

# Symmetries in large deviations of additive observables: what one gains from forgetting probabilities and turning to the quantum world

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Nice – June 9th 2015

# Classical and quantum dynamics

- Correspondence
  - generator of **stochastic** classical system
  - Hamiltonian of **quantum** XXZ chain

(Well known at least in the stat. mech. community.)
- Use: dictionary between
  - regimes of **large deviations** of *dynamical* observables
  - phases across a Quantum Phase Transition

[particles hopping]

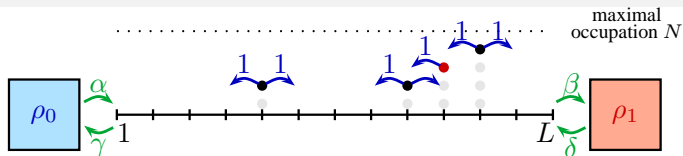
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- Use: dictionary between
  - regimes of **large deviations** of *dynamical* observables
  - phases across a Quantum Phase Transition
- Perspectives opened ; questions raised
  - finite-size effects
  - large/small scale spectrum
  - **import/export techniques from/to stat. mech.**

(I will ask questions to *you*.)

# Exclusion Processes – generic settings



- Configurations: occupation numbers  $\{n_i\}$
- Exclusion rule:  $0 \leq n_i \leq N$
- Markov evolution for the **probability**  $P(\{n_i\}, t)$

$$\partial_t P(\{n_i\}, t) = \sum_{n'_i} [W(n'_i \rightarrow n_i) P(\{n'_i\}, t) - W(n_i \rightarrow n'_i) P(\{n_i\}, t)]$$

- **Large deviation function** of “additive” observables  $A$

$$\langle e^{-sA} \rangle \sim e^{t\psi(s)}$$

( $\Leftrightarrow$  determining  $P(A, t)$ )

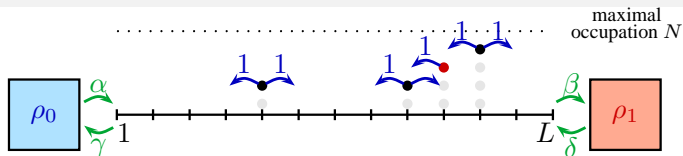
$A$  = total current  $Q$  on time window  $[0, t]$

$$= \# \overrightarrow{\text{jumps}} - \# \overleftarrow{\text{jumps}}$$

$A$  = total activity  $K$  on time window  $[0, t]$

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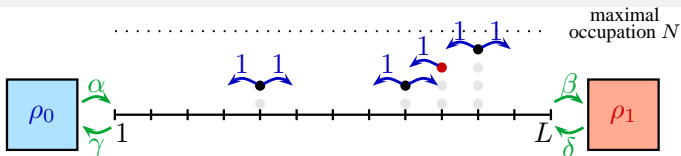
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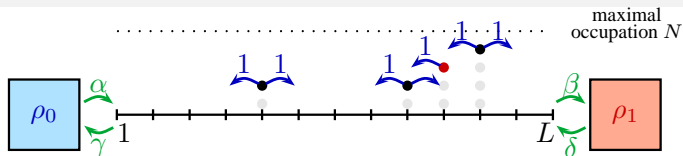
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## Operator representation

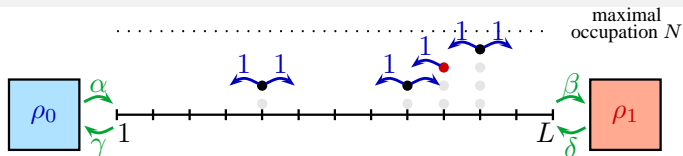
[Schütz & Sandow PRE **49** 2726]Evolution of probability vector  $P$ :

$$\partial_t P = \mathbb{W} P$$

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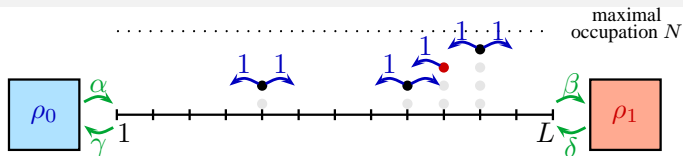
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densities  $\rho_0 = \frac{\alpha}{\alpha + \gamma}$  ;  $\rho_1 = \frac{\delta}{\delta + \beta}$  ; contact rates  $a_0 = \frac{\alpha}{\gamma}$  ;  $a_1 = \frac{\delta}{\beta}$



