Exact solution for the macroscopic fluctuation theory for the symmetric simple exclusion process

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(Based on a collaboration with K. Mallick, H. Moriya)

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Reference: arXiv:2202.05213

0. Introduction and Result

- Large deviation properties of SEP have been believed to be described by MFT developed by Jona-Lasinio et al since around 2000. The large deviation principle had been established by Kipnis, Olla, Varadhan 1989. The MFT equations for SEP are coupled nonlinear PDEs.

- Microscopic calculations using Bethe ansatz

  2009 Derrida-Gershenfeld: Current at the origin

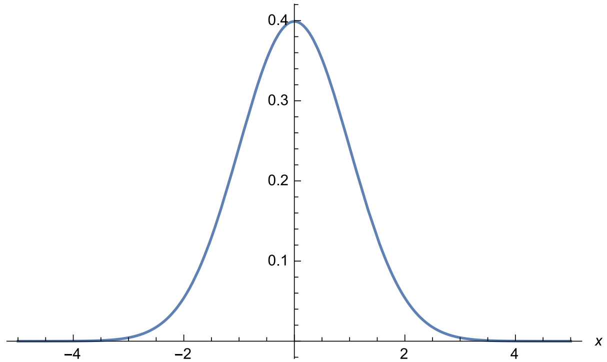
  2017 Imamura-Mallick-TS: Any position and tagged particle

- For the first time we solve t-dependent MFT equations for SEP by mapping them to a classical integrable system (AKNS system). We use a non-local generalization of the canonical Cole-Hopf transformation.

Typical fluctuations and large deviation: a random walk

Let $\xi_i, i = 1, 2, \ldots$ be i.i.d. Bernoulli random variables:
$\mathbb{P}[\xi_i = 1] = \mathbb{P}[\xi_i = -1] = \frac{1}{2}$ and set

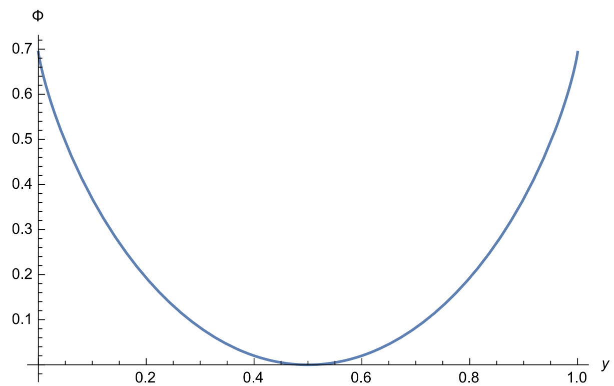
$$X_n = \xi_1 + \cdots + \xi_n$$



Average and variance

$$\langle X_n \rangle = 0, \quad \langle X_n^2 \rangle_C = n$$

Typical fluctuation is on the scale $X_n = O(\sqrt{n})$ and is Gaussian.



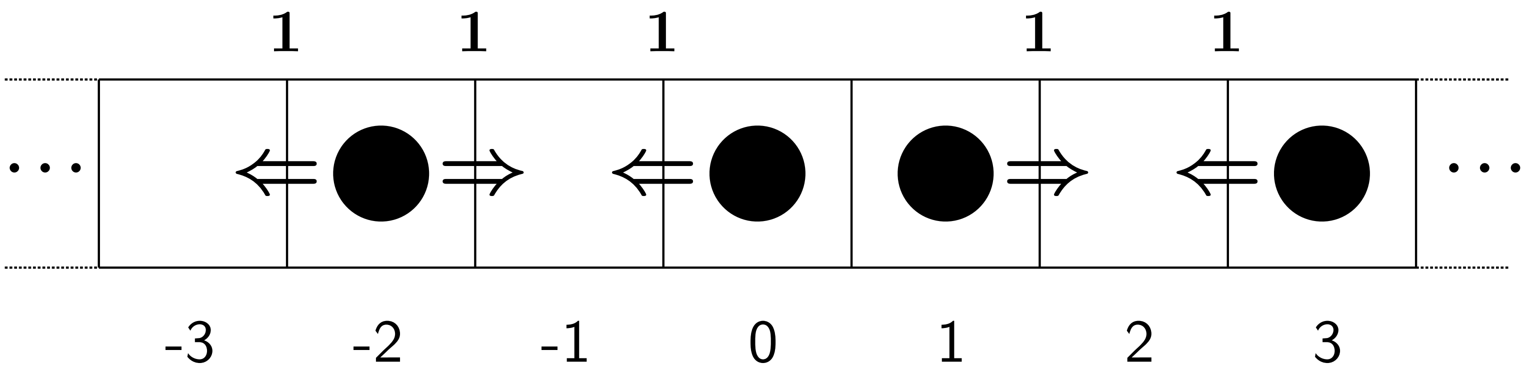
The large deviation is described as

$\mathbb{P}[X_n = ny] \sim e^{-\Phi(y)n}$ $\Phi(y)$: rate function

$$\Phi(y) = y \log y + (1-y)\log(1-y) + \log 2$$

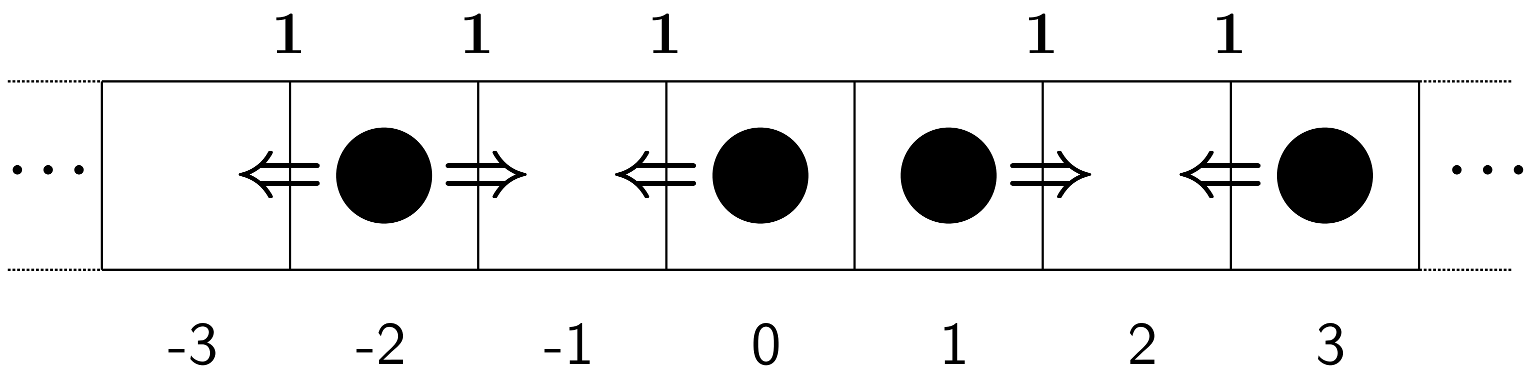
1. The model

1D SEP(symmetric simple exclusion process) on $\mathbb{Z}$



Let $\eta_x(t) = 0$ (or 1) when site x is empty (or occupied) at t.

