Exclusion processes and quantum phase transitions in XXZ spin chains.

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Kyoto – 19th 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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- Use: dictionary between
  - regimes of **large deviations** of dynamical observables
  - phases across a Quantum Phase Transition
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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 \( P(\{n_i\}, t) \)
  \[
  \partial_t P(\{n_i\}, t) = \sum_{n'_i} \left[ W(n'_i \rightarrow n_i) P(\{n'_i\}, t) - W(n_i \rightarrow n'_i) P(\{n_i\}, t) \right]
  \]
- 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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Exclusion Processes – generic settings

- Configurations: occupation numbers \{n_i\}
- Exclusion rule: $0 \leq n_i \leq N$
- Markov evolution for the **probability** $P(\{n_i\}, t)$
  $$\partial_t P(\{n_i\}, t) = \sum_{\text{transitions}} W(n_i' \rightarrow n_i) P(\{n_i'\}, t) - W(n_i \rightarrow n_i') P(\{n_i\}, t)$$
- **Large deviation function** of time-integrated observables $A$
  $$\langle e^{-sA} \rangle \sim e^{t \psi(s)} \quad (\Leftrightarrow \text{determining } P(A, t))$$
  - $A = \text{total current } Q \text{ on time window } [0, t]$
  - $A = \text{total activity } K \text{ on time window } [0, t]$
  - $A = \# \text{jumps} - \text{jumps}$
  - $A = \# \text{jumps} + \text{jumps}$
Operator representation

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.
Operator representation

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**XXX spin chain Hamiltonian** (up to boundary terms and constants).
Operator representation for large deviations

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

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

**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: $\rho_0 = N_0/L$
Focus on a simple situation

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

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Ring geometry
Focus on a simple situation

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

Periodic boundary conditions

Fixed total particle number $N_0$

density: $\rho_0 = N_0 / L$

\[
W_s = \sum_{k=1}^{L-1} \left[ e^{-s} (\sigma_k^- \sigma_{k+1}^- + \sigma_k^- \sigma_{k+1}^+) - \hat{n}_k (1 - \hat{n}_{k+1}) - (1 - \hat{n}_k) \hat{n}_{k+1} \right]
\]
Focus on a simple situation

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\]

\[
= \frac{L - 1}{2} - \frac{e^{-s}}{2} \mathbb{H} \Delta
\]

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

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

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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

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

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

Repartition of Bethe roots in the complex plane

•, •: finite-size solution
- : infinite-size limit
Finite-size effects

large deviation function

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

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

\[ F(u) = \sum_{k\geq2} \frac{(-2u)^kB_{2k-2}}{\Gamma(k)\Gamma(k+1)} \]
Finite-size effects

- large deviation function

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

with \( u = L^2\rho_0(1 - \rho_0)s \)

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\[ F(u) \]

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

non-analyticity → dynamical phase transition

at \( s_c = \frac{\pi^2}{2L^2\rho_0(1 - \rho_0)} \)
Macroscopic limit

[Tailleur, Kurchan, VL, JPA 41 505001]

A reminder: propagator in quantum mechanics

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

Analogy with quantum mechanics

Macroscopic limit

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

[Tailleur, Kurchan, VL, JPA 41 505001]

A reminder: propagator in quantum mechanics

\[
\langle \text{final} | e^{it\mathcal{H}} | \text{initial} \rangle = \int dz_1 \ldots dz_n \langle \text{final} | e^{i\Delta t\mathcal{H}} | z_n \rangle \langle z_{n-1} | e^{i\Delta t\mathcal{H}} | z_{n-2} \rangle \ldots \\
\ldots \langle z_1 | e^{i\Delta t\mathcal{H}} | \text{initial} \rangle \\
= \int \mathcal{D}p \mathcal{D}q \exp \left\{ i \frac{1}{\hbar} S[p, q] \right\}
\]

\[S[p, q] = \text{action}\]
Macroscopic approach

Analogy with quantum mechanics

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[Tailleur, Kurchan, VL, JPA 41 505001]

A reminder: propagator in quantum mechanics

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\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 
\]

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

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

\[
p = p(x, t) \text{ and } q = q(x, t)
\]

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:

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

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

Again: use saddle-point to handle the large $L$ limit.
For exclusion processes

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

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

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

\[
\frac{1}{Lt} \langle Q \rangle \propto D(\rho) \tag{Fourier’s law}
\]

\[
\frac{1}{Lt} \langle Q^2 \rangle_c = \sigma(\rho) \tag{For the SSEP, }\sigma(\rho) = \rho(1 - \rho)
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\( \psi(s): \text{ again} \) [Appert, Derrida, VL, van Wijland, PRE 78 021122]