## Operator representation

[Schütz &amp; Sandow PRE 49 2726]

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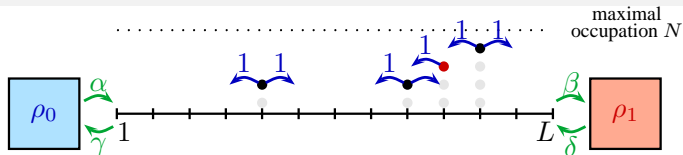
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**XXX spin chain Hamiltonian** (up to boundary terms and constants).

# Operator representation for large deviations

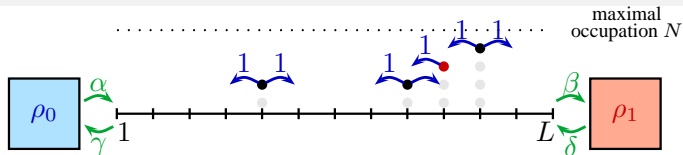


$$\langle e^{-sK} \rangle \sim e^{t\psi(s)} \quad \text{with} \quad \psi(s) = \max \text{Sp } \mathbb{W}_s$$

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for the activity  $K$ : **XXZ spin chain Hamiltonian**

# Operator representation for large deviations



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

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for the **current**  $Q$ : “asymmetric” **XXZ** spin chain **Hamiltonian**

## Example 1: use of rotational symmetry

map non-equilibrium current fluctuations  
to equilibrium current fluctuations

## Mapping non-eq to eq

[Imparato, VL, van Wijland, PTPS 184 276 ]

## Large deviations of the current

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

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

$$+ \alpha [S_1^+ - \check{n}_1] + \gamma [S_1^- - \hat{n}_1]$$

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$$+ \alpha [S_1^+ - \check{n}_1] + \gamma [S_1^- - \hat{n}_1]$$

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

## Local transformation

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

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

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

describes contact with reservoirs of same densities

# SO(3) symmetry

[Imparato, VL, van Wijland, PTPS 184 276 ]

Detailed transformation:

(on **one** site)

$$Q = \mathbf{1} + xS^x - iyS^y + zS^z \quad (\text{invertible})$$

performs a **rotation** of the vector  $\mathbf{S} = (S^x, S^y, S^z)$  of spin operators

$$Q^{-1}S^xQ = (RS)_1 \quad Q^{-1}S^yQ = (RS)_2 \quad Q^{-1}S^zQ = (RS)_3$$

for some SO(3) rotation matrix  $R$ .

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Form of the matrix:

(Cayley form)

$$R = (I + A)(I - A)^{-1}$$

$$A = \begin{pmatrix} 0 & -iz & y \\ iz & 0 & -ix \\ -y & ix & 0 \end{pmatrix}$$



## Large deviations

[Imparato, VL, van Wijland, PTPS 184 276 ]

Result:

(transforming **all** sites)

$$\mathcal{Q}^{-1} \mathbb{W}_{\text{res}}(s; \rho_0, \rho_1; a_0, a_1) \mathcal{Q} = \mathbb{W}_{\text{res}}(s'; \rho'_0, \rho'_1; a_0, a_1)$$

with “primed” variables

$$\rho'_0 = \frac{(1+x)\rho_0 - x - z}{1-x}$$

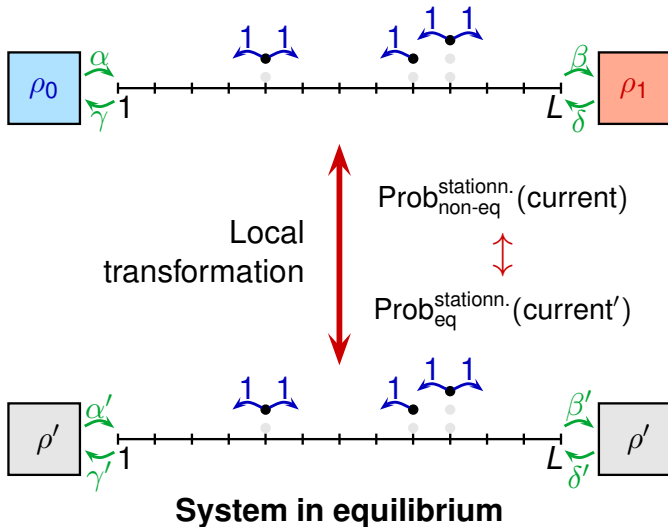
$$\rho'_1 = (x + e^{-s} - z(1 - e^{-s})) \frac{[x + e^s + z(1 - e^s)]\rho_1 - x - z}{1 - x^2}$$

$$e^{-s'} = \frac{x + e^{-s} + z(e^{-s} - 1)}{1 + xe^{-s} + z(e^{-s} - 1)}$$

# Summary

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

Symmetric  
exclusion  
process



# Probabilistic interpretation

Measure  $\hat{P}(\mathbf{n}, s, t)$  biased by  $e^{-sQ}$

Mapping:

$$\begin{aligned} & \hat{P}(\mathbf{n}, s, t; \rho_0, \rho_1; \mathbf{a}_0, \mathbf{a}_1) \\ &= \langle \mathbf{n} | e^{t\mathbb{W}(s; \rho_0, \rho_1; \mathbf{a}_0, \mathbf{a}_1)} | P_{\text{init}} \rangle \\ &= \underbrace{\langle \mathbf{n} | Q}_{\text{new projection state}} e^{t\mathbb{W}(s'; \rho'_0, \rho'_1; \mathbf{a}_0, \mathbf{a}_1)} \underbrace{Q^{-1} | P_{\text{init}} \rangle}_{\text{new initial condition}} \end{aligned}$$

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Question:

What is the mathematical embedding (in terms of process&prob.)?  
(Duality, Radon-Nykodym? **caveat**: prob. not preserved)

Generalization:

- ★ higher dimensions
- ★ generic network and current
- ★ more than two reservoirs
- ★ see also: Derrida & Gerschenfeld ( $\omega$  variable)  
Akkermans, Bodineau, Derrida & Shpielberg (1d LDF for  $d > 1$ )

## Example 2: exclusion process on a ring

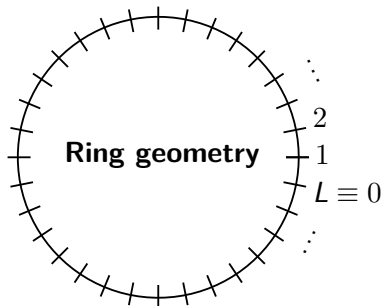
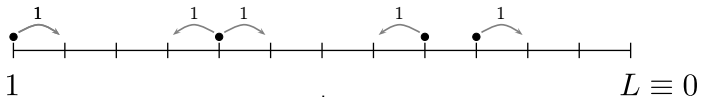
## Focus on a simple situation

**Simple** exclusion process (SSEP): maximal occupation  $N = 1$

Periodic boundary conditions

Fixed total particle number  $N_0$

density:  $\rho_0 = N_0/L$



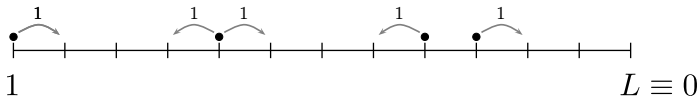
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$$= \frac{L-1}{2} - \frac{e^{-s}}{2} \mathbb{H}_\Delta$$

$$\mathbb{H}_\Delta = - \sum_{k=1}^{L-1} \left[ \sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y + \Delta \sigma_k^z \sigma_{k+1}^z \right] \quad \text{with} \quad \Delta = e^s$$

# Classical/Quantum dictionary

| SSEP  | Quantum Spin Chain  |
|---|---|
| local occupation number $n_k$ ( $1 \leq k \leq L$ )<br>$n_k = 0, 1 \equiv \circ, \bullet$ | local spin $\sigma_k^z$ ( $1 \leq k \leq L$ )<br>$\sigma_k^z = 1, -1 \equiv \uparrow, \downarrow$ |
| (fixed) total occupation $N_0 \equiv \rho_0 L$  | (fixed) total magnetization $M \equiv m_0 L$  |
| (mesoscopic) density $\rho(x)$ ( $0 \leq x \leq 1$ )                                      | (mesoscopic) magnet. $m(x)$ ( $0 \leq x \leq 1$ )   |



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| (mesoscopic) density $\rho(x)$ ( $0 \leq x \leq 1$ )   | (mesoscopic) magnet. $m(x)$ ( $0 \leq x \leq 1$ )   |
| evolution operator<br>$\mathbb{W}_s = \frac{L-1}{2} - \frac{e^{-s}}{2} \mathbb{H}_\Delta$                          | ferromagnetic XXZ Hamiltonian ( $J_{xy} = -1$ )<br>$\mathbb{H}_\Delta = \sum_{k=1}^{L-1} \left[ J_{xy} (\sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y) + J_z \sigma_k^z \sigma_{k+1}^z \right]$<br>$= - \sum_{k=1}^{L-1} \left[ \sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y + \Delta \sigma_k^z \sigma_{k+1}^z \right]$ |
| counting factor $\Delta = e^s$ of the activity $K$   | anisotropy $\Delta = -J_z$ along direction Z  |
| cumulant generating function<br>$\psi(s) = \max \text{Sp } \mathbb{W}_s = \frac{L-1}{2} - \frac{e^{-s}}{2} E_L(s)$ | ground state energy<br>$E_L(s) = \min \text{Sp } \mathbb{H}_\Delta$   |

# Bethe Ansatz

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

# Bethe Ansatz

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Coordinate Bethe Ansatz: Integrability known from long ; difficulty:  $L \rightarrow \infty$

- eigenvector of components

$$\sum_{\mathcal{P}} \mathcal{A}(\mathcal{P}) \prod_{i=1}^{N_0} [\zeta_{\mathcal{P}(i)}]^{x_i}$$

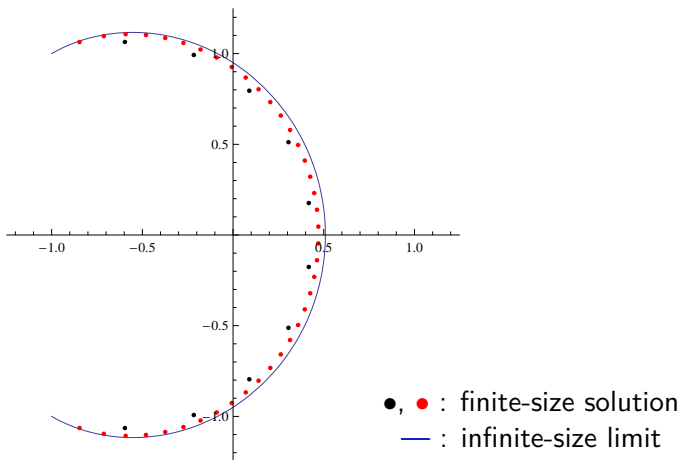
- eigenvalue

$$\psi(s) = -2N_0 + e^{-s} [\zeta_1 + \dots + \zeta_{N_0}] - e^{-s} \left[ \frac{1}{\zeta_1} + \dots + \frac{1}{\zeta_{N_0}} \right]$$

- Bethe equations

$$\zeta_i^L = \prod_{\substack{j=1 \\ j \neq i}}^{N_0} \left[ -\frac{1 - 2e^s \zeta_i + \zeta_i \zeta_j}{1 - 2e^s \zeta_j + \zeta_i \zeta_j} \right]$$

## Bethe Ansatz

[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

$$\psi(s) = \underbrace{-2L\rho_0(1-\rho_0)s}_{\text{order 0}} + \underbrace{L^{-2}\mathcal{F}(u)}_{\text{finite-size}} + \dots \quad \text{with} \quad u = L^2\rho_0(1-\rho_0)s$$

- **universal function** (singular in  $u = \frac{\pi^2}{2}$ )

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

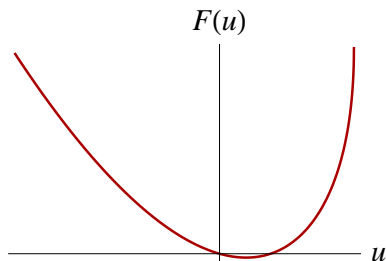
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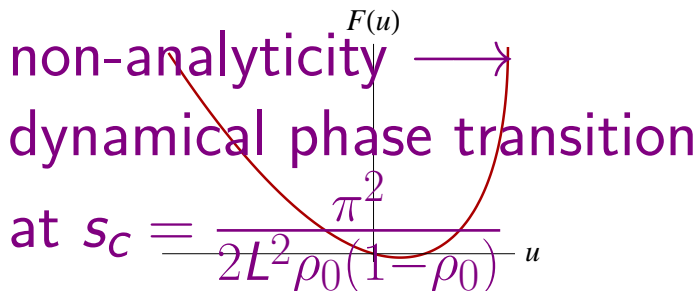
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# Macroscopic limit

a way to derive MFT

A reminder: propagator in quantum mechanics

$$\langle \text{final} | e^{it\mathbb{H}} | \text{initial} \rangle$$



# Macroscopic limit

a way to derive MFT

A reminder: propagator in quantum mechanics

$$\begin{aligned}
 \langle \text{final} | e^{i t \mathbb{H}} | \text{initial} \rangle &= \int dz_1 \dots dz_n \langle \text{final} | e^{i \Delta t \mathbb{H}} | \underline{z}_n \rangle \langle \underline{z}_{n-1} | e^{i \Delta t \mathbb{H}} | \underline{z}_{n-2} \rangle \dots \\
 &\quad \dots \langle \underline{z}_1 | e^{i \Delta t \mathbb{H}} | \text{initial} \rangle \\
 &= \int \mathcal{D}p \mathcal{D}q \exp \left\{ i \frac{1}{\hbar} \underbrace{\mathcal{S}[p, q]}_{\text{action}} \right\}
 \end{aligned}$$

$p = p(x, t)$  and  $q = q(x, t)$

are generically space- & time-dependent **fields**.

“semi-classical limit” recovered in the large  $\frac{1}{\hbar}$  limit

[saddle-point]

# Macroscopic limit

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

For exclusion processes

Using  $SU(2)$  coherent states:

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# Macroscopic limit

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

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Again: use **saddle-point** to handle the large  $L$  limit.

# Macroscopic limit

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

For exclusion processes

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

$$\begin{aligned}\partial_t \rho(x, t) &= -\partial_x \left[ -\partial_x \rho(x, t) + \xi(x, t) \right] \\ \langle \xi(x, t) \xi(x', t') \rangle &= \frac{1}{L} \rho(x, t) (1 - \rho(x, t)) \delta(x' - x) \delta(t' - t)\end{aligned}$$

One recovers the action of fluctuating hydrodynamics

[Spohn; 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

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

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

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Large deviation function

[assuming **uniform** profile  $\rho(x) = \rho$ ]

$$\psi(s) = \underbrace{-s \frac{\langle K \rangle_c}{t}}_{\text{at saddle-point}} + \underbrace{L^{-2} D\mathcal{F}(u)}_{\int \text{ of quadratic fluctuations}} \quad \text{with} \quad u = L^2 s \frac{\sigma(\rho_0) \sigma''(\rho_0)}{8D^2}$$

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

More general?



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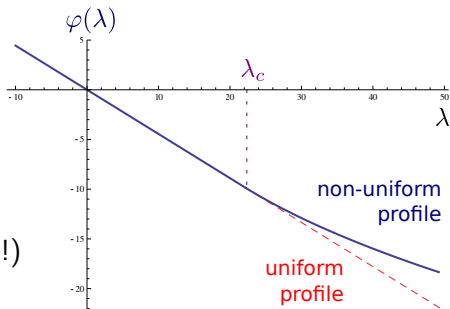
Fluctuating hydrodynamics for quantum chains?

