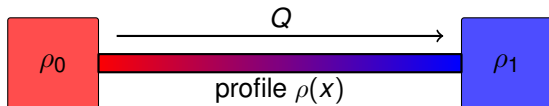
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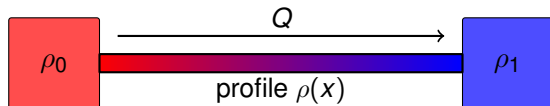
Same $\mathcal{S}_s[\hat{\rho}, \rho]$ as the MSR action of the Langevin evolution:

$$\partial_t \rho = -\partial_x [-\partial_x \rho + \xi]$$

$$\langle \xi(x, t) \xi(x', t') \rangle = \underbrace{\frac{1}{L} \rho(1 - \rho)}_{\text{density-dependent}} \delta(x' - x) \delta(t' - t)$$

Macroscopic limit

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One recovers the action of fluctuating hydrodynamics

[Bertini De Sole Gabrielli Jona-Lasinio Landim]

$\psi(s)$: again[Appert, Derrida, VL, van Wijland, PRE **78** 021122]

Periodic boundary conditions

More general fluctuating hydrodynamics

$$\frac{1}{Lt} \langle Q \rangle \propto D(\rho) \quad (\text{Fourier's law})$$

$$\frac{1}{Lt} \langle Q^2 \rangle_c = \sigma(\rho) \quad (\text{For the SSEP, } \sigma = \rho(1 - \rho))$$

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Saddle point evaluation

$$\langle e^{-sQ} \rangle \sim \int \mathcal{D}\rho \mathcal{D}\hat{\rho} \exp\{L S_s[\hat{\rho}, \rho]\}$$

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[Appert, Derrida, VL, van Wijland, PRE 78 021122]

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Large deviation function

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Correspondence between
(Gaussian) integration of small fluctuations
AND
discreteness of Bethe root repartition.

More general?

With a field

[Appert, Derrida, VL, van Wijland, PRE **78** 021122]

Periodic boundary conditions

Driving field E

With a field

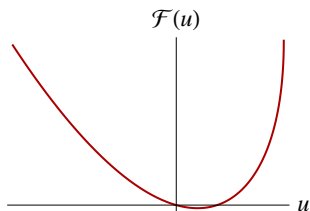
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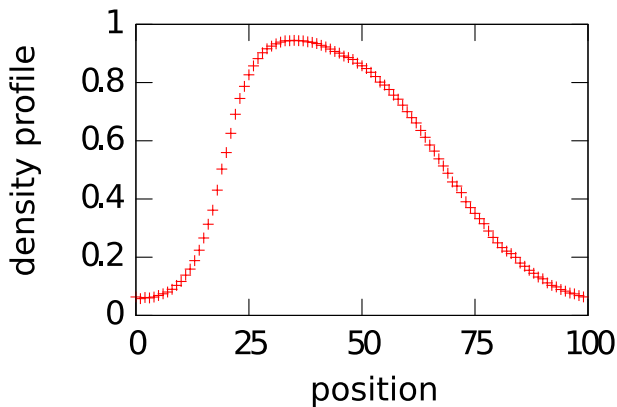
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Dynamical phase transition
between
stationary and non-stationary
profiles

After the transition

(numerical approach)



Non-steady and non-uniform density profile

Microscopic approach [Imparato, VL, van Wijland, PTP **184** 276 (2010)]

Large deviations of the current

$$\psi(\mathbf{s}) = \max_{\text{Sp}} \mathbb{W}(\mathbf{s})$$

$$\mathbb{W}(\mathbf{s}) = \overbrace{\sum_{1 \leq k \leq L-1} \vec{S}_k \cdot \vec{S}_{k+1}}^{\text{invariant by rotation}}$$

$$+ \alpha [S_1^+ - (1 - \hat{n}_1)] + \gamma [S_1^- - \hat{n}_1]$$

$$+ \delta [S_L^+ e^{\mathbf{s}} - (1 - \hat{n}_L)] + \beta [S_L^- e^{-\mathbf{s}} - \hat{n}_L]$$