Current



Q_t: Integrated current at the bond (0,1) for time $[0, t]$

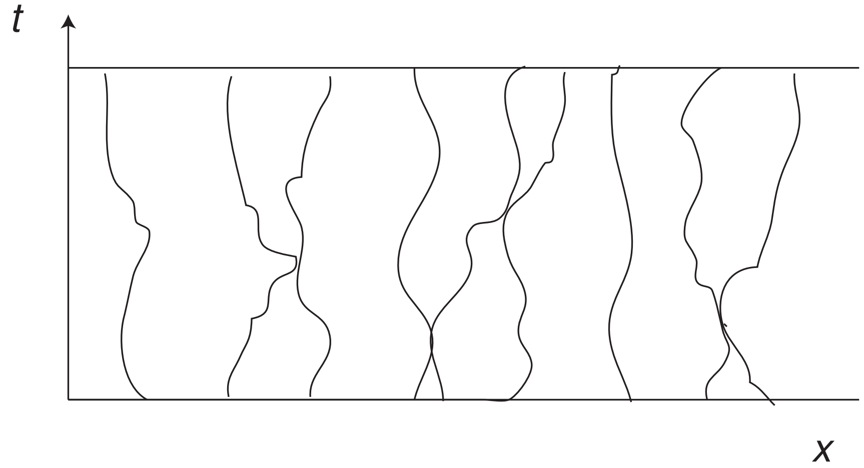
X_t: Tagged particle position starting from the origin

We are interested in fluctuations of these quantities.

Browinian motions with reflection (RBM)

Also called the Harris system

Can be obtained as Brownian motion limit of SEP



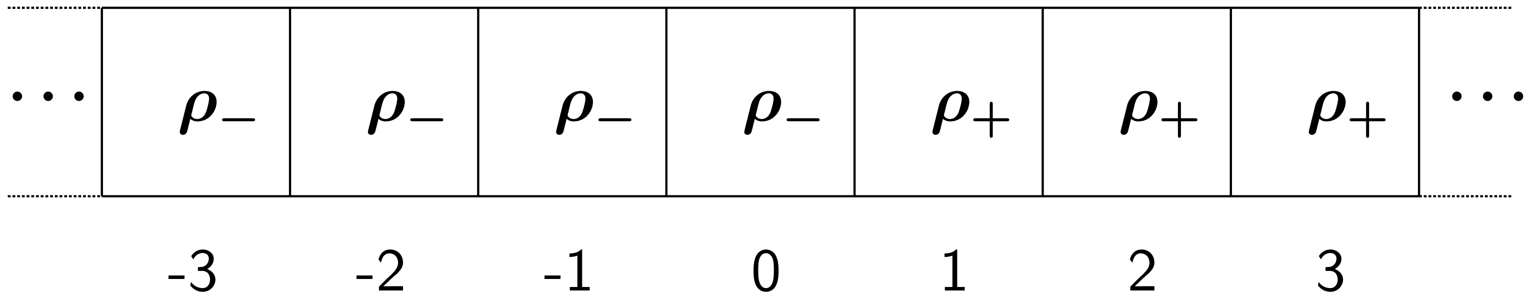
We can consider the corresponding $\boldsymbol{Q_t}$ and $\boldsymbol{X_t}$.

Can be reduced to those of independent BMs.

Initial condition

In principle our scheme should work for general initial condition.

Here mainly step i.c. with two densities: All sites are independent and each site is occupied with prob. ρ_- on left and ρ_+ on right.



Stationary when $\rho_+ = \rho_- = \rho$.

Typical fluctuations of X_T, Q_T for uniform density ρ

SEP Gaussian on the scale $O(T^{1/4})$

Tagged particle (Arratia 1983)

$$\langle X_t \rangle = 0$$

$$\langle X_T^2 \rangle \simeq \frac{2(1-\rho)}{\rho}\sqrt{\frac{T}{\pi}}$$

Current at the origin

$$\langle Q_t \rangle = 0$$

$$\langle Q_T^2 \rangle \simeq 2\rho(1-\rho)\sqrt{\frac{T}{\pi}}$$

The exponent $\frac{1}{4}$ has been confirmed in experiments (colloids).

Large deviation

Large deviation for the current at the origin Q_T

$$\mathbf{Prob}\left(\frac{Q_T}{\sqrt{T}} = q\right) \simeq \exp[-\sqrt{T}\Phi(q)]$$

Can we compute the rate function Φ for SEP?

The problem is equivalent to the calculation of μ in

$$\langle e^{\lambda Q_T} \rangle \simeq e^{\sqrt{T}\mu(\lambda)}$$

Φ and μ are related by Legendre transform

$$\Phi(q) = \min_{\lambda}[\lambda q - \mu(\lambda)]$$

We are also interested in density profiles realizing the rare event.

2. Macroscopic fluctuation theory (MFT)

For a system described by the Langevin equation

$$\partial_t \rho = \partial_x [\partial_x \rho + \sqrt{\sigma(\rho)}\xi(x,t)]$$

where $\sigma(\rho)$ is the mobility ($\sigma(\rho) = 2\rho(1-\rho)$ for SEP),

$$\langle e^{\lambda Q_T} \rangle = \int \mathcal{D}[\rho, H] e^{S[\rho,H]}$$

$$S[\rho, H] = \lambda Q_T - \mathcal{F}_0[\rho(x,0)] - \int_0^T dt \int_{-\infty}^{\infty} dx (H \partial_t \rho + \mathcal{H})$$

$$\mathcal{F}_0[\rho(x,0)] = \int_{-\infty}^{\infty} dx \int_{\bar{\rho}(x)}^{\rho(x,0)} dr \frac{\rho(x,0) - r}{\sigma(r)}$$

$$\mathcal{H}[\rho, H] = (\partial_x \rho)(\partial_x H) - \frac{1}{2}\sigma(\rho)(\partial_x H)^2$$

for local equilibrium state with density $\bar{\rho}(x)$.

MFT equations

Large T behavior is dominated by the maximum of the action S.

The equations for the optimal path in ρ, H are given by

$$\partial_t \rho = \partial_x[\partial_x \rho - \sigma(\rho)\partial_x H]$$

$$\partial_t H = -\partial_x^2 H - (1-2\rho)(\partial_x H)^2$$

accompanied by the conditions at the initial and the final times:

$$H(x,T) = \lambda\theta(x)$$

$$H(x,0) = \lambda\theta(x) + f'(\rho(x,0)) - f'(\bar{\rho}(x))$$

where $f'(\rho) = \log \frac{\rho}{1-\rho}$.

Below we focus on the case $\bar{\rho}(x) = \rho_-\theta(-x) + \rho_+\theta(x)$.

For RBM with $\sigma(\rho) = 2\rho$, the equations are linearlized by the canonical Cole-Hopf transformation $Q = \rho e^{-H}, P = e^{H}$.

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where $f'(\rho) = \log \frac{\rho}{1-\rho}$.

Below we focus on the case $\bar{\rho}(x) = \rho_-\theta(-x) + \rho_+\theta(x)$.

For SEP with $\sigma(\rho) = 2\rho(1 - \rho)$.

Today we solve the equations for SEP!

3. Mapping MFT equations for SEP to AKNS system

Generalized canonical Cole-Hopf transformation

$$u(x,t) = \frac{1}{1-2\rho}\frac{\partial}{\partial x}\frac{\sigma(\rho)}{2}\exp\left[-\int_{-\infty}^{x} dy(1-2\rho)\partial_y H\right]$$

$$v(x,t) = -\frac{1}{1-2\rho}\frac{\partial}{\partial x}\exp\left[\int_{-\infty}^{x} dy(1-2\rho)\partial_y H\right]$$

MFT equations become

$$\partial_t u(x,t) = \partial_{xx} u(x,t) - 2u(x,t)^2 v(x,t)$$

$$\partial_t v(x,t) = -\partial_{xx} v(x,t) + 2u(x,t) v(x,t)^2$$

This is the AKNS (Ablowitz-Kaup-Newell-Segur) system!

When $\rho \to 0$ (RBM limit), the map becomes canonical CH.

Three constants ω, Λ, K

In terms of u, v, the conditions at $t = 0, T$ for ρ, H become

$$u(x, 0) = \omega\delta(x)$$
$$v(x, T) = \delta(x)$$

Using the freedom, $u \to Ku$ and $v \to K^{-1}v$, we write

$$u(x, T) = \begin{cases} K\partial_x\rho(x, T) & x < 0 \\ Ke^{-\Lambda}\partial_x\rho(x, T) & x > 0 \end{cases}$$

$$v(x, 0) = \begin{cases} -2K^{-1}\sigma(\rho_-)^{-1}\partial_x\rho(x, 0) & x < 0 \\ -2K^{-1}\sigma(\rho_+)^{-1}e^{\Lambda}\partial_x\rho(x, 0) & x > 0 \end{cases}$$

$\Lambda = \int_{-\infty}^{+\infty} dy(1 - 2\rho)\partial_y H(y, T)$ is a conserved quantity.

Related works

2007 Tailleur Kurchan Lecomte Mapping to a classical spin system

2009 Derrida Gershenfeld Large deviation for current at origin

2016 Janas Kamenev Meerson Integrability for weak noise KPZ

2017 Imamura Mallick TS Large deviation for tracer

2021 Krajenbrink Le Douss sal Solution for weak noise KPZ

2021 Grabsch Poncet Rizkallah Illien Benichou

Study final density profile of SEP (not MFT)

2021 Bettelheim Smith Meerson Solution to MFT for KMP model

2022 Mallick Moriya TS Solution to MFT for SEP

2022 Tsai, BSM, KLD,...

From abstract of a talk by Jona-Lasinio on May 11

Title: "Integrability in the macroscopic fluctuation theory (MFT)"

A natural question is to what extent this theory [MFT] can be supported by mathematically controllable models. So far it has been confirmed for the stationary states of various models but the time evolution is more difficult. Recent works have used successfully the inverse scattering method (ISM) to solve exactly the time dependent variational equations of the weak noise KPZ equation (Krajenbrink, Le Doussal), of the Kipnis-Marchioro-Presutti model (Bettelheim, Smith, Meerson) and very recently Mallick, Mor[i]ya and Sasamoto have solved exactly the difficult case of the symmetric simple exclusion process (SSEP). These results open new perspectives.

4. Solving AKNS system

Auxiliary linear problem

$$\frac{\partial}{\partial x}\Psi(x,t) = U(x,t;k)\Psi(x,t)$$
$$\frac{\partial}{\partial t}\Psi(x,t) = V(x,t;k)\Psi(x,t)$$

where

$$U = \begin{pmatrix} -ik & v(x,t) \\ u(x,t) & ik \end{pmatrix}$$

$$V = \begin{pmatrix} 2k^2 + u(x,t)v(x,t) & 2ikv(x,t) - \partial_x v(x,t) \\ 2iku(x,t) + \partial_x u(x,t) & -2k^2 - u(x,t)v(x,t) \end{pmatrix}$$

Compatibility $\frac{\partial U}{\partial t} - \frac{\partial V}{\partial x} + [U,V] = 0$ gives the AKNS system.

Scattering data

Scattering data: $a(k), \bar{a}(k), b(k), \bar{b}(k)$

The incoming/outgoing plane waves from $x \to -\infty$

$$\phi(x;k) \sim \begin{pmatrix} e^{-ikx} \\ 0 \end{pmatrix} \quad \text{and} \quad \bar{\phi}(\mathrm{x};\mathrm{k}) \sim - \begin{pmatrix} 0 \\ e^{ikx} \end{pmatrix}$$

will scatter at $x \to +\infty$ as follows

$$\phi(x;k) \sim \begin{pmatrix} a(k)e^{-ikx} \\ b(k)e^{ikx} \end{pmatrix} \quad \text{and} \quad \bar{\phi}(x;k) \sim \begin{pmatrix} \bar{b}(k)e^{-ikx} \\ -\bar{a}(k)e^{ikx} \end{pmatrix}$$

Scattering

Solve the scattering problem for $\partial\Psi/\partial x = U\Psi$ in terms of

$\hat{u}_{\pm}(k) = \int_{\mathbb{R}_{\mp}} u(x,T) e^{-2ikx} dx$, $\hat{v}_{\pm}(k) = \int_{\mathbb{R}_{\pm}} v(x,0) e^{2ikx} dx$,
$\hat{u}(k) := \hat{u}_{+}(k) + \hat{u}_{-}(k)$, $\hat{v}(k) := \hat{v}_{+}(k) + \hat{v}_{-}(k)$.

