Large deviations of additive observables in simple interacting particle systems: of equilibrium, non-equilibrium (& XXZ spin chains)

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Classical and quantum dynamics

What one gains from forgetting probabilities and turning to the quantum world

- Correspondence
  - generator of **stochastic** classical system [particles hopping]
  - Hamiltonian of **quantum** XXZ chain

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

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  - regimes of **large deviations** of *dynamical* (*i.e.* additive) observables
  - phases across a Quantum Phase Transition

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- Use: dictionary between
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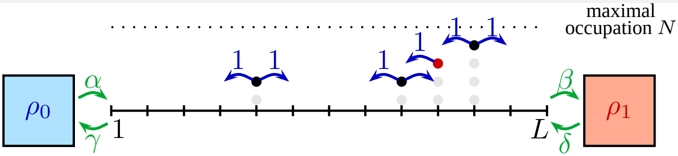
  - phases across a Quantum Phase Transition

- Perspectives opened ; questions raised
  - finite-size effects
  - large-/small-scale spectrum [hidden symmetries]
  - **import/export techniques from/to stat. mech.**

  (I will ask questions to *you*.)

Exclusion Processes – generic settings



- Configurations: occupation numbers $\{n_i\}$
- Exclusion rule: $0 \le n_i \le N$
- 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 "additive" observables A

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

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

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

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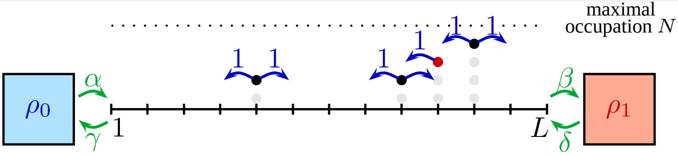

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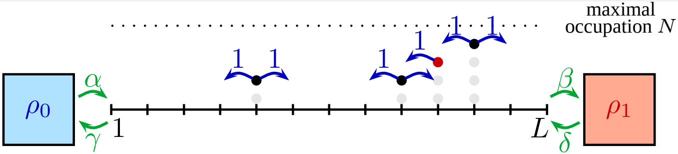

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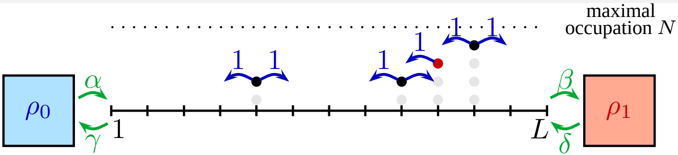
Operator representation [Schütz & Sandow PRE **49** 2726]



Evolution of probability vector P:

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

$$\mathbb{W} = \sum_{1\leq k\leq L-1} \Big[S_k^+ S_{k+1}^- + S_k^- S_{k+1}^+ - \hat{n}_k \check{n}_{k+1} - \hat{n}_{k+1}\check{n}_k \Big]$$
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$S^\pm = S^x \pm i S^y$ and $S^z = \hat{n} - \frac{N}{2}$ are spin operators (of “spin” $j = \frac{N}{2}$)

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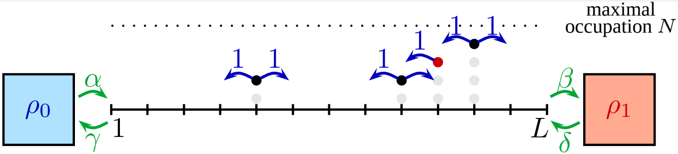

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densities $\rho_0 = \frac{\alpha}{\alpha+\gamma}$; $\rho_1 = \frac{\delta}{\delta+\beta}$; contact rates $a_0 = \frac{\alpha}{\gamma}$; $a_1 = \frac{\delta}{\beta}$

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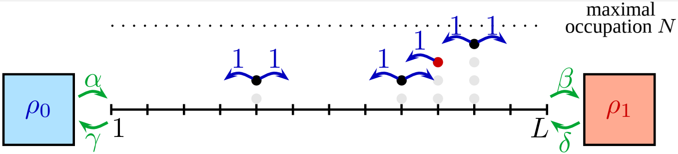

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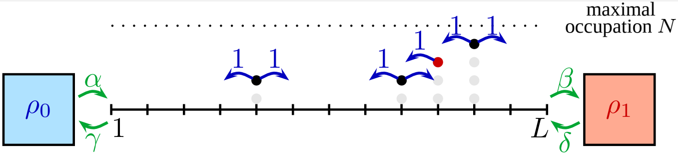
XXX spin chain Hamiltonian (up to boundary terms and constants).

Operator representation for **large deviations**



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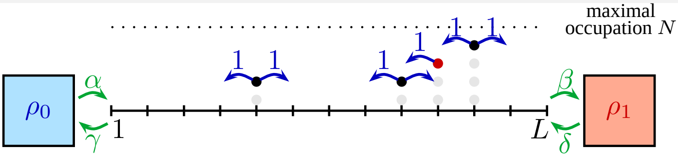
for the **activity** K: **XXZ spin chain Hamiltonian**

Operator representation for **large deviations**



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

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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

$$\psi(s) = \max \mathrm{Sp}\, \mathbb{W}(s)$$

$$\mathbb{W}(s) = \overbrace{\sum_{1\le k\le L-1} \vec{S}_k \cdot \vec{S}_{k+1}}^{\text{invariant by rotation}} + \text{ constant}$$
$$+ \alpha \left[S_1^+ - \check{n}_1\right] + \gamma \left[S_1^- - \hat{n}_1\right]$$
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$$+ \delta \left[S_L^+ \mathrm{e}^{s} - \check{n}_L\right] + \beta \left[S_L^- \mathrm{e}^{-s} - \hat{n}_L\right]$$

Local transformation

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

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

$$\underbrace{+\delta' \left[S_L^+ \mathrm{e}^{s'} - \check{n}_L\right] + \beta' \left[S_L^- \mathrm{e}^{-s'} - \hat{n}_L\right]}_{\text{describes contact with reservoirs of same densities}}$$

SO(3) symmetry [Imparato, VL, van Wijland, PTPS 184 276]

Detailed transformation: (on **one** site)

$$\mathcal{Q} = \mathbf{1} + xS^x - \mathrm{i}yS^y + zS^z \qquad \text{(invertible)}$$

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

$$\mathcal{Q}^{-1} S^x \mathcal{Q} = (R\mathbf{S})_1 \qquad \mathcal{Q}^{-1} S^y \mathcal{Q} = (R\mathbf{S})_2 \qquad \mathcal{Q}^{-1} S^z \mathcal{Q} = (R\mathbf{S})_3$$

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)

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

with "primed" variables

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

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

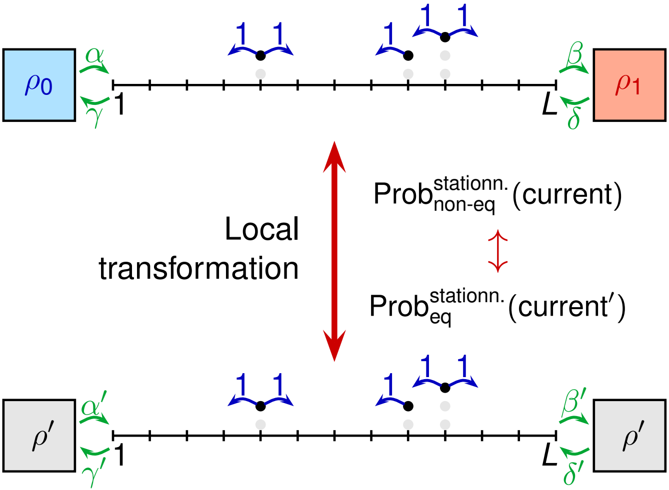
$$e^{-s'} = \frac{x+e^{-s}+z(e^{-s}-1)}{1+xe^{-s}+z(e^{-s}-1)}$$

[Only at $s\neq 0$.]

Summary

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

Symmetric exclusion process



System in equilibrium

Probabilistic interpretation

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

Mapping:

$$\begin{aligned}\hat{P}(\mathbf{n},s, t; \rho_0, \rho_1; a_0, a_1) &= \langle \mathbf{n}| e^{t\mathbb{W}(s;\rho_0,\rho_1;a_0,a_1)} |P_{\text{init}}\rangle \\ &= \underbrace{\langle \mathbf{n}|\mathcal{Q}}_{\substack{\text{new projection}\\ \text{state}}} e^{t\mathbb{W}(s';\rho_0',\rho_1';a_0,a_1)} \underbrace{\mathcal{Q}^{-1}|P_{\text{init}}\rangle}_{\substack{\text{new initial}\\ \text{condition}}}\end{aligned}$$

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Question:

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

Generalizations:

- ⋆ higher dimensions
- ⋆ generic network and current
- ⋆ more than two reservoirs
- ⋆ see also: Derrida & Gerschenfeld (ω 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): max. occupation $N = 1$; spins $S \mapsto \sigma$
Periodic boundary conditions

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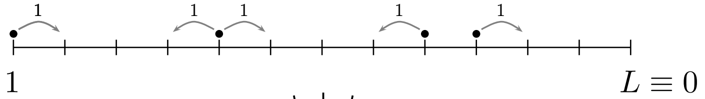

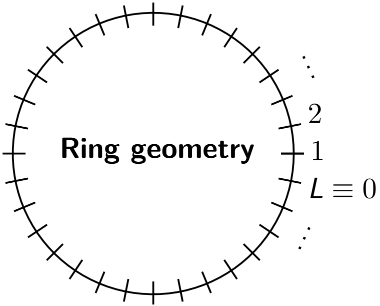

Focus on a simple situation $\quad s \leftrightarrow$ activity K

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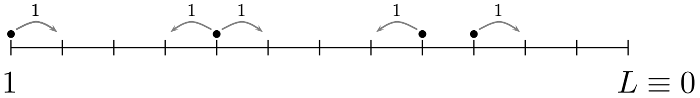

$$\mathbb{W}_s = \sum_{k=1}^{L-1} \Big[e^{-s} \big(\sigma_k^+ \sigma_{k+1}^- + \sigma_k^- \sigma_{k+1}^+ \big) - \hat{n}_k (1 - \hat{n}_{k+1}) - (1 - \hat{n}_k) \hat{n}_{k+1} \Big]$$

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

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

Classical/Quantum dictionary

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

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

Bethe Ansatz

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

Bethe Ansatz

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

- eigenvector of components

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

- eigenvalue

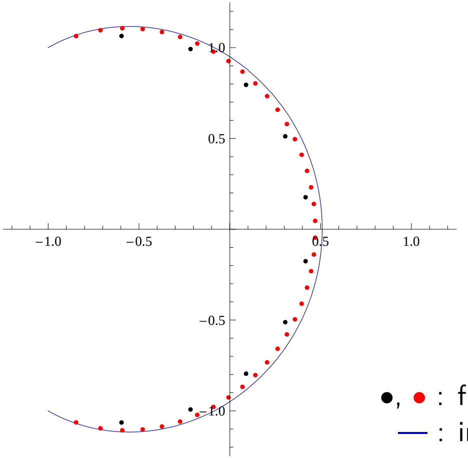
$$\psi(s) = -2N_0 + e^{-s}\left[\zeta_1 + \ldots + \zeta_{N_0}\right] - e^{-s}\left[\frac{1}{\zeta_1} + \ldots + \frac{1}{\zeta_{N_0}}\right]$$

- 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

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

- **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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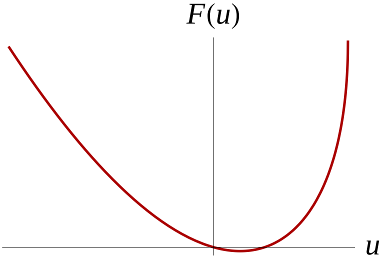

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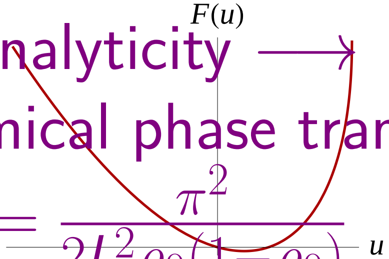

non-analyticity $\longrightarrow$ dynamical phase transition at $s_c = \dfrac{\pi^2}{2L^2\rho_0(1-\rho_0)}$

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

For exclusion processes

Using $SU(2)$ coherent states:

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

Macroscopic limit

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

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Use saddle-point to handle the large L limit. $[L = \hbar^{-1}]$

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

$$\partial_t \rho(x,t) = -\partial_x\big[-\partial_x \rho(x,t) + \xi(x,t)\big]$$
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One recovers the action of fluctuating hydrodynamics $[L\to\infty]$

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[Spohn; Bertini, De Sole, Gabrielli, Jona-Lasinio, Landim]

And obtains non-trivial finite-size corrections [lattice contribs.]

