Exclusion processes and quantum phase transitions in XXZ spin chains.

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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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- Use: dictionnary between
  - regimes of **large deviations** of *dynamical* observables
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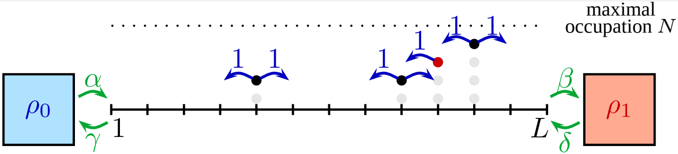
- Perspectives opened / questions raised
  - finite-size effects
  - large/small scale spectrum

  (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** $P(\{n_i\},t)$

$$\partial_t P(\{n_i\},t) = \sum_{n_i'} \left[W(n_i' \to n_i) P(\{n_i'\},t) - W(n_i \to n_i') P(\{n_i\},t) \right]$$

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

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

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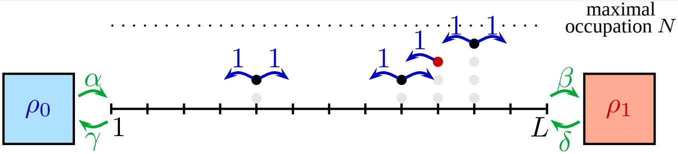

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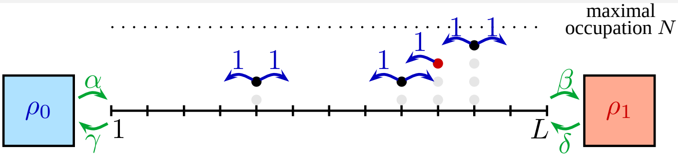

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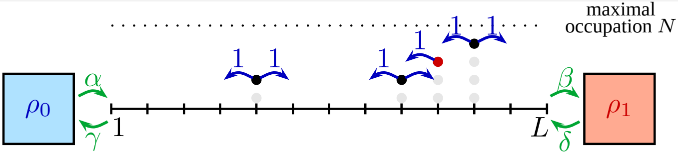

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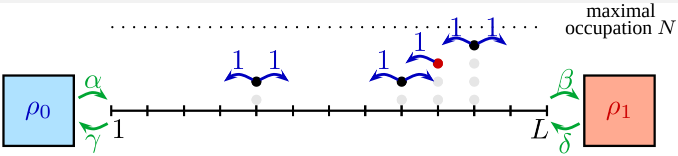
$$A = \text{total current } Q \text{ on time window } [0,t] \qquad = \#\overrightarrow{\text{jumps}} - \overleftarrow{\text{jumps}}$$

$$A = \text{total activity } K \text{ on time window } [0,t] \qquad = \#\overrightarrow{\text{jumps}} + \overleftarrow{\text{jumps}}$$

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**

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

$$\mathbb{W} = \sum_{1\le k\le L-1} \left[\sigma_k^+\sigma_{k+1}^- + \sigma_k^-\sigma_{k+1}^+ - \hat n_k(1-\hat n_{k+1}) - \hat n_{k+1}(1-\hat n_k)\right] + \alpha\left[\sigma_1^+ - (1-\hat n_1)\right] + \gamma\left[\sigma_1^- - \hat n_1\right] + \delta\left[\sigma_L^+ - (1-\hat n_L)\right] + \beta\left[\sigma_L^- - \hat n_L\right]$$

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

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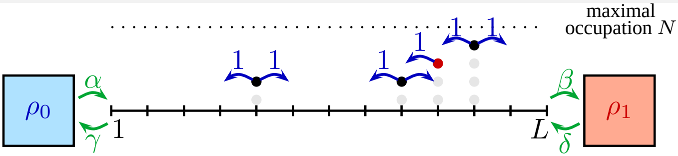

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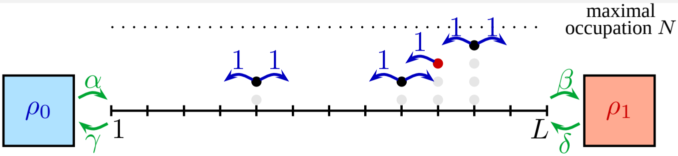
XXX spin chain Hamiltonian (up to boundary terms and constants).

Operator representation for **large deviations**



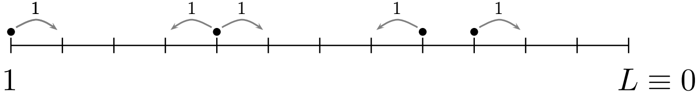
$$\left\langle e^{-sK} \right\rangle \sim e^{t\psi(s)} \qquad \text{with} \qquad \psi(s) = \max \operatorname{Sp} \mathbb{W}_s$$

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

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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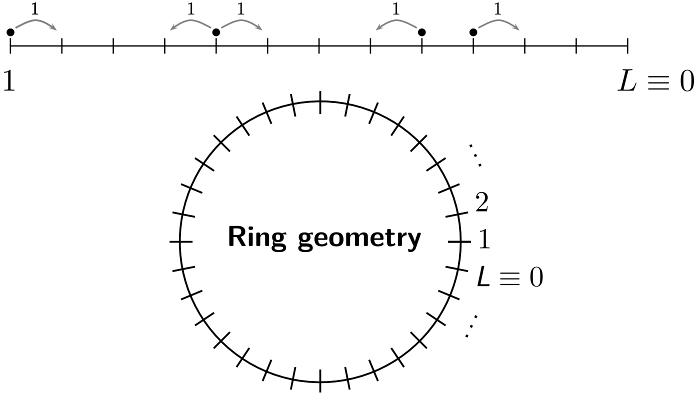

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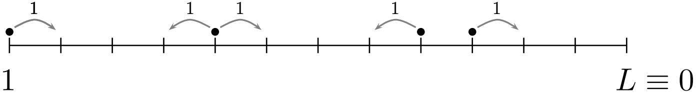

$$\mathbb{W}_s = \sum_{k=1}^{L-1} \Big[e^{-s} \big(\sigma_k^+ \sigma_{k+1}^- + \sigma_k^- \sigma_{k+1}^+ \big) - \hat{n}_k (1 - \hat{n}_{k+1}) - (1 - \hat{n}_k) \hat{n}_{k+1} \Big]$$

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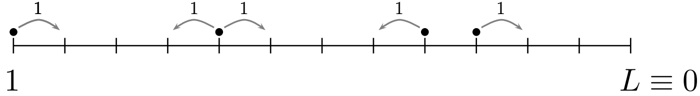

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$$= \frac{L-1}{2} - \frac{e^{-s}}{2} \mathbb{H}_\Delta$$

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

Classical/Quantum dictionnary

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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(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 $\mathbb{W}_s = \frac{L-1}{2} - \frac{e^{-s}}{2}\mathbb{H}_\Delta$	ferromagnetic XXZ Hamiltonian $(J_{xy} = -1)$ $\mathbb{H}_\Delta = \sum_{k=1}^{L-1} \Big[J_{xy}\big(\sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y\big) + J_z \sigma_k^z \sigma_{k+1}^z \Big]$ $= -\sum_{k=1}^{L-1} \Big[\sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y + \Delta \sigma_k^z \sigma_{k+1}^z \Big]$
counting factor $\Delta = e^s$ of the activity K	anisotropy $\Delta = -J_z$ along direction Z
cumulant generating function $\psi(s) = \max \mathrm{Sp}\, \mathbb{W}_s = \frac{L-1}{2} - \frac{e^{-s}}{2} E_L(s)$	ground state energy $E_L(s) = \min \mathrm{Sp}\, \mathbb{H}_\Delta$

Bethe Antsatz

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

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Bethe Ansatz:

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

- eigenvector of components

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

- eigenvalue

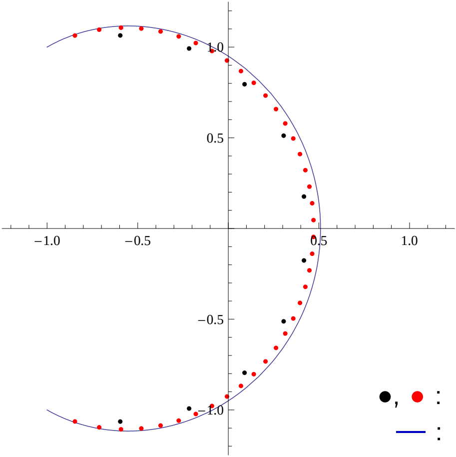
$$\psi(s) = -2N_0 + e^{-s}\left[\zeta_1 + \ldots + \zeta_{N_0}\right] - e^{-s}\left[\frac{1}{\zeta_1} + \ldots + \frac{1}{\zeta_{N_0}}\right]$$

- Bethe equations

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

Bethe Ansatz

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



●, 🔴 : finite-size solution

— : infinite-size limit

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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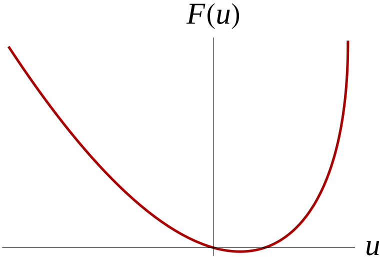

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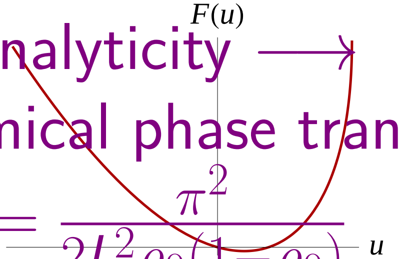

non-analyticity $\longrightarrow$

dynamical phase transition

at $s_c = \dfrac{\pi^2}{2L^2\rho_0(1-\rho_0)}$

Macroscopic limit

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

A reminder: propagator in quantum mechanics

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

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$p = p(x,t)$ 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:

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

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

Macroscopic limit

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

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

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

Macroscopic limit

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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

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

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

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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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More general?

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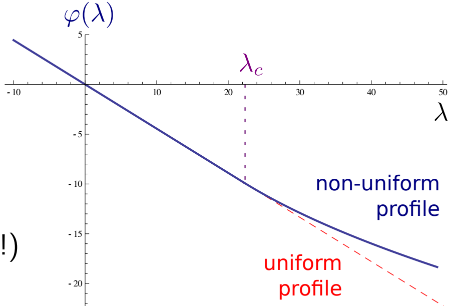
Fluctuating hydrodynamics for quantum chains?

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

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

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

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



$\lambda_c = \frac{\pi^2}{\sigma(\rho_0)}$
(can be large!)

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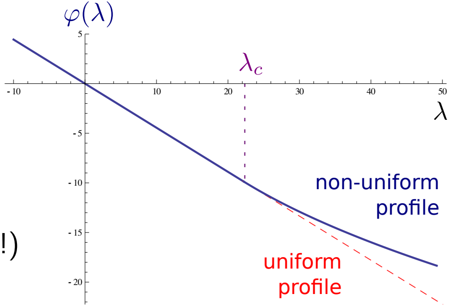
$$\varphi(\lambda) = \lim_{L\to\infty} L\psi(\lambda/L^2)$$

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

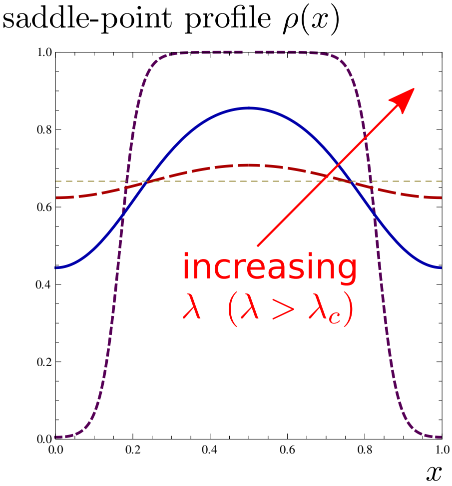


$\lambda_c = \frac{\pi^2}{\sigma(\rho_0)}$
(can be large!)

[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



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 $\mathbb{H}_\triangle$ ground state energy $E_L(s)$

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

Sketch of derivation [VL, Garrahan, van Wijland, JPA **45** 175001]

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

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

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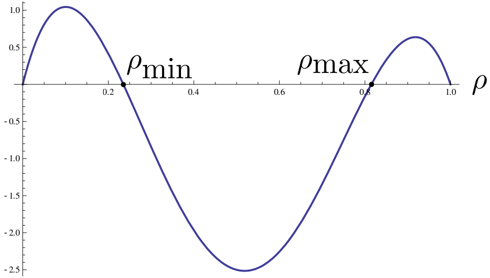
"Potential energy" $E_P(\rho)$



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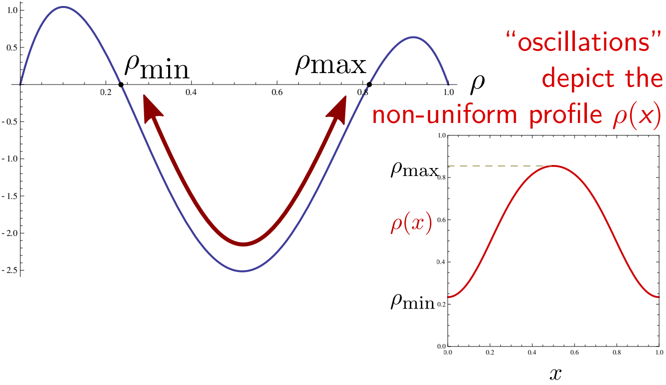


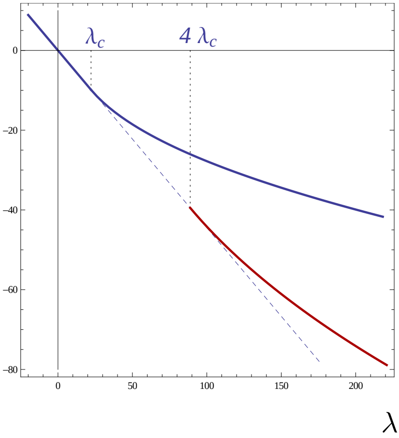
"oscillations" depict the non-uniform profile $\rho(x)$

Excitations

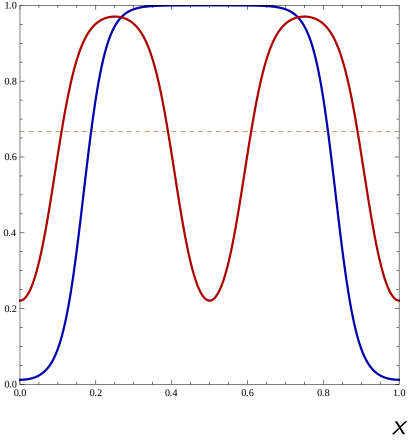
[Cheneau, VL, *work in progress*]

What about solutions with *more than one* kink+anti-kink?