At $t = 0$, we have

$$a(k,0) = 1 + \omega \hat{v}_{+}(k), \quad b(k,0) = \omega,$$

$$\bar{a}(k,0) = 1 + \omega \hat{v}_{-}(k), \quad \bar{b}(k,0) = -\left[\hat{v}(k) + \omega \hat{v}_{+}(k) \hat{v}_{-}(k)\right].$$

At $t = T$, we have

$$a(k,T) = 1 + \hat{u}_{+}(k), \quad b(k,T) = \hat{u}(k) + \hat{u}_{+}(k)\hat{u}_{-}(k),$$

$$\bar{a}(k,T) = 1 + \hat{u}_{-}(k), \quad \bar{b}(k,T) = -1.$$

Time evolutioin

Solving time evolution $\partial\Psi/\partial t = V\Psi$ in terms of $a, \bar{a}, b, \bar{b}$,

$$a(k,t) = a(k,0), \quad b(k,t) = b(k,0)e^{-4k^2 t}$$
$$\bar{a}(k,t) = \bar{a}(k,0), \quad \bar{b}(k,t) = \bar{b}(k,0)e^{4k^2 t}$$

Time evolutions of the MFT equations for SEP become so simple!

Riemann-Hilbert problem

Combining the above, the problem reduces to

$$[\hat{u}_+(k) + 1]\,[\hat{u}_-(k) + 1] = 1 + \omega e^{-4k^2 T}$$

By taking log, we find

$$\hat{u}_\pm(k) + 1 = \exp\left[\pm\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{\log(1+\omega e^{-4q^2T})}{q-k\mp i\epsilon}dq\right]$$

$$\left[\text{Use} \quad \pm\frac{1}{\pi i}\int_{-\infty}^{\infty}\frac{e^{-q^2}}{q-k\mp i\epsilon}dq = e^{-k^2}\mathrm{erfc}(\mp ik)\right]$$

$$= \exp\left[-\frac{1}{2}\sum_{n=1}^{\infty}\frac{(-\omega e^{-4k^2T})^n}{n}\mathrm{erfc}(\mp i\sqrt{4nT}k)\right]$$

We can also determine $\hat{v}_\pm(k)$ and calculate $u(x,T)$ and $v(x,0)$.

Formulas of ω, Λ, K

The results are

$$\omega = (e^{\lambda} - 1)\rho_-(1 - \rho_+) + (e^{-\lambda} - 1)\rho_+(1 - \rho_-)$$

$$e^{\Lambda} = e^{\lambda}\frac{1 + (e^{-\lambda} - 1)\rho_+}{1 + (e^{\lambda} - 1)\rho_-}$$

$$K = -2\sinh(\lambda/2)e^{\Lambda/2}$$

Rem: The parameter ω has been known to appear in various related problems for SEP.

Determination of ω, Λ

The solution to

$$\frac{\partial}{\partial x}\Omega(x,t) = U(x,t;0)\Omega(x,t)$$

is written in the form

$$\Omega(x,t) = \begin{pmatrix} Ce^{\int_{-\infty}^{x} dy(1-\rho)\partial_y H} & Ce^{-\int_{-\infty}^{x} dy\rho\partial_y H} \\ -(1-\rho)e^{\int_{-\infty}^{x} dy\rho\partial_y H} & \rho e^{-\int_{-\infty}^{x} dy(1-\rho)\partial_y H} \end{pmatrix}$$