(those affecting the saddle, not the fluctuations around it)

$\psi(s)$: 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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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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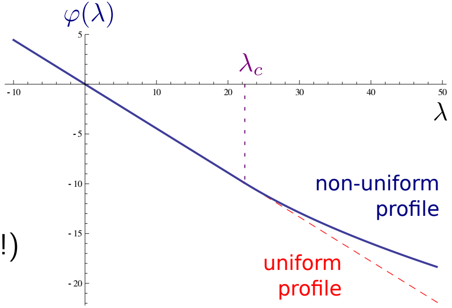
Fluctuating hydrodynamics for quantum chains?

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

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

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

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



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(can be large!)

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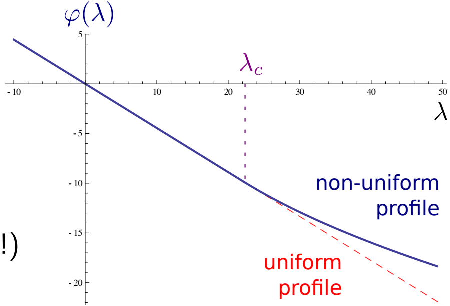

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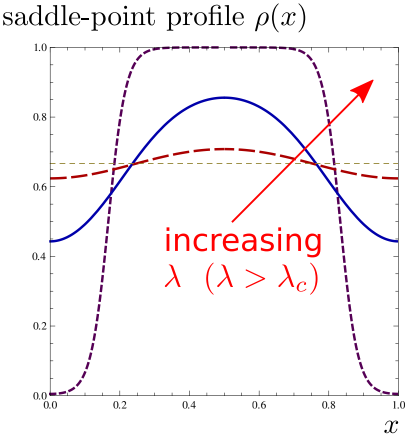
see also: for LDF of Q [Bodineau, Derrida, PRE **78** 021122] phase transition in WASEP for large dev. (**non-stationary** profile) [Jona-Lasinio *et al.*] generic criterion for instability

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

Optimal



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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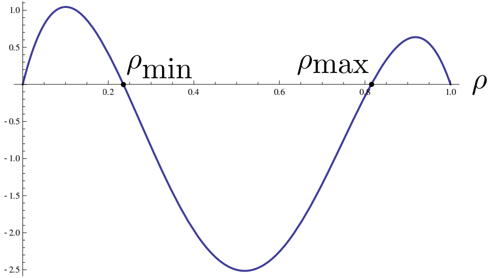
"Potential energy" $E_P(\rho)$



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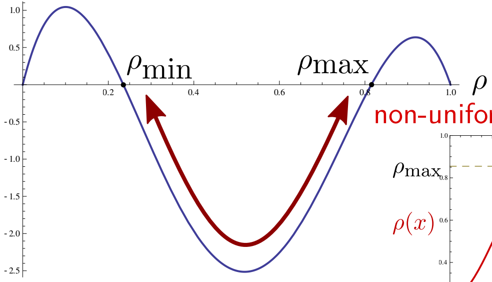
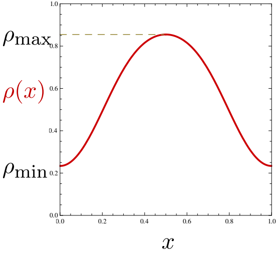


"oscillations" depict the non-uniform profile $\rho(x)$

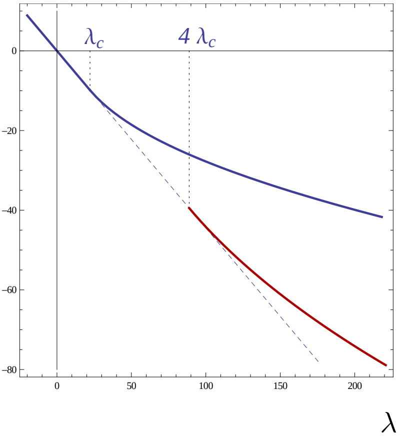


Excitations

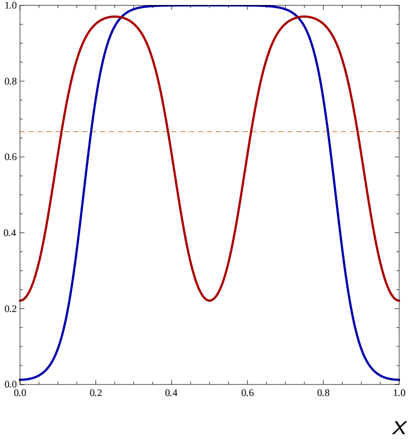
[Cheneau, VL, *work in progress*]

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

$\varphi(\lambda)$

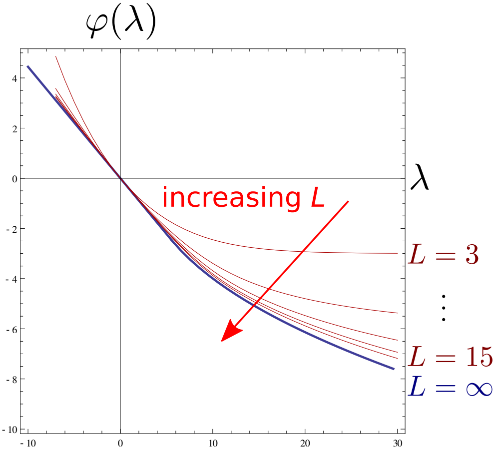


corresponding profiles $\rho(x)$



Small sizes: the ground state

Aim: experimental realizations with cold atoms
$\to$ non-periodic (but isolated, 1D) system
$\to$ smaller sizes & finite-temperature & excited state



Small sizes: the full spectrum [preliminary!]

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

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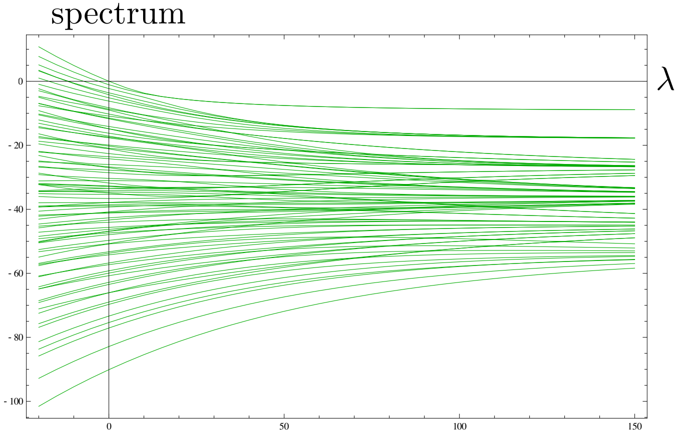

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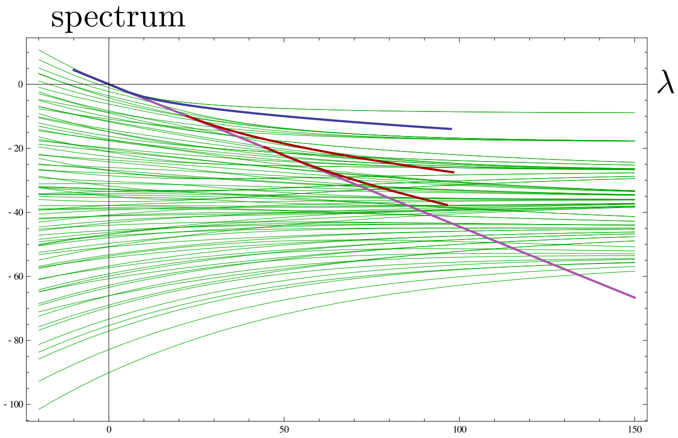
infinite-size ground state
infinite-size excited states



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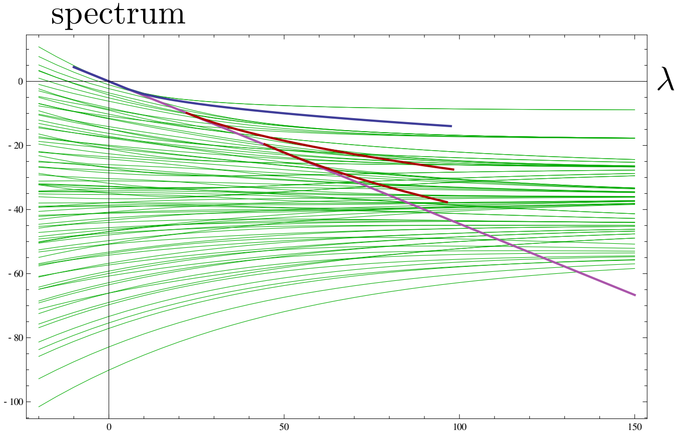

gathering(?) of microscopic eigenvalues $\longrightarrow$ macroscopic ($L = \infty$) states

Summary

Microscopic approach:

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

Macroscopic approach:

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

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Microscopic approach:

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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 $\to$ 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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- ⋆ Vivien Lecomte, Juan P. Garrahan, Frédéric van Wijland
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- ⋆ Vivien Lecomte, Alberto Imparato, Frédéric van Wijland
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