$\varphi(\lambda)$



corresponding profiles $\rho(x)$

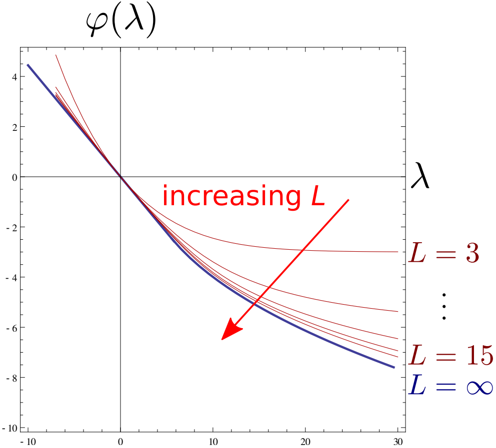


Small sizes: the ground state

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

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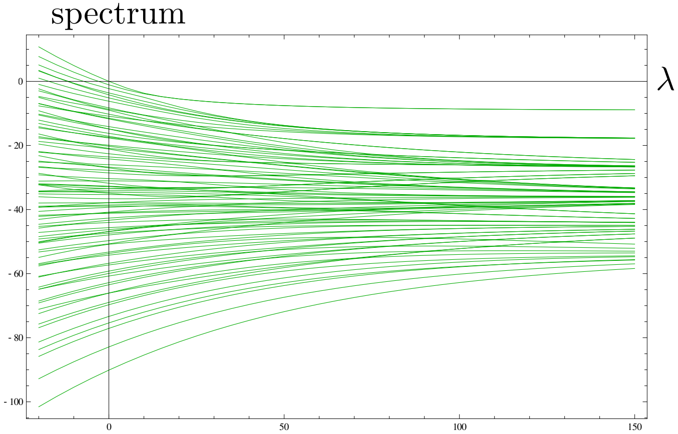

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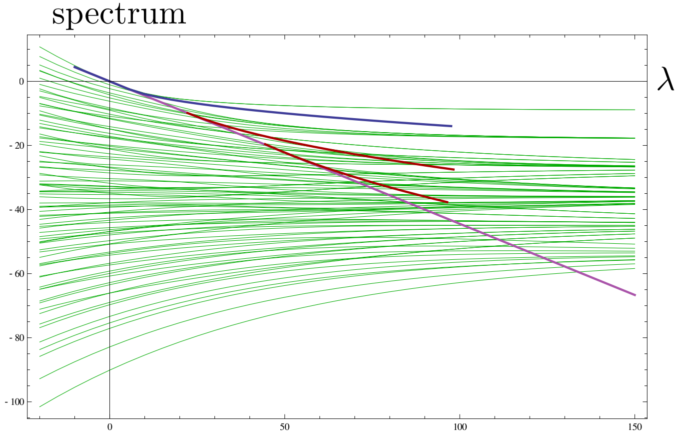
infinite-size ground state
infinite-size excited states



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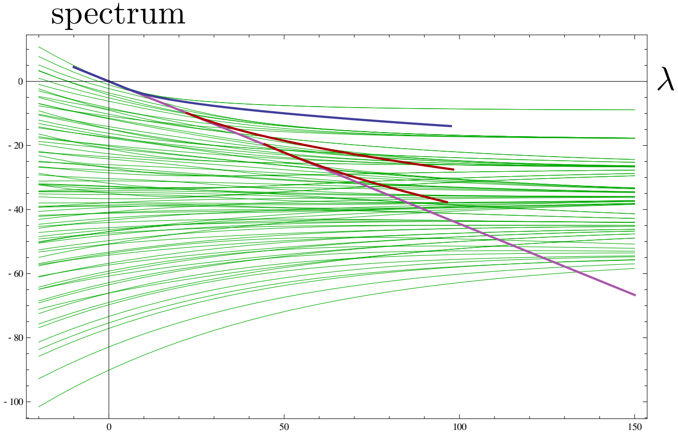

gathering(?) of microscopic eigenvalues $\longrightarrow$ macroscopic ($L = \infty$) states

Summary

Microscopic approach:

- ⋆ operator formalism ⋆ XXZ spin chain ⋆ Bethe Ansatz

Macroscopic approach:

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

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- ⋆ saddle-point method, dynamical phase transition

Questions:

- ⋆ Finite-size crossover around a quantum phase transition? Between:
  - · Luttinger Liquid ($s \to -\infty$)
  - · Phase-separated ferromagnet ($s \to +\infty$)
- ⋆ Across the transition: continuum spectrum → 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
  J. Phys. A **45** 175001 (2012)
- Cécile Appert-Rolland, Bernard Derrida, Vivien Lecomte and Frédéric van Wijland
  Phys. Rev. E **78** 021122 (2008)