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Local transformation

$$\mathcal{Q}^{-1} \mathbb{W}(\mathbf{s}) \mathcal{Q} = \sum_{1 \leq k \leq L-1} \vec{S}_k \cdot \vec{S}_{k+1}$$

$$+ \alpha' [S_1^+ - (1 - \hat{n}_1)] + \gamma' [S_1^- - \hat{n}_1]$$

$$+ \delta' [S_L^+ e^{\mathbf{s}'} - (1 - \hat{n}_L)] + \beta' [S_L^- e^{-\mathbf{s}'} - \hat{n}_L]$$

describes contact with reservoirs of same densities

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Local transformation Fluctuations@eq \leftrightarrow Fluctuations@non-eq

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describes contact with reservoirs of same densities

Macroscopic approach

[Imparato, VL, van Wijland, **PRE** 80 011131]

$$\langle e^{-sQ} \rangle \sim \int \mathcal{D}\rho \mathcal{D}\hat{\rho} \exp\{L\mathcal{S}_s[\hat{\rho}, \rho]\}$$

Fluctuations $\phi, \hat{\phi}$ around the saddle

$$\rho(\mathbf{x}, t) = \rho_c(\mathbf{x}) + \phi(\mathbf{x}, t)$$

$$\hat{\rho}(\mathbf{x}, t) = \hat{\rho}_c(\mathbf{x}) + \hat{\phi}(\mathbf{x}, t)$$

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Mapping of non-eq. fluctuations $\phi, \hat{\phi}$ to eq. fluctuations $\phi', \hat{\phi}'$

$$\phi(\mathbf{x}, t) = (\partial_x \hat{\rho}_c)^{-1} \phi'(\mathbf{x}, t) + (\partial_x \rho_c)^{-1} \hat{\phi}'(\mathbf{x}, t)$$

$$\hat{\phi}(\mathbf{x}, t) = (\partial_x \hat{\rho}_c) \hat{\phi}'(\mathbf{x}, t)$$

Macroscopic approach

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Fluctuations $\phi, \hat{\phi}$ around the saddle

$$\rho(\mathbf{x}, t) = \rho_c(\mathbf{x}) + \phi(\mathbf{x}, t) \qquad \hat{\rho}(\mathbf{x}, t) = \hat{\rho}_c(\mathbf{x}) + \hat{\phi}(\mathbf{x}, t)$$

Mapping of non-eq. fluctuations $\phi, \hat{\phi}$ to eq. fluctuations $\phi', \hat{\phi}'$

$$\phi(\mathbf{x}, t) = (\partial_x \hat{\rho}_c)^{-1} \phi'(\mathbf{x}, t) + (\partial_x \rho_c)^{-1} \hat{\phi}'(\mathbf{x}, t)$$

$$\hat{\phi}(\mathbf{x}, t) = (\partial_x \hat{\rho}_c) \hat{\phi}'(\mathbf{x}, t)$$

Large deviation function

$$\psi(\mathbf{s}) = \underbrace{\frac{1}{L} \mu(\mathbf{s})}_{\text{saddle}} + \underbrace{\frac{D}{8L^2} \mathcal{F} \left(\frac{\sigma''}{2D^2} \mu(\mathbf{s}) \right)}_{\text{fluctuations}} \quad \text{same } \mathcal{F} \text{ as at eq.}$$

Macroscopic approach

[Imparato, VL, van Wijland, **PRE** 80 011131]

Physical remark

In contact with reservoirs, neither SSEP nor KMP present a 'dynamical phase transition' (\Leftarrow no singularity in $\psi(s)$).

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one way to compute these finite-size corrections to **saddle**:

- start from $\mathbb{W}(\mathbf{s})$
- use coherent states to obtain a *spatially-discrete* action $S_s[\rho, \hat{\rho}]$
- solve the *spatially-discrete* stationary saddle-point equations

