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\textbf{ stochastic} classical system [particles hopping]
  - Hamiltonian of quantum XXZ chain

(Well known at least in the stat. mech. community.)
Classical and quantum systems

- **Correspondence**
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- **Use:** dictionary between
  - regimes of *large deviations* of *dynamical* observables
  - phases across a Quantum Phase Transition
Classical and quantum systems

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- Use: dictionary 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)}
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  (\( \leftrightarrow \) determining \( P(A, t) \))
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  \( \iff \) determining \( P(A, t) \)
  \[
  A = \text{total current } Q \text{ on time window } [0, t] = \# \text{jumps} - \text{jumps}
  \]
  \[
  A = \text{total activity } K \text{ on time window } [0, t] = \# \text{jumps} + \text{jumps}
  \]
**Operator representation**

![Diagram](image)

**Evolution of probability vector $P$:**

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

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

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

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

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

**Similar to Schrödinger eq. but eq. for the probability instead of the wave function**
Evolution of probability vector $P$:

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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

\[ \langle e^{-sK} \rangle \sim e^{t\psi(s)} \quad \text{with} \quad \psi(s) = \max \text{Sp } W_s \]

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

XXZ spin chain Hamiltonian

Vivien Lecomte (LPMA – Paris VI-VII)
Focus on a simple situation

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

Periodic boundary conditions

Fixed total particle number $N_0$

Density: $\rho_0 = N_0/L$

\[ L \equiv 0 \]
Focus on a simple situation

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Periodic boundary conditions
Fixed total particle number $N_0$

density: $\rho_0 = N_0 / L$

Ring geometry

$\cdot \cdot \cdot$

$L \equiv 0$

$1$

$1 \cdot 1 \cdot 1$

$2$

$1$

$L \equiv 0$

$\cdot \cdot \cdot$
Focus on a simple situation

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

Periodic boundary conditions

Fixed total particle number \( N_0 \)

Density: \( \rho_0 = N_0 / L \)

\[
\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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$$= \frac{L - 1}{2} - \frac{e^{-s}}{2} \mathcal{H} \Delta$$

$$\mathcal{H} \Delta = - \sum_{k=1}^{L-1} \left[ \sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y + \Delta \sigma_k^z \sigma_{k+1}^z \right]$$

with $\Delta = e^s$
# Classical/Quantum dictionary

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<td>$= - \sum_{k=1}^{L-1} \left[ \sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y + \Delta \sigma_k^z \sigma_{k+1}^z \right]$</td>
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<td>counting factor $\Delta = e^s$ of the activity $K$</td>
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<td>$\psi(s) = \max \text{Sp} \ W_s = \frac{L-1}{2} - \frac{e^{-s}}{2} E_L(s)$</td>
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Bethe Ansatz

[Appert, Derrida, VL, van Wijland, PRE 78 021122]
Bethe Ansatz

Bethe Ansatz:

- eigenvector of components

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

- eigenvalue

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

- Bethe equations

\[ \zeta_i^L = \prod_{\substack{j=1 \, \text{to} \, N_0 \, \text{except} \, i}} \left[ -\frac{1 - 2e^s\zeta_i + \zeta_i\zeta_j}{1 - 2e^s\zeta_j + \zeta_i\zeta_j} \right] \]
Bethe Ansatz

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

Repartition of Bethe roots in the complex plane

●, ○: finite-size solution
—: infinite-size limit
Finite-size effects

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

- large deviation function

\[
\psi(s) = -2L\rho_0(1 - \rho_0)s + L^{-2}\mathcal{F}(u) + \ldots \text{ with } u = L^2\rho_0(1-\rho_0)s
\]

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

\[
\mathcal{F}(u) = \sum_{k \geq 2} \frac{(-2u)^kB_{2k-2}}{\Gamma(k)\Gamma(k+1)}
\]
Finite-size effects

