

Exclusion processes and quantum phase transitions in XXZ spin chains.

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Trieste – 15th July 2014

Classical and quantum systems

- Correspondence
 - evolution operator for **stochastic** classical system [particles hopping]
 - Hamiltonian of quantum XXZ chain

(Well known at least in the stat. mech. community.)

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 - phases across a Quantum Phase Transition

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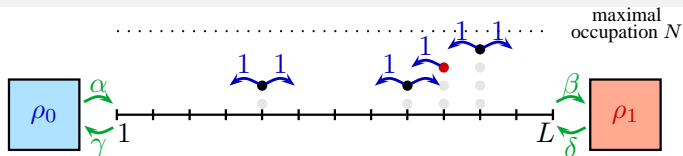
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- Use: dictionary between
 - regimes of **large deviations** of *dynamical* observables
 - phases across a Quantum Phase Transition

- Perspectives opened / questions raised
 - finite-size effects
 - large/small scale spectrum

(I will ask questions to *you*.)

Exclusion Processes – generic settings



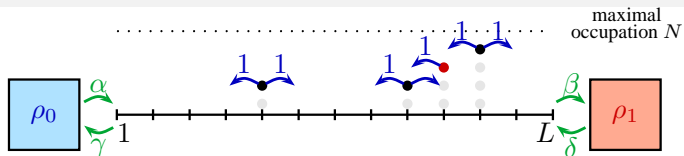
- Configurations: occupation numbers $\{n_i\}$
- Exclusion rule: $0 \leq n_i \leq N$
- Markov evolution for the **probability** $P(\{n_i\}, t)$

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

- **Large deviation function** of time-integrated observables A

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

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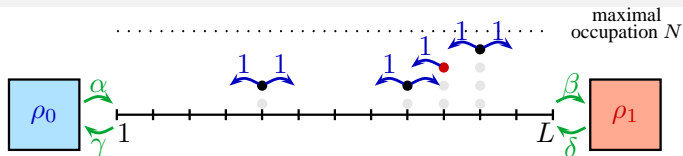
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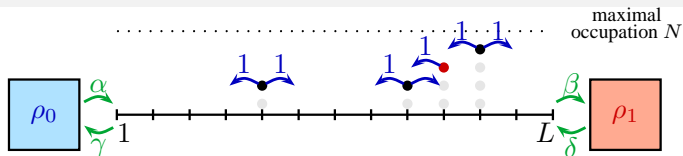
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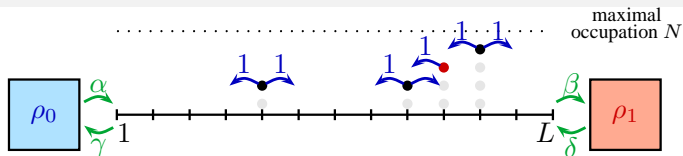
A = total current Q on time window $[0, t]$

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

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

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

Operator representation

[Schütz & Sandow PRE **49** 2726]Evolution of probability vector P :similar to Schrödinger eq.
but eq. for the **probability**
instead of the **wave function**

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

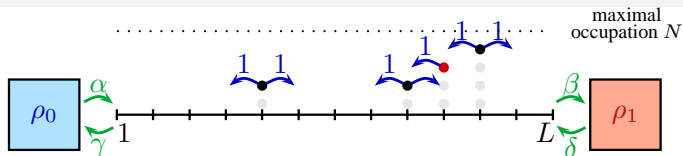
$$\mathbb{W} = \sum_{1 \leq k \leq L-1} [\sigma_k^+ \sigma_{k+1}^- + \sigma_k^- \sigma_{k+1}^+ - \hat{n}_k (1 - \hat{n}_{k+1}) - \hat{n}_{k+1} (1 - \hat{n}_k)]$$

$$+ \alpha [\sigma_1^+ - (1 - \hat{n}_1)] + \gamma [\sigma_1^- - \hat{n}_1]$$

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

$$\sigma^\pm = \sigma^x \pm i\sigma^y \quad \text{and} \quad \sigma^z = \hat{n} - \frac{N}{2} \quad \text{are spin operators (with } j = \frac{N}{2} \text{)}$$

