

Large deviations of additive observables in simple interacting particle systems: equilibrium & non-equilibrium

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Classical and quantum dynamics

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

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- Correspondence

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

[particles hopping]

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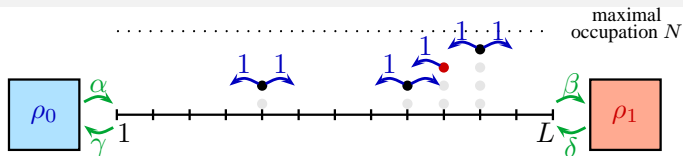
- Use: dictionary between
 - regimes of **large deviations** of *dynamical* (i.e. additive) observables
 - phases across a Quantum Phase Transition

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

[hidden symmetries]

(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 $P(A, t)$)

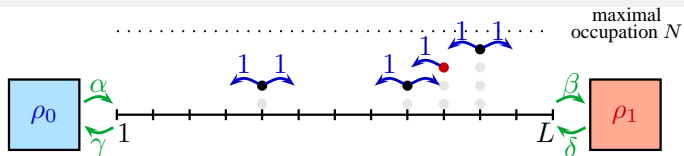
A = total current Q on time window $[0, t]$

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

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

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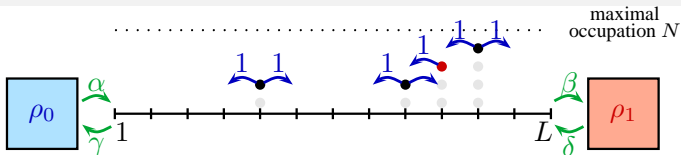
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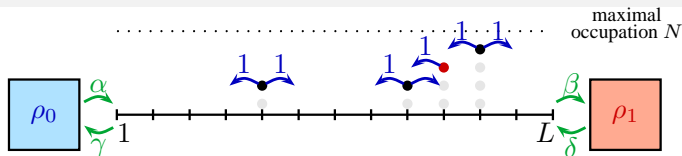
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Operator representation

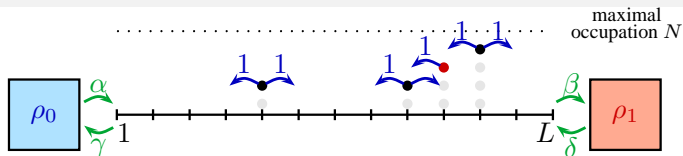
[Schütz & Sandow PRE **49** 2726]Evolution of probability vector P :

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

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

 $S^\pm = S^x \pm iS^y$ and $S^z = \hat{n} - \frac{N}{2}$ are spin operators (of “spin” $j = \frac{N}{2}$)

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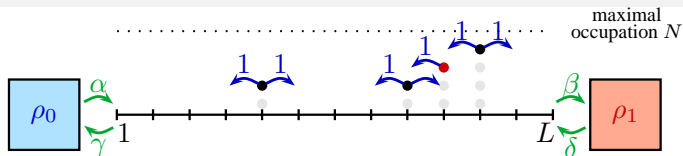
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densities $\rho_0 = \frac{\alpha}{\alpha + \gamma}$; $\rho_1 = \frac{\delta}{\delta + \beta}$; contact rates $a_0 = \frac{\alpha}{\gamma}$; $a_1 = \frac{\delta}{\beta}$

Operator representation

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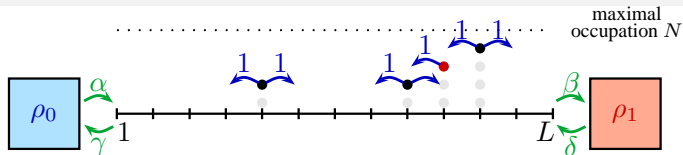
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XXX spin chain Hamiltonian (up to boundary terms and constants).