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\[ \psi(s) = -2L\rho_0(1 - \rho_0)s + L^{-2}F(u) + \ldots \quad \text{with} \quad u = L^2\rho_0(1 - \rho_0)s \]

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\[ F(u) \]

Non-analyticity \( \rightarrow \)

Dynamical phase transition at \( s_c = \frac{\pi^2}{2L^2\rho_0(1 - \rho_0)}u \)
A reminder: propagator in quantum mechanics

$$\langle \text{final} | e^{it\hat{H}} | \text{initial} \rangle$$
Macroscopic approach

Analogy with quantum mechanics

Macroscopic limit

[Tailleur, Kurchan, VL, JPA 41 505001]

A reminder: propagator in quantum mechanics

\[
\langle \text{final} | e^{it\hat{H}} | \text{initial} \rangle = \int dz_1 \ldots dz_n \langle \text{final} | e^{i\Delta t \hat{H}} | z_n \rangle \langle z_{n-1} | e^{i\Delta t \hat{H}} | z_{n-2} \rangle \ldots \\
\ldots \langle z_1 | e^{i\Delta t \hat{H}} | \text{initial} \rangle
\]
Macroscopic limit

A reminder: propagator in quantum mechanics

\[ \langle \text{final} | e^{it\mathcal{H}} | \text{initial} \rangle = \int dz_1 \ldots dz_n \langle \text{final} | e^{i\Delta t \mathcal{H}} | z_n \rangle \langle z_{n-1} | e^{i\Delta t \mathcal{H}} | z_{n-2} \rangle \ldots \]

\[ \ldots \langle z_1 | e^{i\Delta t \mathcal{H}} | \text{initial} \rangle \]

\[ = \int \mathcal{D}p \mathcal{D}q \exp \left\{ i \frac{1}{\hbar} S[p, q] \right\} \]

where \( S[p, q] \) is the action.
A reminder: propagator in quantum mechanics

\[ \langle \text{final} | e^{i t \hat{H}} | \text{initial} \rangle = \int dz_1 \ldots dz_n \langle \text{final} | e^{i \Delta t \hat{H}} | z_n \rangle \langle z_{n-1} | e^{i \Delta t \hat{H}} | z_{n-2} \rangle \ldots \]
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\[ = \int \mathcal{D}p \mathcal{D}q \ exp \left\{ i \frac{1}{\hbar} S[p, q] \right\} \]

\( p = p(x, t) \) 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

For exclusion processes

Using $SU(2)$ coherent states:

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

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

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

For exclusion processes

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

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

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

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One recovers the action of fluctuating hydrodynamics

[Spohn, Bertini De Sole Gabrielli Jona-Lasinio Landim]
\[ \psi(s): \text{ again} \]

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

Periodic boundary conditions
More general fluctuating hydrodynamics

\[ \frac{1}{L_t} \langle Q \rangle \propto D(\rho) \quad \text{(Fourier’s law)} \]

\[ \frac{1}{L_t} \langle Q^2 \rangle_c = \sigma(\rho) \quad \text{(For the SSEP, } \sigma(\rho) = \rho(1 - \rho)) \]
ψ(ϕ): again

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Saddle point evaluation

\[\langle e^{-sK} \rangle \sim \int D\rho D\hat{\rho} \exp\{L S_s[\hat{\rho}, \rho]\}\]
**ψ(s): again**

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

Periodic boundary conditions
More general fluctuating hydrodynamics

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\frac{1}{Lt} \langle Q^2 \rangle_c = \sigma(\rho)
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(Fourier’s law)

(For the SSEP, \(\sigma(\rho) = \rho(1 - \rho)\))

Saddle point evaluation

\[
\langle e^{-sK} \rangle \sim \int D\rho D\hat{\rho} \exp\{LS_s[\hat{\rho}, \rho]\}
\]

Large deviation function

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

\[
\psi(s) = -s\frac{\langle K \rangle_c}{t} + \int \text{of quadratic fluctuations} \quad \text{with} \quad u = L^2 s \frac{\sigma(\rho_0)\sigma''(\rho_0)}{8D^2}
\]

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

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

More general?