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Saddle point evaluation

\[
\langle e^{-sK} \rangle \sim \int \mathcal{D} \rho \mathcal{D} \hat{\rho} \exp \{ L S_s[\hat{\rho}, \rho] \}
\]
Macroscopic approach

Large deviation function

\( \psi(s) \): again

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

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Saddle point evaluation

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

Large deviation function

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

\[
\psi(s) = -s \frac{\langle K \rangle_c}{t} + L^{-2} D\mathcal{F}(u) \quad \text{at saddle-point,}\int \text{of quadratic fluctuations}
\]

with

\[
u = L^2 s \frac{\sigma(\rho_0)\sigma''(\rho_0)}{8D^2}
\]
Correspondence between the (Gaussian) integration of small fluctuations AND discreteness of Bethe root repartition.

More general?
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
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More general?

Repartition of Bethe roots for $s > s_c$?

Fluctuating hydrodynamics for quantum chains?
Dynamical phase transition \cite{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 non-uniform saddle-point profile for \( \lambda > \lambda_c \)

\( \lambda_c = \frac{\pi^2}{\sigma(\rho_0)} \) (can be large!)
Dynamical phase transition [VL, Garrahan, van Wijland, JPA 45 175001]

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

Scaling

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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</tr>
<tr>
<td>( \circ \circ \circ \circ \circ \circ \circ \circ \circ \circ \circ \circ \circ \circ \circ \circ \circ ) &amp; ( \downarrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \downarrow \downarrow \downarrow \downarrow \downarrow ) ( \text{(in fact, superp. of } e^{i\theta} \downarrow \downarrow \uparrow \uparrow \downarrow \downarrow \ldots )</td>
<td></td>
</tr>
<tr>
<td>time ( t ) ((\text{steady state: } t \to +\infty))</td>
<td>inverse temp. ( \beta ) ((\text{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}^{XXZ}(\Delta) = \text{Tr } e^{-\beta \mathbb{H}_\Delta} )</td>
</tr>
</tbody>
</table>
Saddle-point equations for the profile $\rho(x)$ take the form

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

![Graph showing the oscillations and the non-uniform profile](image-url)
Sketch of derivation

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

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

Motion in “time” $x$ of a particle of “position” $\rho$ in a “Potential energy” $E_P(\rho)$

“oscillations” depict the non-uniform profile $\rho(x)$
Excitations

[Cheneau, VL, work in progress]

What about solutions with \textit{more than one} kink\textendash{}anti-kink?

\[ \varphi(\lambda) \]

\[ \begin{align*}
\lambda_c & \quad 4\lambda_c \\
0 & \quad 50 \quad 100 \quad 150 \quad 200
\end{align*} \]

Corresponding profiles \( \rho(x) \)

\[ \begin{align*}
0.0 & \quad 0.2 \quad 0.4 \quad 0.6 \quad 0.8 \quad 1.0 \\
0.0 & \quad 0.2 \quad 0.4 \quad 0.6 \quad 0.8 \quad 1.0
\end{align*} \]
Beyond the critical point

Smaller sizes

Small sizes: the ground state

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

\( \varphi(\lambda) \)

Vivien Lecomte (LPMA – Paris VI-VII)

SSEP and QPT in XXZ spin chains

Kyoto – 19/09/2014
Small sizes: the full spectrum

$L = 9$ sites

$N_0 = 3$ particles
Small sizes: the full spectrum [preliminary!]

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

\begin{figure}
\centering
\includegraphics[width=\textwidth]{spectrum.png}
\end{figure}
Small sizes: the full spectrum

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

infinite-size ground state
infinite-size excited states
Small sizes: the full spectrum

\[ L = 9 \text{ sites} \]
\[ N_0 = 3 \text{ particles} \]

infinite-size ground state
infinite-size excited states

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

[preliminary!]
Summary

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

Macroscopic approach:
- action of fluctuating hydrodynamics
- saddle-point method, dynamical phase transition
Summary

Microscopic approach:
- operator formalism
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Macroscopic approach:
- action of fluctuating hydrodynamics
- saddle-point method, dynamical phase transition

Questions:
- Finite-size crossover around a quantum phase transition? Between:
  - Luttinger Liquid ($s \rightarrow -\infty$)
  - 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:

- Vivien Lecomte, Juan P. Garrahan, Frédéric van Wijland  
- Cécile Appert-Rolland, Bernard Derrida, Vivien Lecomte and  
  Frédéric van Wijland  