Operator representation for large deviations

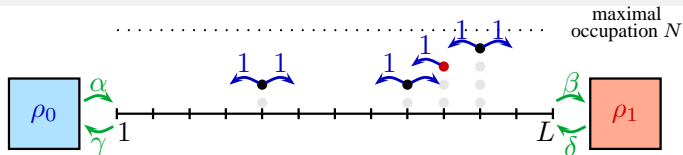


$$\langle e^{-sK} \rangle \sim e^{t\psi(s)} \quad \text{with} \quad \psi(s) = \max \text{Sp } \mathbb{W}_s$$

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

Operator representation for large deviations



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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

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

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

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

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

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

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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for some SO(3) rotation matrix R .

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

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

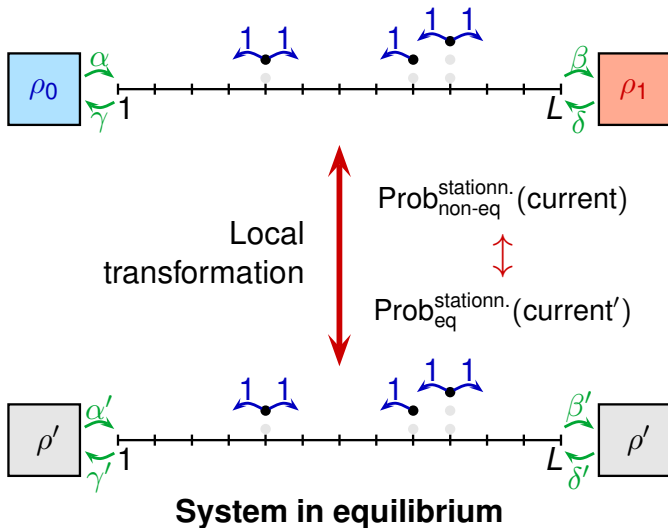
$$\rho'_1 = (x + e^{-s} - z(1 - e^{-s})) \frac{[x + e^s + z(1 - e^s)]\rho_1 - x - z}{1 - x^2}$$

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

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 (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

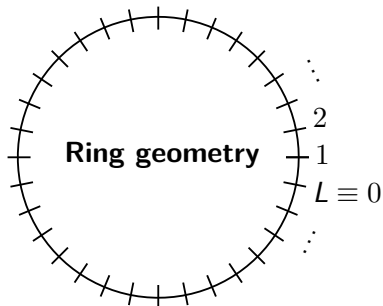
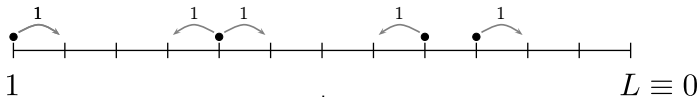
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Fixed total particle number N_0

density: $\rho_0 = N_0/L$



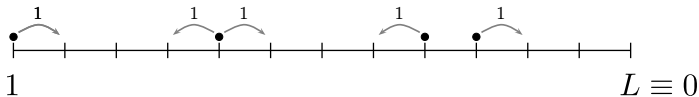
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 $s \leftrightarrow$ activity K

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

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

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

Classical/Quantum dictionary

SSEP	Quantum Spin Chain
local occupation number n_k ($1 \leq k \leq L$) $n_k = 0, 1 \equiv \circ, \bullet$	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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evolution operator \mathbb{W}_s $s \leftrightarrow$ activity K $\mathbb{W}_s = \frac{L-1}{2} - \frac{e^{-s}}{2} \mathbb{H}_\Delta$	ferromagnetic XXZ Hamiltonian ($J_{xy} = -1$) $\mathbb{H}_\Delta = \sum_{k=1}^{L-1} \left[J_{xy} (\sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y) + J_z \sigma_k^z \sigma_{k+1}^z \right]$ $= - \sum_{k=1}^{L-1} \left[\sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y + \Delta \sigma_k^z \sigma_{k+1}^z \right]$
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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Coordinate Bethe Ansatz: Integrability known from long ; difficulty: $L \rightarrow \infty$

- eigenvector of components

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

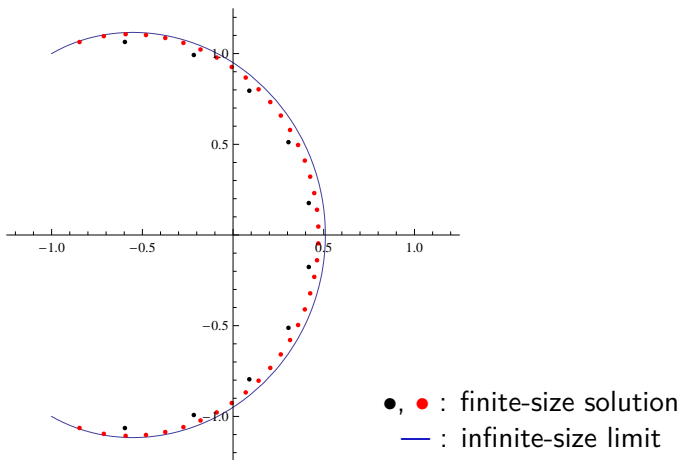
- eigenvalue

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

- 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

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

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

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

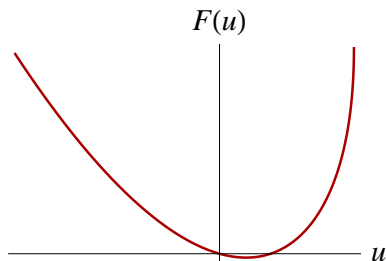
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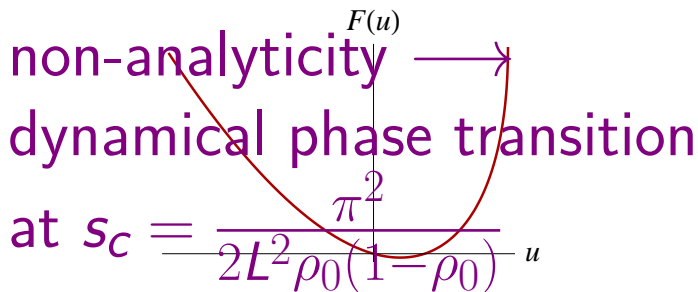
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[Apert, Derrida, VL, van Wijland, PRE 78 021122]

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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

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

$p = p(x, t)$ 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:

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

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Using $SU(2)$ coherent states:

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

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:

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

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

One recovers the action of fluctuating hydrodynamics [$L \rightarrow \infty$]

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

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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

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

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

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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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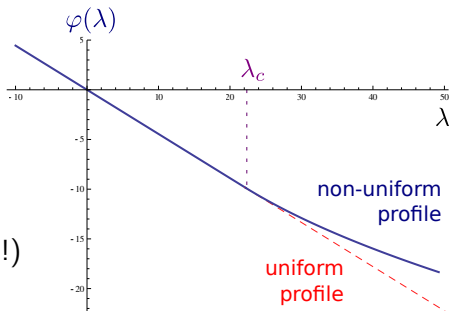
Fluctuating hydrodynamics for quantum chains?

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 $\lambda > \lambda_c$



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

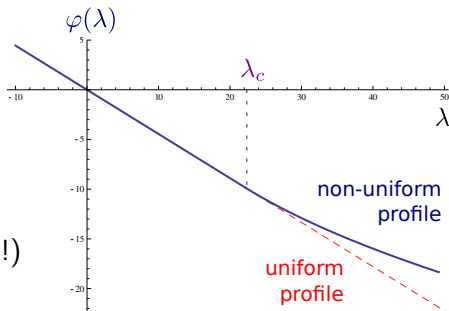
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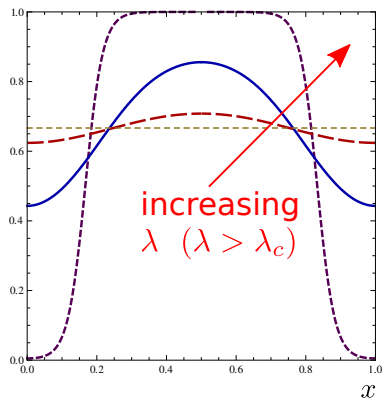
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see also: for LDF of Q
 [Bodineau, Derrida,
 PRE **78** 021122]
 phase transition
 in WASEP for large dev.
 (**non-stationary** profile)
 [Jona-Lasinio *et al.*]
 generic criterion for
 instability