$\Omega(x,t)\Omega^{-1}(y,t)$ connects the solutions at x and y and so

$$\lim_{\substack{x\to+\infty \\ y\to-\infty}} \Omega(x,t)\Omega^{-1}(y,t) = \begin{pmatrix} a(0,t) & -\bar{b}(0,t) \\ b(0,t) & \bar{a}(0,t) \end{pmatrix}$$

Using

$$\rho(x,t) \sim \rho_-, \quad H(x,t) \sim 0, \quad \text{as} \quad x \to -\infty,$$
$$\rho(x,t) \sim \rho_+, \quad H(x,t) \sim \lambda, \quad \text{as} \quad x \to +\infty,$$

Ω is written as

$$\begin{pmatrix} C_1[1+(e^{\lambda}-1)\rho_-] & -C_2(e^{\lambda}-1) \\ -C_2^{-1}[r_- - e^{-\lambda}r_+] & C_1^{-1}[1+(e^{-\lambda}-1)\rho_+] \end{pmatrix}$$

with $r_\pm = \rho_\pm(1-\rho_\mp)$ and two constants given by $C_1 = e^{\Lambda/2-\lambda/2}$ and $C_2 = CC_1$.

Λ can be evaluated by taking the ratio of the diagonal elements.

Multiplying the off-diagonal elements and using $\bar{b}(0,0) = \bar{b}(0,T) = -1$, one can determine $\omega = b(0,0)$.

Determination of K

We use the mass conservation law

$$\int_{\mathbb{R}} dx[\rho(x,T) - \rho(x,0)] = 0.$$

Insert $\rho(x,0), \rho(x,T)$ as integrals of $u(x,T), v(x,0)$ and use

$$\int_{\mathbb{R}_\mp} xu(x,T)dx = \frac{\hat{u}'_\pm(0)}{-2i} = \pm\frac{\sqrt{T}}{\sqrt{\pi}}\mathrm{Li}_{1/2}(-\omega)\sqrt{1+\omega}$$

$$\int_{\mathbb{R}_\pm} xv(x,0)dx = \frac{\hat{v}'_\pm(0)}{2i} = \mp\frac{\sqrt{T}}{\sqrt{\pi}}\mathrm{Li}_{1/2}(-\omega)\frac{\sqrt{1+\omega}}{\omega}$$

with the polylogarithm of order s, $\mathrm{Li}_s(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^s}$.

5. Results: Profiles of ρ, H at $t = T$

At $t = T$, for ρ,

$$\rho(x,T) = \rho_- + A_- \int_{-\infty}^{x} u(y,T)dy, \quad x < 0$$

$$\rho(x,T) = \rho_+ + A_+ \int_{x}^{\infty} u(y,T)dy, \quad x > 0$$

$$A_\pm = -\frac{1}{e^{\mp\lambda} - 1}\sqrt{\frac{1 + (e^{\mp\lambda} - 1)\rho_\pm}{1 + (e^{\pm\lambda} - 1)\rho_\mp}}$$

For H,

$$H(x,T) = \lambda\theta(x)$$

Profiles of ρ, H at $t = 0$

At $t = 0$, for ρ,

$$\rho(x,0) = \rho_- + B_- \int_{-\infty}^{x} v(y,0)dy, \quad x < 0$$

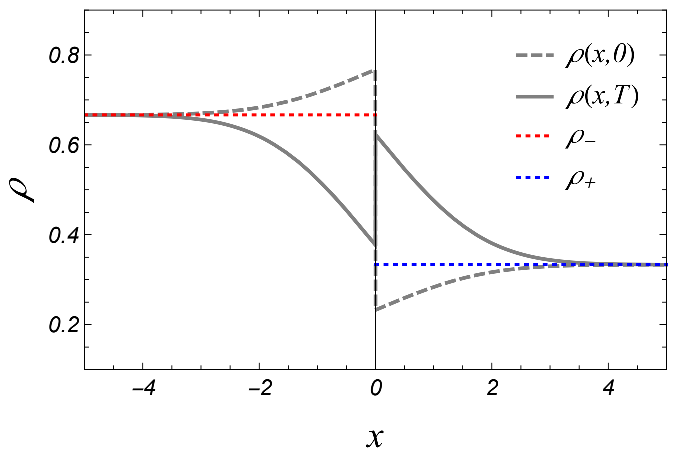
$$\rho(x,0) = \rho_+ + B_+ \int_{x}^{\infty} v(y,0)dy, \quad x > 0$$