# Dynamical phase transition [VL, Garrahan, van Wijland, JPA **45** 175001]

Rescaling of the large deviation function [singularity at  $\lambda_c > 0$  as  $L \rightarrow \infty$ ]

$$\varphi(\lambda) = \lim_{L \rightarrow \infty} L\psi(\lambda/L^2)$$

Using the correct *non-uniform* saddle-point profile for  $\lambda > \lambda_c$



$$\lambda_c = \frac{\pi^2}{\sigma(\rho_0)}$$

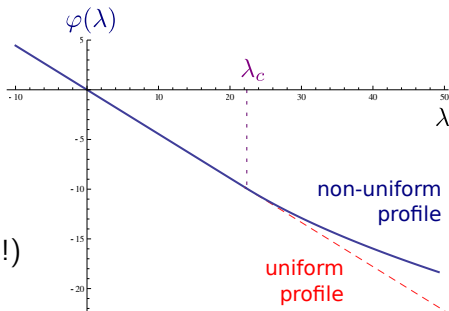
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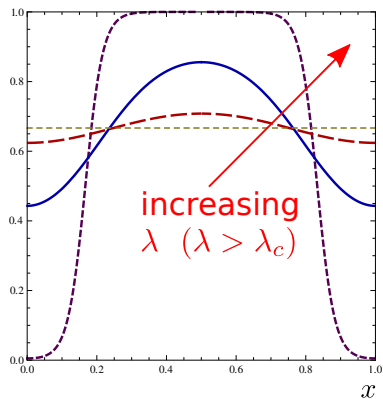
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see also: for LDF of  $Q$   
 [Bodineau, Derrida,  
 PRE **78** 021122]  
 phase transition  
 in WASEP for large dev.  
 (**non-stationary** profile)  
 [Jona-Lasinio *et al.*]  
 generic criterion for  
 instability

# Dynamical phase transition [VL, Garrahan, van Wijland, JPA **45** 175001]

Optimal

saddle-point profile  $\rho(x)$



| SSEP  | Quantum Spin Chain  |
|---|---|
| local occupation number $n_k$ ( $1 \leq k \leq L$ )<br>$n_k = 0, 1 \equiv \circ, \bullet$ | local spin $\sigma_k^z$ ( $1 \leq k \leq L$ )<br>$\sigma_k^z = 1, -1 \equiv \uparrow, \downarrow$ |
| (fixed) total occupation $N_0 \equiv \rho_0 L$  | (fixed) total magnetization $M \equiv m_0 L$  |
| (mesoscopic) density $\rho(x)$ ( $0 \leq x \leq 1$ )                                      | (mesoscopic) magnet. $m(x)$ ( $0 \leq x \leq 1$ )   |
| evolution operator $\mathbb{W}_s$<br>cumulant generating function $\psi(s)$               | ferromagnetic XXZ Hamiltonian $\mathbb{H}_\Delta$<br>ground state energy $E_L(s)$                 |

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| minimal activity phase ( $s \rightarrow +\infty$ )<br>$\bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \circ \circ \circ \circ$  | Ising ferromagnetic order ( $\Delta \rightarrow +\infty$ )<br>$\downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \uparrow \uparrow \uparrow \uparrow \uparrow$   |
| maximal activity phase ( $s \rightarrow -\infty$ )<br>$\bullet \circ \circ \circ \circ \circ \circ \circ \circ \circ \circ \bullet \circ \circ \circ$<br>& $\circ \circ \circ \circ \bullet \circ \circ \circ \bullet \circ \circ \circ \bullet \circ \circ \bullet$ | XY degenerate groundstate ( $\Delta = 0$ )<br>$\downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow$<br>(in fact, superp. of $e^{i\theta} \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \dots$ ) |
| time $t$ (steady state: $t \rightarrow +\infty$ )  | inverse temp. $\beta$ (zero-temp. limit: $\beta \rightarrow +\infty$ )   |
| dynamical partition function<br>$\langle e^{-sK} \rangle \simeq \text{Tr} e^{t\mathbb{W}_s}$   | partition function<br>$Z_\beta^{\text{XXZ}}(\Delta) = \text{Tr} e^{-\beta \mathbb{H}_\Delta}$  |