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 ($1 \leq k \leq L$) $n_k = 0, 1 \equiv \circ, \bullet$	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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minimal activity phase ($s \rightarrow +\infty$) $\bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \circ \circ \circ \circ \circ \circ$	Ising ferromagnetic order ($\Delta \rightarrow +\infty$) $\downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow$
maximal activity phase ($s \rightarrow -\infty$) $\bullet \circ \circ \circ \circ \circ \circ \circ \circ \circ \circ \circ \bullet \bullet \bullet \bullet \bullet \bullet$ & $\circ \circ \circ \circ \circ \circ \circ \circ \circ \circ \circ \bullet \bullet \bullet \bullet \bullet \bullet$	XY degenerate groundstate ($\Delta = 0$) $\downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow$ (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

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

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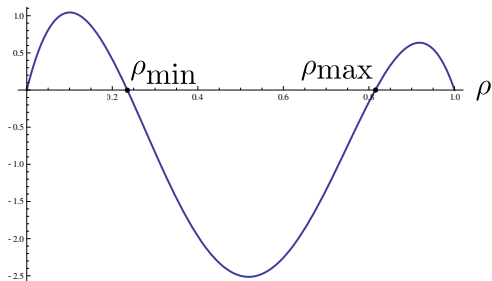
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“Potential energy” $E_P(\rho)$



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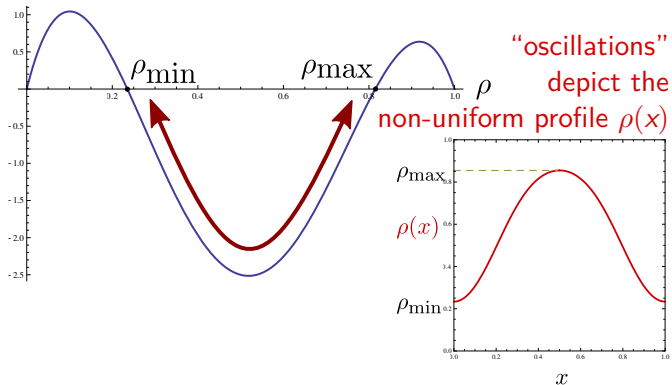
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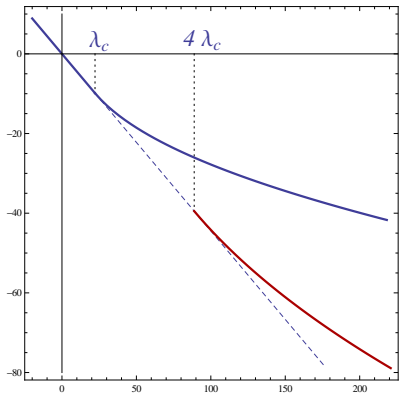
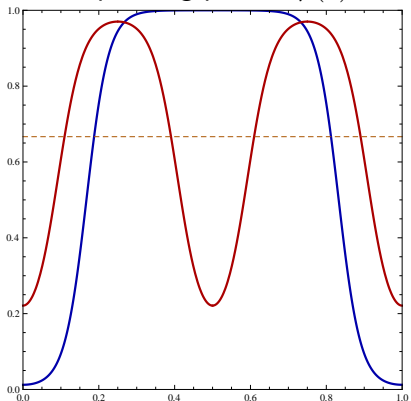
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Excitations

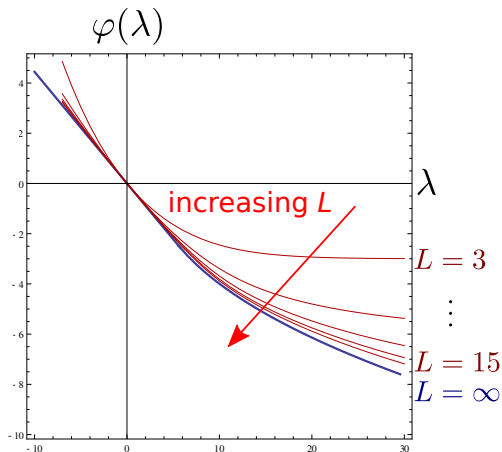
[Cheneau, VL, *work in progress*]What about solutions with *more than one* kink+anti-kink? $\varphi(\lambda)$  λ corresponding profiles $\rho(x)$  x

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

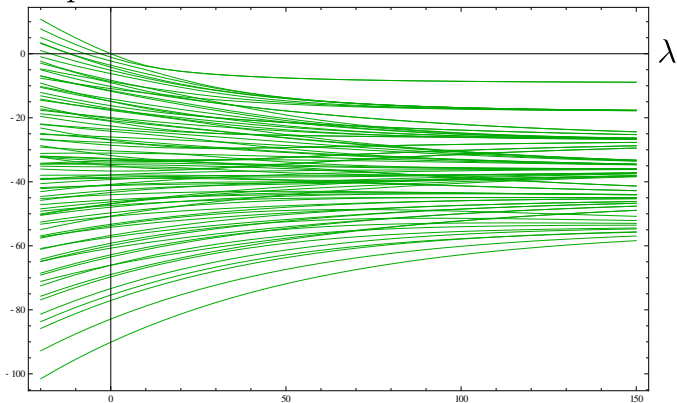
$N_0 = 3$ particles

Small sizes: the full spectrum

[preliminary!]

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

spectrum



Small sizes: the full spectrum

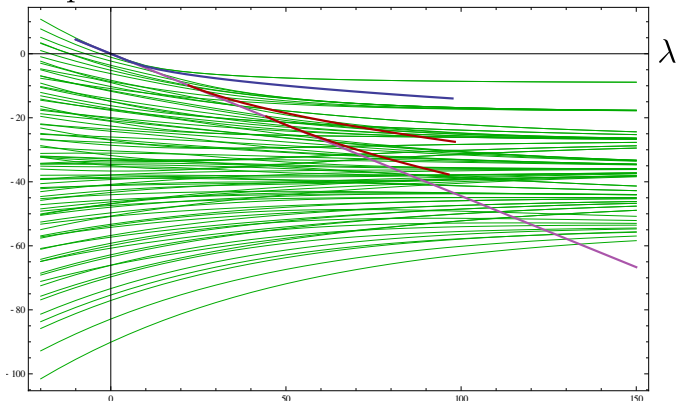
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infinite-size ground state

infinite-size excited states

spectrum



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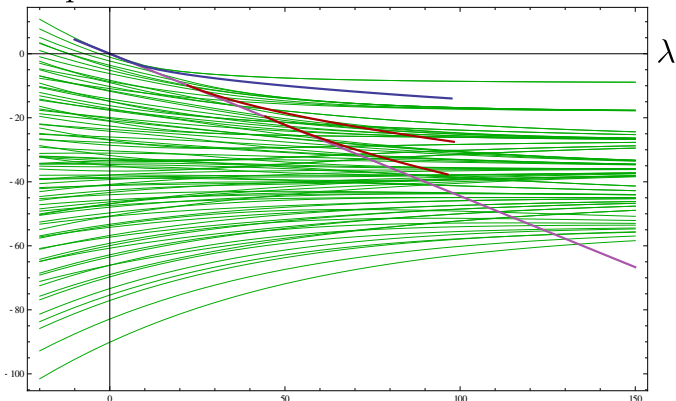
[preliminary!]

 $L = 9$ 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:

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

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Macroscopic approach:

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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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work in progress (2014-)
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