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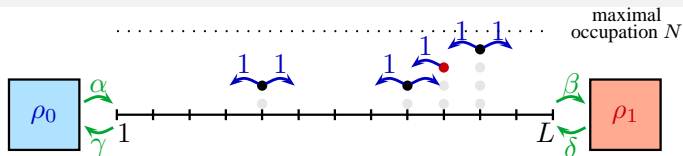
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$\sigma^\pm = \sigma^x \pm i\sigma^y$ and $\sigma^z = \hat{n} - \frac{N}{2}$ are spin operators (with $j = \frac{N}{2}$)

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

Operator representation for large deviations



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

$$\begin{aligned} \mathbb{W}_s = & \sum_{1 \leq k \leq L-1} [e^{-s} \sigma_k^+ \sigma_{k+1}^- + e^{-s} \sigma_k^- \sigma_{k+1}^+ - \hat{n}_k(1 - \hat{n}_{k+1}) - \hat{n}_{k+1}(1 - \hat{n}_k)] \\ & + \alpha [e^{-s} \sigma_1^+ - (1 - \hat{n}_1)] + \gamma [e^{-s} \sigma_1^- - \hat{n}_1] \\ & + \delta [e^{-s} \sigma_L^+ - (1 - \hat{n}_L)] + \beta [e^{-s} \sigma_L^- - \hat{n}_L] \end{aligned}$$

XXZ spin chain Hamiltonian

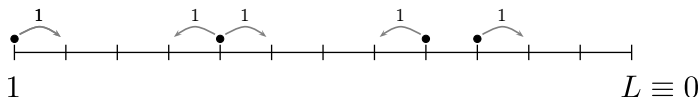
Focus on a simple situation

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

Periodic boundary conditions

Fixed total particle number N_0

density: $\rho_0 = N_0/L$



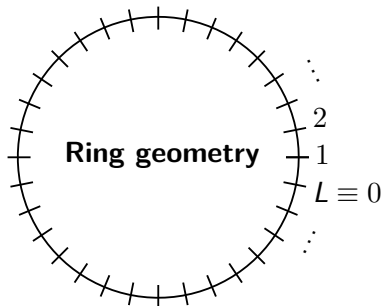
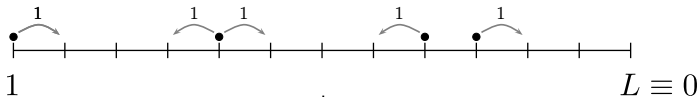
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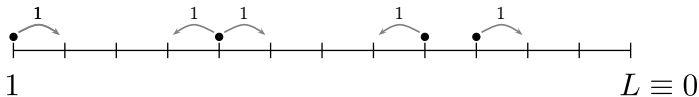
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$$\mathbb{W}_s = \sum_{k=1}^{L-1} \left[e^{-s} (\sigma_k^+ \sigma_{k+1}^- + \sigma_k^- \sigma_{k+1}^+) - \hat{n}_k (1 - \hat{n}_{k+1}) - (1 - \hat{n}_k) \hat{n}_{k+1} \right]$$

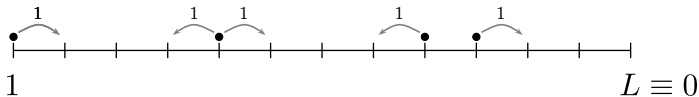
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$$= \frac{L-1}{2} - \frac{e^{-s}}{2} \mathbb{H}_\Delta$$

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

Classical/Quantum dictionary

SSEP	Quantum Spin Chain
local occupation number n_k ($1 \leq k \leq L$) $n_k = 0, 1 \equiv \circ, \bullet$	local spin σ_k^z ($1 \leq k \leq L$) $\sigma_k^z = 1, -1 \equiv \uparrow, \downarrow$
(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 $\mathbb{W}_s = \frac{L-1}{2} - \frac{e^{-s}}{2} \mathbb{H}_\Delta$	ferromagnetic XXZ Hamiltonian ($J_{xy} = -1$) $\mathbb{H}_\Delta = \sum_{k=1}^{L-1} \left[J_{xy} (\sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y) + J_z \sigma_k^z \sigma_{k+1}^z \right]$ $= - \sum_{k=1}^{L-1} \left[\sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y + \Delta \sigma_k^z \sigma_{k+1}^z \right]$
counting factor $\Delta = e^s$ of the activity K	anisotropy $\Delta = -J_z$ along direction Z
cumulant generating function $\psi(s) = \max \text{Sp } \mathbb{W}_s = \frac{L-1}{2} - \frac{e^{-s}}{2} E_L(s)$	ground state energy $E_L(s) = \min \text{Sp } \mathbb{H}_\Delta$

Bethe Ansatz

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

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Bethe Ansatz:

i Do not apply [Kim, PRE **52** 3512] **!**

- eigenvector of components

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

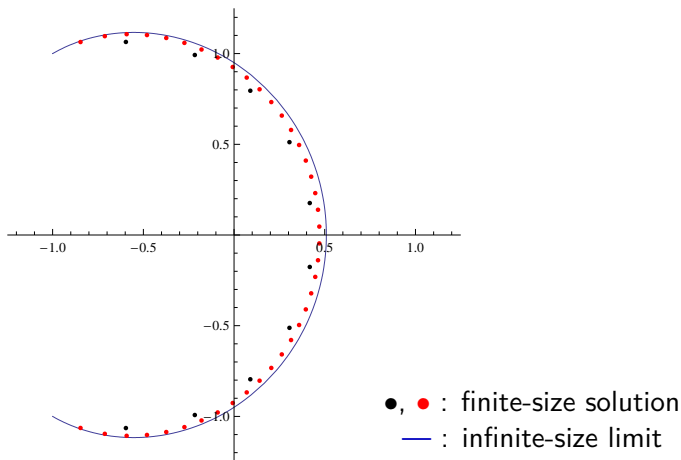
- eigenvalue

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

- 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 $u = \frac{\pi^2}{2}$)

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

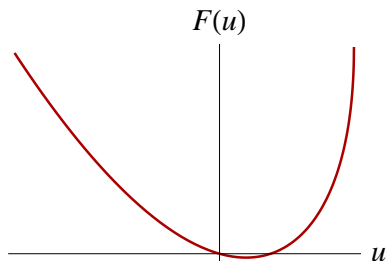
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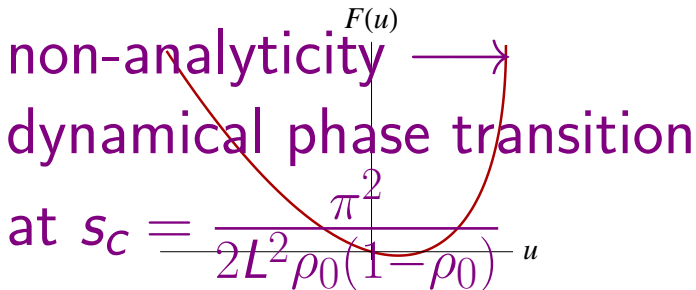
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Macroscopic limit

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

A reminder: propagator in quantum mechanics

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$$\langle \text{final} | e^{it\mathbb{H}} | \text{initial} \rangle = \int dz_1 \dots dz_n \langle \text{final} | e^{i\Delta t\mathbb{H}} | \underline{z_n} \rangle \langle \underline{z_{n-1}} | e^{i\Delta t\mathbb{H}} | \underline{z_{n-2}} \rangle \dots \\ \dots \langle \underline{z_1} | e^{i\Delta t\mathbb{H}} | \text{initial} \rangle$$

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 &\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\}
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 \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:

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

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

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

$$\partial_t \rho(x, t) = -\partial_x \left[-\partial_x \rho(x, t) + \xi(x, t) \right]$$

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

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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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Saddle point evaluation

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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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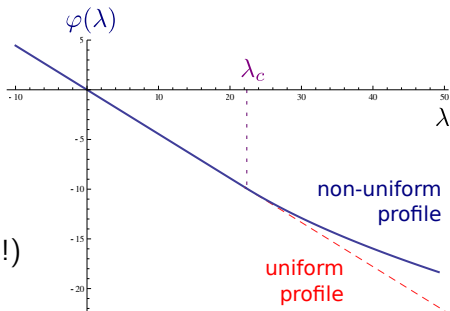
Fluctuating hydrodynamics for quantum chains?

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 $\lambda > \lambda_c$



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

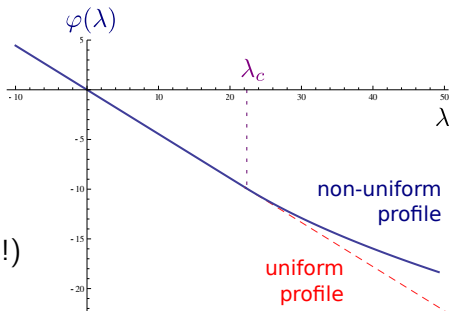
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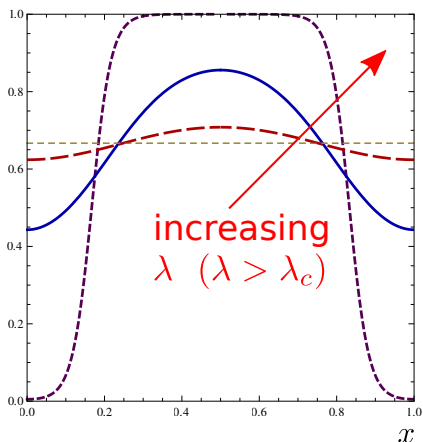
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[Bodineau, Derrida,
PRE **78** 021122]
phase transition
in WASEP for large dev.
of the current Q
(**non-stationary** profile)

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

Optimal (i.e. **saddle-point**) profile

saddle-point profile $\rho(x)$



SSEP	Quantum Spin Chain
local occupation number n_k ($1 \leq k \leq L$) $n_k = 0, 1 \equiv \circ, \bullet$	local spin σ_k^z ($1 \leq k \leq L$) $\sigma_k^z = 1, -1 \equiv \uparrow, \downarrow$
(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 cumulant generating function $\psi(s)$	ferromagnetic XXZ Hamiltonian \mathbb{H}_Δ ground state energy $E_L(s)$

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

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

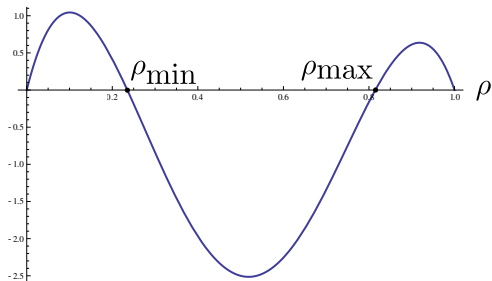
[VL, Garrahan, van Wijland, JPA **45** 175001]

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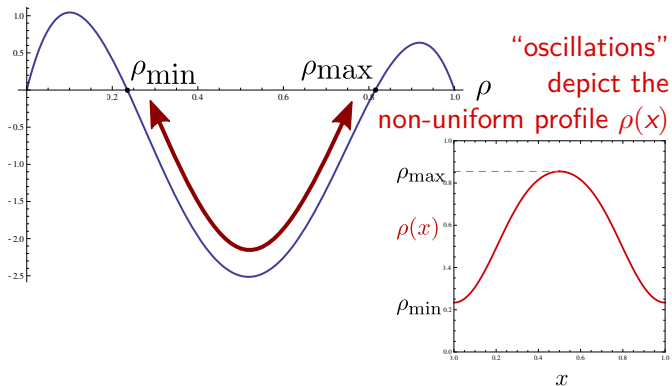
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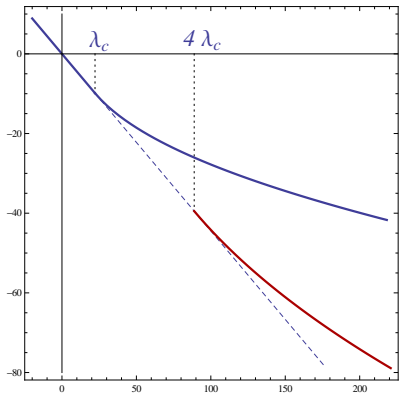
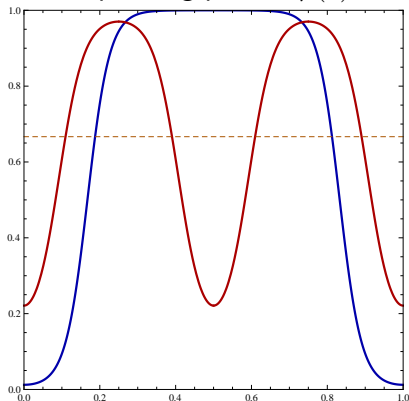
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Excitations

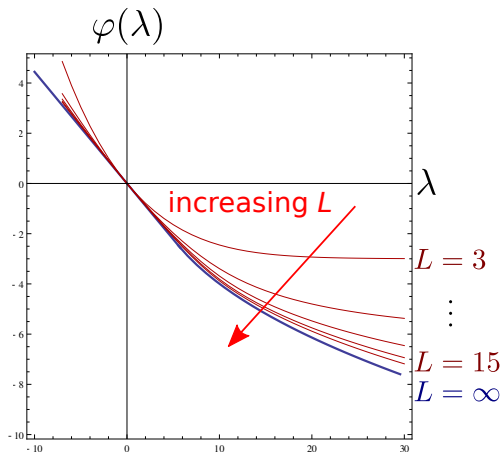
[Cheneau, VL, *work in progress*]What about solutions with *more than one* kink+anti-kink? $\varphi(\lambda)$  λ corresponding profiles $\rho(x)$  x

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

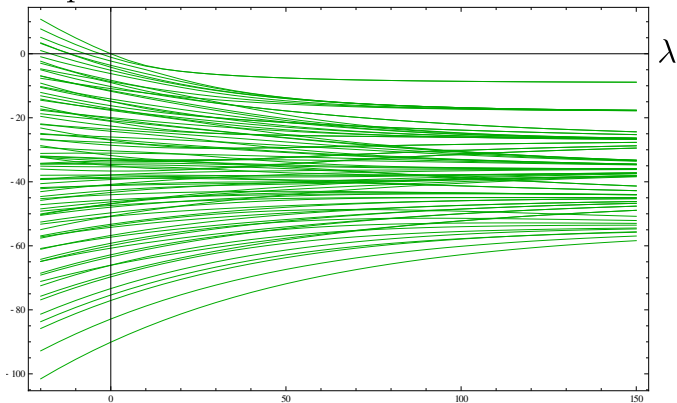
$N_0 = 3$ particles

Small sizes: the full spectrum

[preliminary!]

 $L = 9$ sites $N_0 = 3$ particles

spectrum



Small sizes: the full spectrum

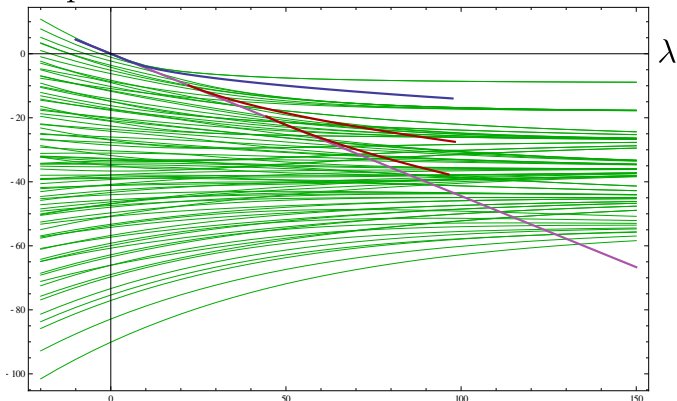
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 $L = 9$ sites $N_0 = 3$ particles

infinite-size ground state

infinite-size excited states

spectrum



Small sizes: the full spectrum

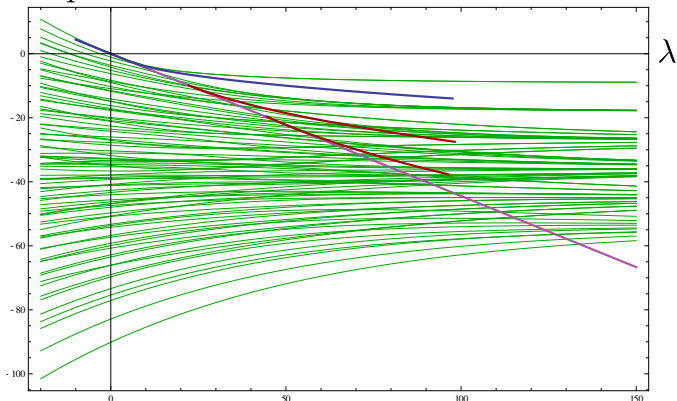
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 $L = 9$ sites $N_0 = 3$ particles

infinite-size ground state

infinite-size excited states

spectrum

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

Summary

Microscopic approach:

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

Macroscopic approach:

- ★ action of fluctuating hydrodynamics
- ★ saddle-point method, dynamical phase transition

Summary

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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?

Thank you for your attention!

References:

- ★ Marc Cheneau, Vivien Lecomte et al.
work in progress (2014)
- ★ Vivien Lecomte, Juan P. Garrahan, Frédéric van Wijland
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- ★ Cécile Appert-Rolland, Bernard Derrida, Vivien Lecomte and
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