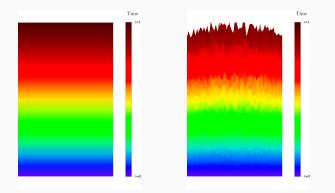
A journey from classical integrability to the large deviations of the Kardar-Parisi-Zhang equation

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Quantinuum & Cambridge Quantum Computing

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The stochastic Kardar-Parisi-Zhang growth of an interface



Kardar-Parisi-Zhang equation ('85)

Consider a height field h(x, t) obeying

$$\partial_t h(x,t) = \partial_x^2 h(x,t) + (\partial_x h(x,t))^2 + \sqrt{2} \xi(x,t) ,$$

where $\xi(x, t)$ is a standard white noise.

Physics motivation

Since its birth in 1985, the KPZ equation was applied to describe

- Growth of interfaces
- Burgers turbulence
- Directed polymers in random media
- Chemical reaction fronts
- Slow combustion
- Coffee stains
- Conductance fluctuations in Anderson localization
- Bose Einstein superfluids
- Quantum entanglement growth
- Spin-chain correlations

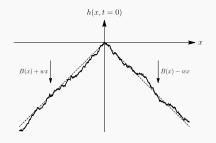
▶ ...

A few geometries of interest

Full-space

 $x \in \mathbb{R}$

- Flat h(x, t = 0) = 0
- Brownian $h(x, t = 0) = \mathcal{B}(x) - w|x|$
- ► Droplet (wedge) $h(x, t = 0) = -w|x| + \log(\frac{w}{2}),$ with a slope $w \gg 1$



Exact solutions have been found

DropletSasamoto, Spohn ; Calabrese, Le Doussal, Rosso ;
Dotsenko ; Amir, Corwin, Quastel ('10)FlatCalabrese, Le Doussal ('11)BrownianImamura, Sasamoto ('12),
Borodin, Corwin, Ferrari, Veto ('14)

Important recent effort on the half-space problem with b.c. $\partial_x h(x, t) |_{x=0} = A$

Exact solution to the KPZ equation with droplet data

Recall that the droplet data is $h(x, 0) = -w|x| + \log(w/2)$ with $w \gg 1$, or equivalently $\exp[h(x, 0)] = \delta(x)$, then

Result (Exact solution for the droplet initial condition)

$$\mathbb{E}_{\mathrm{KPZ}}\left[\exp\left(-ze^{h(0,t)+\frac{t}{12}}\right)\right] = \mathrm{Det}[I - \sigma_{z,t}K_{\mathrm{Ai}}]_{\mathbb{L}^{2}(\mathbb{R})}.$$

where $\mathbb{E}_{\text{KPZ}} \equiv$ average over the KPZ white noise. K_{Ai} is the Airy kernel, $K_{\text{Ai}}(u, u') = \int_0^\infty dr \operatorname{Ai}(r+u) \operatorname{Ai}(r+u')$, the weight $\sigma_{z,t}$ is the Fermi factor

$$\sigma_{z,t}(u) = \frac{z}{z + e^{-t^{1/3}u}}$$

Can we extract direct information on the height from this ? Let us focus on short times!

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Height distribution at short times

The probability density of the centered height $H(t) = h(0, t) - \langle h(0, t) \rangle$ is given by a Large Deviation Principle at short time $t \ll 1$

$$P(H,t) \sim \exp\left(-rac{\Phi(H)}{\sqrt{t}}
ight)$$

where the large deviation function $\boldsymbol{\Phi}$ has the universal properties

$$\Phi(H)\simeq egin{cases} c_{-\infty}|H|^{5/2}, & H
ightarrow -\infty\ c_0\,H^2, & |H|\ll 1\ c_{+\infty}H^{3/2}, & H
ightarrow +\infty \end{cases}$$

the coefficients $c_{-\infty}, c_0, c_{+\infty}$ depend on the initial condition.

Why studying the large deviations ?

The large deviations of KPZ correspond to excess or deficit of growth. If the growing substrate is sufficiently long, disparate regions will see roughly independent growth. The maximal and minimal height of the entire substrate, hence its roughness, will be determined by the one-point tail behaviors. Since the roughness of the substrates determines device performance, large deviations dictate failure rates.