## Sketch of derivation

[VL, Garrahan, van Wijland, JPA **45** 175001]

Saddle-point equations for the profile  $\rho(x)$  take the form

$$(\partial_x \rho(x))^2 + E_P(\rho(x)) = 0$$



## Sketch of derivation

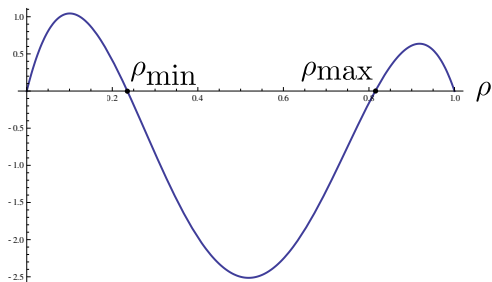
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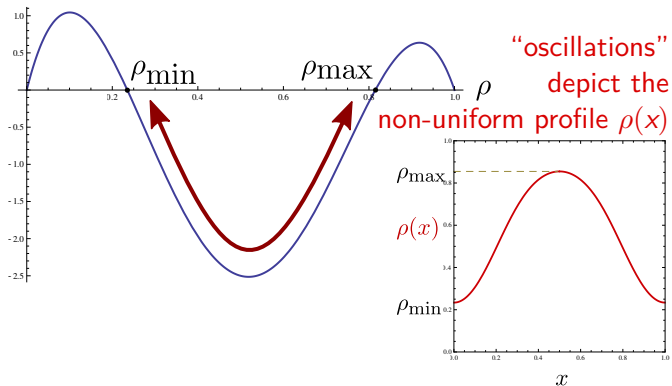
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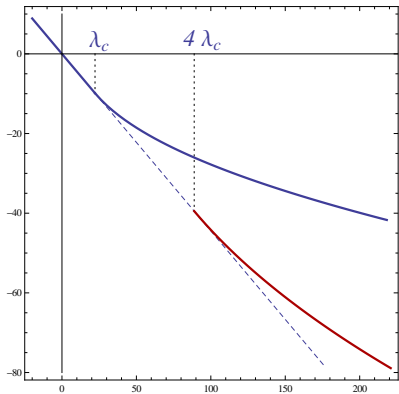
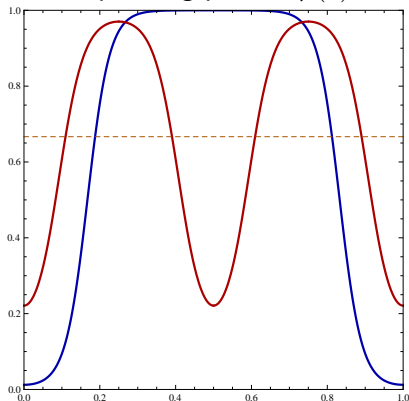
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## Excitations

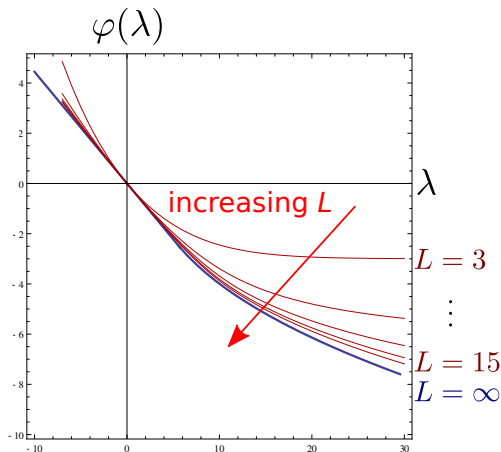
[Cheneau, VL, *work in progress*]What about solutions with *more than one* kink+anti-kink? $\varphi(\lambda)$  $\lambda$ corresponding profiles  $\rho(x)$  $x$

## Small sizes: the ground state

Aim: experimental realizations with cold atoms

→ non-periodic (but isolated, 1D) system

→ smaller sizes & finite-temperature & excited state



# Small sizes: the full spectrum

[preliminary!]