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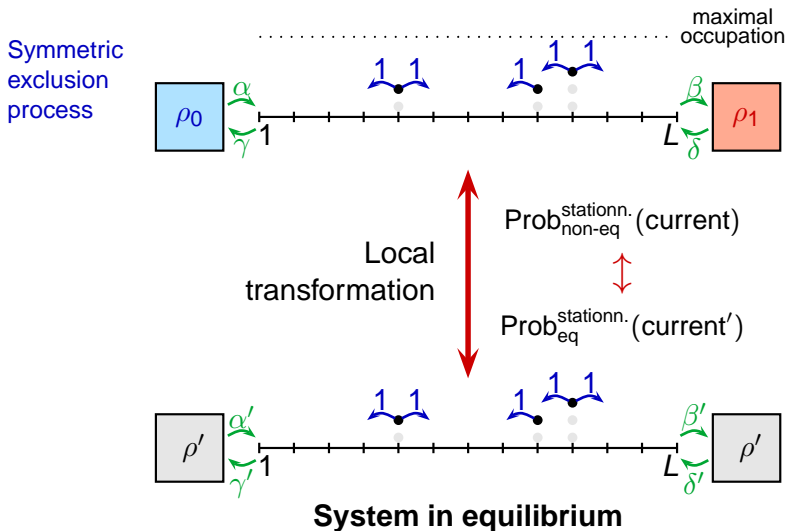
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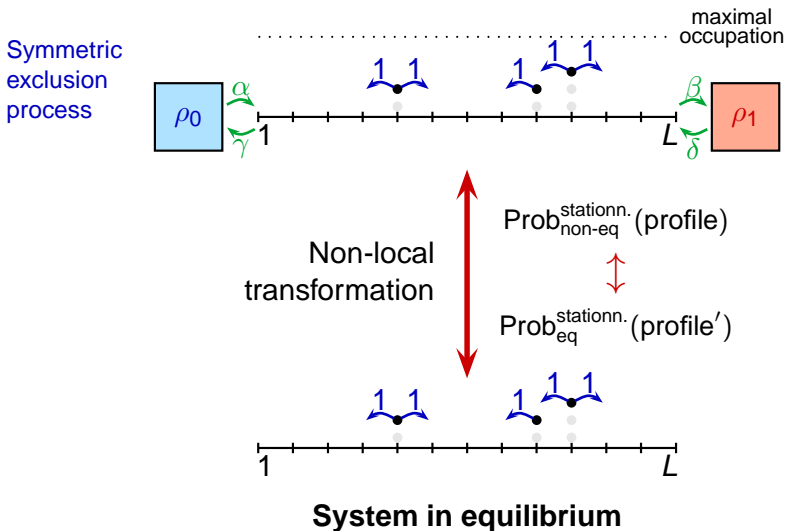
→ How does this translate in the Bethe Ansatz approach?

For the current

[Imparato, VL, van Wijland, **PRE** 80 011131]

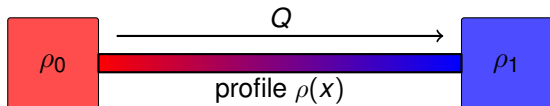
For the density profile

[Tailleur, Kurchan, VL, JPA 41 505001]



Non-local mapping

[Tailleur, Kurchan, VL, JPA **41** 505001]

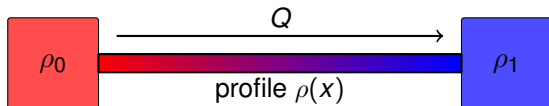


Boundary-driven transport model:

- long-range correlations
- breaking of time-reversal symmetry

Non-local mapping

[Tailleur, Kurchan, VL, JPA **41** 505001]



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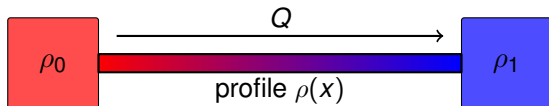
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- yields $\text{Prob}[\rho(x)]$ through a maximisation principle

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[Tailleur, Kurchan, VL, JPA **41** 505001]



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→ Applies to non-equilibrium quantum chains?

Summary

Approach:

- operator formalism
- large deviation function

Extensions:

- fluctuating hydrodynamics
- saddle-point method, instantons
- integration of fluctuations (dynamical phase transition)

Open questions:

- Eq \leftrightarrow non-eq mapping in higher dimensions?
- More generic systems of interacting particles?
- Link btw the eq \leftrightarrow non-eq mappings?
- Crossover to KPZ? Other universal fluctuations?

Other interests

Random manifolds/directed polymers:

- With E. Agoritsas & T. Giamarchi:
roughness of interfaces in short-range correlated disorder
functional renormalization group approach
- With J.-P. Eckmann & T. Giamarchi:
depinning of interfaces with internal degrees of freedom

Fluctuation theorems:

- With R. Garcia-Garcia, A. Kolton, D. Dominguez:
generic symmetries
non-equilibrium fluctuation-dissipation relation