The cheese or the dessert ? the obnoxious French waiter dilemma

$${\sf P}({\sf H},t)\sim \expig(-rac{\Phi({\cal H})}{\sqrt{t}}ig)$$

The cheese

Fredholm determinant approach

- Exploits the few explicit solutions obtained through quantum integrability;
- Provides complete large deviations and sub-contributions.

$$\left\{egin{array}{l} e^{H}=\Psi'(z)\ \Phi(H)=\Psi(z)-z\Psi'(z)\ \Psi(z)=-rac{1}{\sqrt{4\pi}}\mathrm{Li}_{5/2}(-z) \end{array}
ight.$$

The dessert

Weak noise theory

- Hydrodynamic framework valid for any initial condition;
- Describes the optimal height and noise history;
- Provides the variance and the tails only analytically.

$$igapla(H)\simeq \left\{egin{array}{c} rac{4}{15\pi}|H|^{5/2},\ H
ightarrow -\infty\ rac{1}{\sqrt{2\pi}}H^2,\ |H|\ll 1\ rac{4}{3}H^{3/2},\ H
ightarrow +\infty \end{array}
ight.$$

The cheese and the dessert: solving the WNT using classical integrability.

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Outline

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Inverse Scattering of the Zakharov-Shabat System Solves the Weak Noise Theory of the Kardar-Parisi-Zhang Equation

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- 1. The Martin-Siggia-Rose approach to large deviations: the landmark of stochastic field theory
- 2. The direct and inverse scattering transforms: the landmark of classical integrability
- 3. Completion of the large-deviation program

Height distribution at short times

To obtain $\Phi(H)$, one defines an intermediate Large Deviation Principle

$$\mathbb{E}_{\text{KPZ}}\left[\exp\left(-\frac{ze^{H(t)}}{\sqrt{t}}\right)\right] \sim \exp\left(-\frac{\Psi(z)}{\sqrt{t}}\right)$$
$$= \int dH P(H, t) \exp\left(-\frac{ze^{H}}{\sqrt{t}}\right)$$
$$= \int dH \exp\left(-\frac{\Phi(H) + ze^{H}}{\sqrt{t}}\right)$$

The large deviation function $\Phi(H)$ can be determined by a Legendre transform!

 Result (Large deviation problem)

 For $t \ll 1$,

 $\Psi(z) = \min_{H} [ze^{H} + \Phi(H)]$

 This is equivalent to the parametric system

 $\left(e^{H} - \Psi'(z)\right)$

$$\begin{cases} e = \Psi(z) \\ \Phi(H) = \Psi(z) - z\Psi'(z) \end{cases}$$

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Zakharov-Shabat solves the large deviations of KPZ

Martin-Siggia-Rose formalism I

Starting from the KPZ equation

$$\partial_{\tau} h(y,\tau) = \partial_y^2 h(y,\tau) + (\partial_y h(y,\tau))^2 + \sqrt{2}\eta(y,\tau)$$

We want to observe $h(0, T) = H - \log \sqrt{T}$, and use the scale $t = \tau/T$, $x = y/\sqrt{T}$ so that

$$\partial_t h(x,t) = \partial_x^2 h(x,t) + (\partial_x h(x,t))^2 + \sqrt{2} T^{1/4} \tilde{\eta}(x,t)$$

Now $t \in [0, 1]$ and if $T \ll 1$, the new unit white noise has a small magnitude: it is a weak noise.

We now write the generating function

$$\mathbb{E}_{\mathrm{KPZ}}\left[\exp\left(-\frac{ze^{H}}{\sqrt{T}}\right)\right]$$

where the expectation is taken with respect to the white noise

$$\mathcal{D}\tilde{\eta}\exp\big(-\frac{1}{2}\iint_{xt}\mathrm{d}x\mathrm{d}t\,\tilde{\eta}(x,t)^2\big)$$

Martin-Siggia-Rose formalism II

Then the generating function

$$\mathbb{E}_{\mathrm{KPZ}}\left[\exp\left(-\frac{ze^{H}}{\sqrt{T}}\right)\right]$$
$$=\int \mathcal{D}h\mathcal{D}\tilde{\eta}\exp\left(-\frac{ze^{H}}{\sqrt{T}}-\frac{1}{2}\iint_{xt}\tilde{\eta}^{2}\right)\delta(\partial_{t}h-\partial_{x}^{2}h-(\partial_{x}h)^{2}-\sqrt{2}T^{1/4}\tilde{\eta})$$

Response field

One introduces the response field ϱ/\sqrt{T} such that

$$\delta(\partial_t h - \partial_x^2 h - (\partial_x h)^2 - \sqrt{2}T^{1/4}\tilde{\eta}) = \int \mathcal{D}\varrho \exp\left(-\frac{\int\int_{xt} \varrho(\partial_t h - \partial_x^2 h - (\partial_x h)^2 - \sqrt{2}T^{1/4}\tilde{\eta})}{\sqrt{T}}\right)$$

Martin-Siggia-Rose formalism III

One then integrates over the noise and

 Result (MSR large deviation action)

 overall the MSR action at short time reads

 $\mathbb{E}_{\mathrm{KPZ}}\left[\exp\left(-\frac{ze^{H}}{\sqrt{T}}\right)\right]$
 $=\int \mathcal{D}h\mathcal{D}\varrho\exp\left(-\frac{ze^{H}+\iint_{xt}\varrho(\partial_{t}h-\partial_{x}^{2}h-(\partial_{x}h)^{2}-\varrho)}{\sqrt{T}}\right)$

 This action is amonghing to a coddle point evaluation!

This action is amenable to a saddle-point evaluation!

Hydrodynamic description

The optimal height and noise verify the non-linear hydrodynamic system

$$\partial_t h = \partial_x^2 h + (\partial_x h)^2 + 2\varrho$$

 $-\partial_t \varrho = \partial_x^2 \varrho - 2\partial_x (\varrho \partial_x h)$

Define the Cole-Hopf transform

$$Q(x,t) = e^{h(x,t)}, \qquad -zP(x,t)Q(x,t) = \varrho(x,t)$$

Then it is transformed into the $\{P, Q\}$ system

$$\partial_t Q = \partial_x^2 Q - 2zPQ^2$$

 $-\partial_t P = \partial_x^2 P - 2zP^2 Q$

Main takeway I

Both these systems can be solved explicitly without approximation.

Intermediate summary of the large deviation problem

Result (KPZ large deviation function)

The large deviation function is given by

$$\Phi(H) = z^2 \int_0^1 \mathrm{d}t \int_{\mathbb{R}} \mathrm{d}x \ P(x,t)^2 Q(x,t)^2$$

with the $\{P, Q\}$ system

$$\partial_t Q = \partial_x^2 Q - 2zPQ^2$$
$$-\partial_t P = \partial_x^2 P - 2zP^2 Q$$

with initial / boundary conditions

$$\underbrace{Q(x,0) = \delta(x)}_{\text{nitial condition of KPZ}}, \underbrace{P(x,1) = \delta(x)}_{\text{position of the large deviation}}, \underbrace{Q(x = 0, t = 1) = e^{H}}_{\text{value of the conditioned height}}.$$

The optimal height is given by $h = \log Q$ and the optimal noise by $\varrho = -zPQ$.

And now what ? The system is non-linear, not very friendly...

That is where Zakharov and Shabat come to our rescue





Zakharov and Shabat tell us how linearize the problem.

The $\{P, Q\}$ system is classically integrable!

We have the existence of a Lax pair: define a 2-component vector $\vec{v} = (v_1, v_2)^T$ depending on (x, t, k) (space, time, Fourier) and the linear differential system

$$\partial_x \vec{v} = U_1 \vec{v}, \qquad U_1 = \begin{pmatrix} -ik/2 & zP(x,t) \\ Q(x,t) & ik/2 \end{pmatrix}$$

and

$$\partial_t \vec{v} = U_2 \vec{v}$$

Result (Compatibility)

The compatibility equation is

$$\partial_{xt}\vec{v} = \partial_{tx}\vec{v}$$
 or $\partial_t U_1 - \partial_x U_2 + [U_1, U_2] = 0.$

This is precisely the $\{P, Q\}$ system.

The spatial equation is the Zakharov-Shabat system with non-Hermitian potentials *P*, *Q*. The ZS system is the landmark of the AKNS class of integrable non-linear problems (comprising KdV, mKdV, NLS...) solvable using scattering theory.

Definition of the scattering problem

Let $\vec{v} = e^{k^2 t/2} \phi$ with $\phi = (\phi_1, \phi_2)^T$ and $\vec{v} = e^{-k^2 t/2} \bar{\phi}$ be two independent solutions of the ZS linear problem such that

$$\phi \underset{x \to -\infty}{\simeq} \begin{pmatrix} e^{-\mathrm{i}kx/2} \\ 0 \end{pmatrix}, \qquad \bar{\phi} \underset{x \to -\infty}{\simeq} \begin{pmatrix} 0 \\ -e^{\mathrm{i}kx/2} \end{pmatrix}$$

and

$$\phi \underset{x \to +\infty}{\simeq} \begin{pmatrix} \mathsf{a}(k,t)e^{-\frac{ikx}{2}} \\ \mathsf{b}(k,t)e^{\frac{ikx}{2}} \end{pmatrix} , \ \bar{\phi} \underset{x \to +\infty}{\simeq} \begin{pmatrix} \tilde{b}(k,t)e^{-\frac{ikx}{2}} \\ -\tilde{a}(k,t)e^{\frac{ikx}{2}} \end{pmatrix}$$

$(a, \tilde{a}, b, \tilde{b})$ are called the scattering amplitudes.

The following ratios define the reflection coefficients

$$r(k,t) = rac{b(k,t)}{a(k,t)}, \qquad ilde{r}(k,t) = -rac{ ilde{b}(k,t)}{ ilde{a}(k,t)}$$

Scattering transforms

$$\{Q(x, t = 0), P(x, t = 1)\} \xrightarrow[\text{direct}]{\text{direct}} \{a(k, t), b(k, t)\} \xrightarrow[\text{inverse}]{\text{scattering}}} \{Q(x, t), P(x, t)\}$$

Main takeway II

Both of the direct and inverse scattering transforms are done explicitly.

Our plan:

- **1.** Time dependence: $\{a(k, t), b(k, t)\}$
- **2.** Fourier dependence: $\{a(k, t), b(k, t)\}$

DST - Time-dependence of the scattering coefficients

Plugging

$$\phi \underset{x \to +\infty}{\simeq} \begin{pmatrix} \mathsf{a}(k,t)e^{-\frac{ikx}{2}} \\ \mathsf{b}(k,t)e^{\frac{ikx}{2}} \end{pmatrix} , \ \bar{\phi} \underset{x \to +\infty}{\simeq} \begin{pmatrix} \tilde{b}(k,t)e^{-\frac{ikx}{2}} \\ -\tilde{a}(k,t)e^{\frac{ikx}{2}} \end{pmatrix}$$

into the time equation

$$\partial_t \vec{v} = U_2 \vec{v}$$

One finds that

Result (Time-dependence)

$$a(k, t) = a(k)$$

$$\tilde{a}(k, t) = \tilde{a}(k)$$

$$b(k, t) = b(k)e^{-k^{2}t}$$

$$\tilde{b}(k, t) = \tilde{b}(k)e^{k^{2}t}$$

This is universal and independent of the potentials P, Q !

DST - Fourier-dependence of the scattering coefficients

One then solves the spatial part at t = 0 and t = 1

$$\partial_x \vec{v} = U_1 \vec{v}, \qquad U_1 = \begin{pmatrix} -ik/2 & zP(x,t) \\ Q(x,t) & ik/2 \end{pmatrix}$$

Using

$$Q(x,0) = \delta(x), \quad P(x,1) = \delta(x).$$

One finds that

 $\begin{aligned} & \textit{Result (Fourier-dependence)} \\ & \begin{cases} b(k) = 1 \\ \tilde{b}(k) = -ze^{-k^2} \\ \tilde{a}(k) = a(k)^{\dagger} \\ a(k) = \sqrt{1 + ze^{-k^2}}e^{-i\varphi(k)}, \quad \varphi(k) = \int_{\mathbb{R}} \frac{\mathrm{d}g}{2\pi} \frac{k \log(1 + ze^{-q^2})}{q^2 - k^2} \end{aligned}$

We also have the normalization $a\tilde{a} + b\tilde{b} = 1$, this is universal.

IST using Fredholm determinants

The inverse scattering is solvable by the means of Fredholm determinant: define the Fourier transform of the reflection coefficients

$$A_t(x) = \int_{\mathbb{R}} \frac{\mathrm{d}k}{2\pi} r(k) e^{\mathrm{i}kx - k^2 t}, \qquad B_t(x) = \int_{\mathbb{R}} \frac{\mathrm{d}k}{2\pi} \tilde{r}(k) e^{k^2 t - \mathrm{i}kx}$$

and two linear operators from $\mathbb{L}^2(\mathbb{R}^+)$ to $\mathbb{L}^2(\mathbb{R}^+)$ with respective kernels

$$\mathcal{A}_{xt}(v,v') = A_t(x+v+v'), \qquad \mathcal{B}_{xt}(v,v') = B_t(x+v+v')$$

Result (General solution to the $\{P, Q\}$ system)

The general solution to the $\{P, Q\}$ system is

$$Q(x,t) = \langle \delta | \mathcal{A}_{xt} (I - z \mathcal{B}_{xt} \mathcal{A}_{xt})^{-1} | \delta \rangle$$
$$P(x,t) = \langle \delta | \mathcal{B}_{xt} (I - z \mathcal{A}_{xt} \mathcal{B}_{xt})^{-1} | \delta \rangle$$

where $|\delta\rangle$ is the vector with component $\delta(v)$ so that $\langle\delta|\mathcal{O}|\delta\rangle = \mathcal{O}(0,0)$ for any operator \mathcal{O} (~ selecting a matrix element).

The Fredholm determinant is hidden as: $-zPQ = \partial_x^2 \log \operatorname{Det}(I - z\mathcal{B}_{xt}\mathcal{A}_{xt}).$

But where is the large deviation function ?

We don't want to calculate

$$\Phi(H) = z^2 \int_0^1 \mathrm{d}t \int_{\mathbb{R}} \mathrm{d}x \ P(x,t)^2 Q(x,t)^2$$

We want to be more clever!

What else can we exploit in a classically integrable system ? An infinite amount conserved quantities!

The large deviation function is hidden in the conserved quantities.

Conserved quantities I

Define the Ricatti variable $\Gamma = \frac{v_2}{v_1},$ the Zakharov-Shabat system reads

$$\partial_x \Gamma = ik\Gamma + Q + gP\Gamma^2 \quad \Rightarrow \quad \Gamma = \sum_{n \ge 1} \frac{\Gamma_n(x,t)}{(ik)^n}$$

Result (Infinite amount of conserved quantities)

The ZS system has conserved quantities

$$C(k) = z \int_{\mathbb{R}} \mathrm{d}x P(x, t) \Gamma(x, t, k) = \log a(k)$$

The Laurent series of $\log a(k)$ determines all the conserved quantities

$$\log a(k) = \sum_{n \ge 1} \frac{C_n(x, t)}{(ik)^n}, \qquad C_n = z \int_{\mathbb{R}} \mathrm{d}x \, P(x, t) \Gamma_n(x, t)$$

The first few:
$$C_1 = -z \int_{\mathbb{R}} dx \ PQ, \quad C_3 = \int_{\mathbb{R}} dx \ [-zP\partial_x^2Q + z^2P^2Q^2]$$

Conserved quantities II

Recall that $\log a(k) = -i\varphi(k) + \frac{1}{2}\log(1 + ze^{-k^2})$. Since the last term has a vanishing Laurent series, we have

$$-\mathrm{i} \oint_{\mathbb{R}} \frac{\mathrm{d}q}{2\pi} \, \frac{k \log(1 + z e^{-q^2})}{q^2 - k^2} = -\mathrm{i}\varphi(k) = \sum_{n \ge 1} \frac{C_n(g)}{(\mathrm{i}k)^n}$$

The first one reads

$$C_1 = \frac{1}{\sqrt{4\pi}} \mathrm{Li}_{\frac{3}{2}}(-z)$$

On the other side

$$C_1 = -z \int_{\mathbb{R}} \mathrm{d}x \ P(x, t=1)Q(x, t=1) = -ze^{H}$$

Now recall the parametric representation

$$\begin{cases} e^{H} = \Psi'(z) \\ \Phi(H) = \Psi(z) - z\Psi'(z) \end{cases}$$

Result (Parametric large deviation function)

$$\Psi(z) = -\frac{1}{\sqrt{4\pi}} \mathrm{Li}_{5/2}(-z)$$

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Are we done yet ?

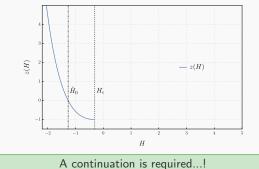
What is the domain of validity of what we have done so far ?

$$\mathbb{E}_{\mathrm{KPZ}}\left[\exp\left(-\frac{ze^{H(t)}}{\sqrt{t}}\right)\right] \sim \exp\left(-\frac{\Psi(z)}{\sqrt{t}}\right)$$

The left hand side exists only for z > 0. Using

$$-ze^{H} = \frac{1}{\sqrt{4\pi}} \mathrm{Li}_{\frac{3}{2}}(-z)$$

and extending to z > -1 allows to obtain $\Phi(H)$ for H < 0.



Zakharov-Shabat solves the large deviations of KPZ

Are we done yet ?

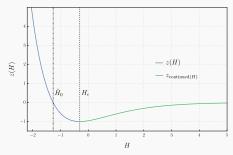
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The left hand side exists only for z > 0. Using

$$-ze^{H}=\frac{1}{\sqrt{4\pi}}\mathrm{Li}_{\frac{3}{2}}(-z)$$

and extending to z > -1 allows to obtain $\Phi(H)$ for $H < H_c$.

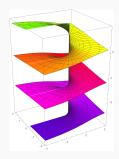


An analytic continuation required...

The phase of $a(k) = \sqrt{1 + ze^{-k^2}}e^{-\mathrm{i}\varphi(k)}$ has a branch cut on i $\mathbb R$

$$\varphi(k) = \int_{\mathbb{R}} \frac{\mathrm{d}q}{2\pi} \, \frac{k \log(1 + z e^{-q^2})}{q^2 - k^2},$$
$$e^{q_0^2} = -z, \qquad q_0 = \mathrm{i}\kappa_0 \in \mathrm{i}\mathbb{R}$$

so we modify the phase $\varphi \Longrightarrow \varphi + \Delta \varphi$ with the contribution $\Delta \varphi(k) = 2 \arctan(\frac{\kappa_0}{k})$.



Result (Continuation of the conserved quantities)

The conserved quantities are continued as

$$C_n \Longrightarrow C_n + \Delta C_n, \qquad \Delta C_n = -\frac{2}{n} \kappa_0^n$$

This implies

$$\Psi(z) \Longrightarrow \Psi(z) + \Delta(z)$$

Solitonic interpretation of the continuation

Recall the $\{P, Q\}$ system

$$\partial_t Q = \partial_x^2 Q - 2zPQ^2$$
$$-\partial_t P = \partial_x^2 P - 2zP^2 Q$$

with initial / boundary conditions

$$Q(x,0) = \delta(x), \quad P(x,1) = \delta(x), \quad Q(x = 0, t = 1) = e^{H}.$$

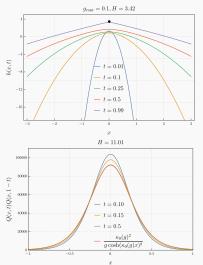
The negative coupling -z < 0 describes the repulsive (defocusing) regime.

Result (Solitonic interpretation)

- -z > 0 is the attractive or focusing regime
 - The same coupling constant z can give rise to two values of H.
 - The analytic continuation corresponds to the spontaneous generation of a soliton of rapidity κ₀ (for H > H_c).

Numerical evaluation of the height and the noise

The solution for the height and the noise is numerically computable using a quadrature scheme (extending the work of Bornemann in random matrix theory).



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Zakharov-Shabat solves the large deviations of KPZ

So far, exact solutions for KPZ universality have been obtained exclusively by exploiting the (quantum/stochastic) integrability of the dynamics. We have derived here a nontrivial quantity directly from the underlying field theory, by exploiting the (classical) integrability of the saddle point equations. We have also completed the program of the weak noise theory.

- \blacktriangleright Extension to the flat and Brownian initial condition in full-space \checkmark
- Extension to the droplet initial condition in half-space ? much much harder...
- Extension to the macroscopic fluctuation theory of diffusive systems? history in the making! work in progress...

Thank you very much for listening! Any questions ?

Bonus: continuation of the reflection coefficients for the IST (*technical*)

Practically, this modifies the reflection coefficients as

Fredholm interpretation

The generation of the soliton induces a rank-one perturbation in the Fredholm determinant.