$L = 9$  sites

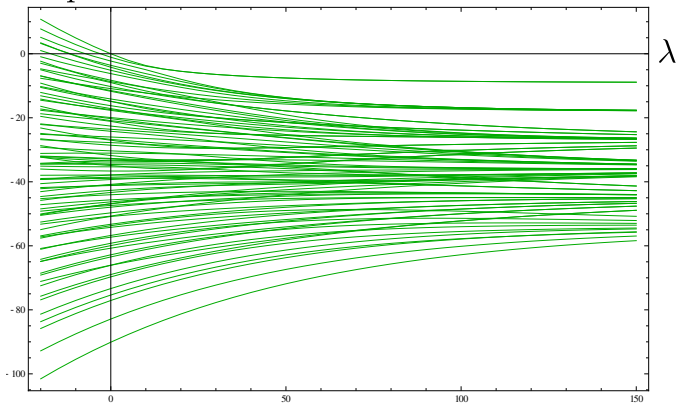
$N_0 = 3$  particles

## Small sizes: the full spectrum

[preliminary!]

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spectrum



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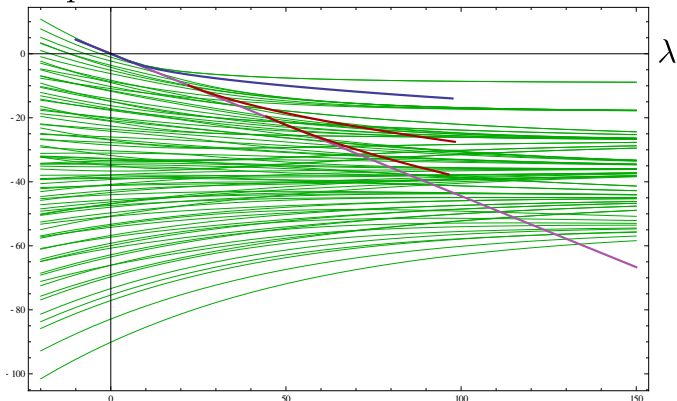
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infinite-size excited states

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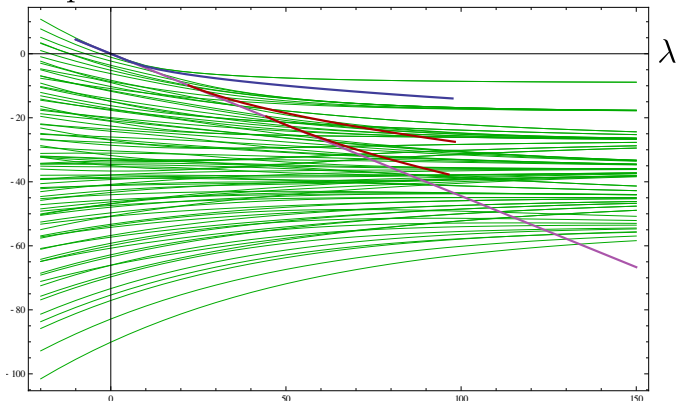
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spectrum

gathering(?) of microscopic eigenvalues  $\rightarrow$  macroscopic ( $L = \infty$ ) states



# Summary

## Microscopic approach:

- ★ operator formalism
- ★ XXZ spin chain
- ★ Bethe Ansatz

## Macroscopic approach:

- ★ MFT, saddle-point method, dynamical phase transition

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## Questions:

- ★ Finite-size crossover around a quantum phase transition? Between:
  - Luttinger Liquid ( $s \rightarrow -\infty$ )
  - Phase-separated ferromagnet ( $s \rightarrow +\infty$ )
- ★ Across the transition: continuum spectrum  $\rightarrow$  gaped spectrum?
- ★ XXZ transition not at  $\Delta = 1$  but at  $\Delta = 1 + \mathcal{O}(L^{-2})$
- ★ Are scaling exponents/functions known? Are they interesting?
- ★ Hydrodynamics approaches for quantum questions?
- ★ Non-Hermitian operators  $\longleftrightarrow$  dissipation in Lindblad?

# Thank you for your attention!

## References:

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