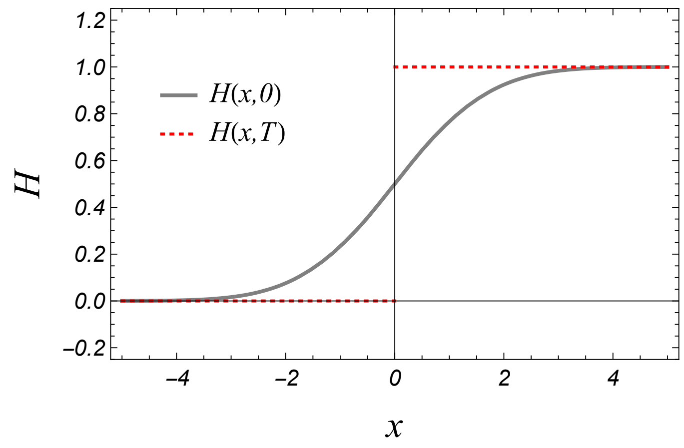
$$B_\pm = -2\sinh^2(\lambda/2)e^{\mp\Lambda}\sigma(\rho_\pm)A_\pm$$

$H(x,0)$ is determined by

$$H(x,0) = \lambda\theta(x) + f'(\rho(x,0)) - f'(\bar{\rho}(x))$$

Figures for the profiles





Optimal profiles of ρ (left) and H (right) at $t = 0$ and at $t = T$, with $\rho_+ = 1/3$, $\rho_- = 2/3$, $\lambda = 1$ and $T = 1$.

Cumulant generating function

Noting $\frac{d\mu}{d\lambda} = Q_T/\sqrt{T}$ and calculating the total current Q_T from the profiles at $t = 0$ and $t = T$, we obtain

$$\mu(\lambda) = \frac{1}{\sqrt{\pi}} \sum_{n=1}^{\infty} \frac{(-1)^{n-1}\omega^n}{n^{3/2}}$$

This agrees with the result of Derrida Gershenfeld 2009, giving the first analytic confirmation of the prediction of MFT for an interacting model in the time dependent regime!

Summary

- We have presented the first exact solution to the MFT equation for SEP by mapping them to the classically integrable AKNS system.

  This was achieved by our new non-local generalization of the canonical Cole-Hopf transformation.

- The solution to the case of step i.c. with two densities agrees with the previous result by microscopic calculation. This is the first analytic confirmation of the prediction of MFT for an interacting model in the time dependent regime. We could also calculate the densities at $t = 0, T$.

- Various generalizations should be possible.

RBM and SEP 4th moment by MFT

Krapivsky Mallick Sadhu 2014

For the uniform density (ρ) case. By solving the MFT equation,

$$\log \text{Prob}[X_t = \xi\sqrt{t}]/\sqrt{t} \sim -\rho(\sqrt{A(\xi)} - \sqrt{A(-\xi)})^2$$

with

$$A(\xi) = \frac{1}{2}\int_{\xi}^{\infty} dz \text{erfc}(z)$$

For SEP, MFT was applied perturbatively. They found

$$\langle X_t^4 \rangle \simeq \frac{2(1-\rho)}{\rho^3} a(\rho)\sqrt{\frac{t}{\pi}}$$

$$a(\rho) = 1 - [4 - (8 - 3\sqrt{2})\rho](1-\rho) + \frac{12}{\pi}(1-\rho)^2$$

The question was to find a formula for general $\langle X_t^n \rangle$.