Repartition of Bethe roots for $s > s_c$?
Correspondence between the (Gaussian) integration of small fluctuations AND discreteness of Bethe root repartition.

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Repartition of Bethe roots for $s > s_c$?

Fluctuating hydrodynamics for quantum chains?
Dynamical phase transition \[\text{[VL, Garrahan, van Wijland, JPA 45 175001]}\]

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

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

Using the correct \textit{non-uniform} saddle-point profile for \(\lambda > \lambda_c\)

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

(non-uniform profile)

(uniform profile)
Dynamical phase transition [VL, Garrahan, van Wijland, JPA 45 175001]

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

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

saddle-point profile $\rho(x)$

increasing $\lambda$ ($\lambda > \lambda_c$)
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<td>XY degenerate groundstate ($\Delta = 0$)</td>
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<td>$\circ \circ \circ \circ \circ \circ \circ \bullet \bullet \bullet \bullet$ &amp; $\circ \circ \circ \circ \circ \circ \circ \bullet \bullet \bullet \bullet$</td>
<td></td>
</tr>
<tr>
<td>time $t$ (steady state: $t \to +\infty$)</td>
<td>inverse temp. $\beta$ (zero-temp. limit: $\beta \to +\infty$)</td>
</tr>
<tr>
<td>dynamical partition function $\langle e^{-sK} \rangle \approx \text{Tr } e^{i\mathbb{W}_s}$</td>
<td>partition function $Z_{\beta}^{\text{XXZ}}(\Delta) = \text{Tr } e^{-\beta \mathbb{H}_{\Delta}}$</td>
</tr>
</tbody>
</table>
Sketch of derivation

[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]

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

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

Motion in “time” $x$ of a particle of “position” $\rho$ in a

“Potential energy” $E_P(\rho)$
Sketch of derivation

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

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

Motion in “time” $x$ of a particle of “position” $\rho$ in a

“Potential energy” $E_P(\rho)$

“oscillations” depict the non-uniform profile $\rho(x)$
What about solutions with *more than one* kink+anti-kink?

\[ \phi(\lambda) \]

[Diagram showing \( \phi(\lambda) \) and corresponding profiles \( \rho(x) \)]

**Excitations**

[Cheneau, VL, *work in progress*]
Small sizes: the ground state

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

\[ \varphi(\lambda) \]

**Graph:**
- Increasing \( L \)
- \( L = 3 \)
- \( L = 15 \)
- \( L = \infty \)
Small sizes: the full spectrum

$L = 9$ sites
$N_0 = 3$ particles
Small sizes: the full spectrum

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

Vivien Lecomte (LPMA – Paris VI-VII)

SSEP and QPT in XXZ spin chains

15/07/2014 23 / 25
Small sizes: the full spectrum

\( L = 9 \) sites
\( N_0 = 3 \) particles

infinite-size ground state
infinite-size excited states

Vivien Lecomte (LPMA – Paris VI-VII)
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Small sizes: the full spectrum

$L = 9$ sites
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infinite-size ground state
infinite-size excited states

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

Questions:
- Finite-size crossover around a quantum phase transition? Between:
  - Luttinger Liquid ($s < 1$)
  - Phase-separated ferromagnet ($s > 1$)
- Across the transition: continuum spectrum $\rightarrow$ gaped spectrum?
- XXZ transition not at $\Delta = 1$ but at $\Delta = 1 + O(L^{-2})$?
Summary

Microscopic approach:
- operator formalism
- XXZ spin chain
- Bethe Ansatz

Macroscopic approach:
- action of fluctuating hydrodynamics
- 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 $\to$ gaped spectrum?
- XXZ transition not at $\Delta = 1$ but at $\Delta = 1 + \mathcal{O}(L^{-2})$
- Are scaling exponents/functions known? Are they interesting?
Thank you for your attention!

References: