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

Alexandre Krajenbrink

Quantinuum & Cambridge Quantum Computing

February 23, 2022
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.
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**
  
  $h(x, t = 0) = B(x) - w|x|$

- **Droplet (wedge)**
  
  $h(x, t = 0) = -w|x| + \log\left(\frac{w}{2}\right)$, with a slope $w \gg 1$

Exact solutions have been found

- **Droplet**: Sasamoto, Spohn ; Calabrese, Le Doussal, Rosso ; Dotsenko ; Amir, Corwin, Quastel (’10)
- **Flat**: Calabrese, Le Doussal (’11)
- **Brownian**: Imamura, 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)**

$$\mathbb{E}_{\text{KPZ}} \left[ \exp \left( -z e^{h(0,t)} + \frac{t}{12} \right) \right] = \text{Det}[1 - \sigma_{z,t} K_{\text{Ai}}]_{L^2(\mathbb{R})}.$$  

where $\mathbb{E}_{\text{KPZ}} \equiv$ average over the KPZ white noise. $K_{\text{Ai}}$ is the Airy kernel, $K_{\text{Ai}}(u, u') = \int_0^\infty dr \ Ai(r + u)Ai(r + u')$, 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!
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 $t \ll 1$

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

where the large deviation function $\Phi$ has the universal properties

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

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

\[ P(H, t) \sim \exp \left( - \frac{\Phi(H)}{\sqrt{t}} \right) \]

**The cheese**

Fredholm determinant approach

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

\[
\begin{align*}
  e^H &= \Psi'(z) \\
  \Phi(H) &= \Psi(z) - z\Psi'(z) \\
  \Psi(z) &= -\frac{1}{\sqrt{4\pi}} \text{Li}_{5/2}(-z)
\end{align*}
\]

**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.

\[
\Phi(H) \simeq \begin{cases} 
  \frac{4}{15\pi} |H|^{5/2}, & H \to -\infty \\
  \frac{1}{\sqrt{2\pi}} H^2, & |H| \ll 1 \\
  \frac{4}{3} H^{3/2}, & H \to +\infty
\end{cases}
\]

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

**The cheese or the dessert? the obnoxious French waiter dilemma**

Alexandre Krajenbrink

Zakharov-Shabat solves the large deviations of KPZ
Outline

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

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

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

where the expectation is taken with respect to the white noise

$$\mathcal{D}\tilde{\eta} \exp \left( -\frac{1}{2} \iint_{xt} dx dt \tilde{\eta}(x, t)^2 \right)$$
Then the generating function

\[ \mathbb{E}_{\text{KPZ}} \left[ \exp \left( -\frac{z e^H}{\sqrt{T}} \right) \right] \]

\[ = \int D h D \tilde{\eta} \exp \left( -\frac{z e^H}{\sqrt{T}} - \frac{1}{2} \int \int_{xt} \tilde{\eta}^2 \right) \delta(\partial_t h - \partial_x^2 h - (\partial_x h)^2 - \sqrt{2} T^{1/4} \tilde{\eta}) \]

**Response field**

One introduces the response field \( \varrho / \sqrt{T} \) such that

\[ \delta(\partial_t h - \partial_x^2 h - (\partial_x h)^2 - \sqrt{2} T^{1/4} \tilde{\eta}) = \int D \varrho \exp \left( -\frac{\int \int_{xt} \varrho (\partial_t h - \partial_x^2 h - (\partial_x h)^2 - \sqrt{2} T^{1/4} \tilde{\eta})}{\sqrt{T}} \right) \]
One then integrates over the noise and

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

\[
= \int \mathcal{D} h \mathcal{D} \varrho \exp \left( - \frac{ze^H + \int_x \varrho (\partial_t h - \partial_x^2 h - (\partial_x h)^2 - \varrho)}{\sqrt{T}} \right)
\]

This action is amenable to a saddle-point evaluation!
The optimal height and noise verify the non-linear hydrodynamic system

\[
\begin{align*}
\partial_t h &= \partial_x^2 h + (\partial_x h)^2 + 2\varrho \\
-\partial_t \varrho &= \partial_x^2 \varrho - 2\partial_x (\varrho \partial_x h)
\end{align*}
\]

Define the Cole-Hopf transform

\[Q(x, t) = e^{h(x, t)} , \quad -zP(x, t)Q(x, t) = \varrho(x, t)\]

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

\[
\begin{align*}
\partial_t Q &= \partial_x^2 Q - 2zPQ^2 \\
-\partial_t P &= \partial_x^2 P - 2zP^2 Q
\end{align*}
\]

Main takeaway 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

\[
\Phi(H) = z^2 \int_0^1 dt \int_{\mathbb{R}} dx \ P(x, t)^2 Q(x, t)^2
\]

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

\[
Q(x, 0) = \delta(x), \quad P(x, 1) = \delta(x), \quad Q(x = 0, t = 1) = e^H.
\]

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

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

and

\[
\partial_t \vec{v} = U_2 \vec{v}
\]

**Result (Compatibility)**

The compatibility equation is

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

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

$$\phi \xrightarrow{x \to -\infty} \begin{pmatrix} e^{-ikx/2} \\ 0 \end{pmatrix}, \quad \bar{\phi} \xrightarrow{x \to -\infty} \begin{pmatrix} 0 \\ -e^{ikx/2} \end{pmatrix}$$

and

$$\phi \xrightarrow{x \to +\infty} \begin{pmatrix} a(k, t)e^{-ikx/2} \\ b(k, t)e^{ikx/2} \end{pmatrix}, \quad \bar{\phi} \xrightarrow{x \to +\infty} \begin{pmatrix} \tilde{b}(k, t)e^{-ikx/2} \\ -\tilde{a}(k, t)e^{ikx/2} \end{pmatrix}$$

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

The following ratios define the reflection coefficients

$$r(k, t) = \frac{b(k, t)}{a(k, t)}, \quad \tilde{r}(k, t) = -\frac{\tilde{b}(k, t)}{\tilde{a}(k, t)}$$
Scattering transforms

\{Q(x, t = 0), P(x, t = 1)\} \rightarrow \{a(k, t), b(k, t)\} \rightarrow \{Q(x, t), P(x, t)\}

**Main takeaway 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
\[
\begin{align*}
\phi & \xrightarrow{x \to +\infty} \begin{pmatrix} a(k, t)e^{-\frac{ikx}{2}} \\ b(k, t)e^{\frac{ikx}{2}} \end{pmatrix}, \\
\bar{\phi} & \xrightarrow{x \to +\infty} \begin{pmatrix} \tilde{b}(k, t)e^{-\frac{ikx}{2}} \\ -\tilde{a}(k, t)e^{\frac{ikx}{2}} \end{pmatrix}
\end{align*}
\]

into the time equation
\[
\partial_t \vec{v} = U_2 \vec{v}
\]

One finds that

**Result (Time-dependence)**

\[
\begin{cases}
a(k, t) = a(k) \\
\tilde{a}(k, t) = \tilde{a}(k) \\
b(k, t) = b(k)e^{-k^2t} \\
\tilde{b}(k, t) = \tilde{b}(k)e^{k^2t}
\end{cases}
\]

This is *universal* and *independent* of the potentials $P, Q$!
One then solves the spatial part at $t = 0$ and $t = 1$

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

Using

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

One finds that

**Result (Fourier-dependence)**

$$\begin{cases} 
    b(k) = 1 \\
    \tilde{b}(k) = -ze^{-k^2} \\
    \tilde{a}(k) = a(k)^\dagger \\
    a(k) = \sqrt{1 + ze^{-k^2}} e^{-i\varphi(k)}, \quad \varphi(k) = \int_{\mathbb{R}} \frac{dq}{2\pi} \frac{k \log(1 + ze^{-q^2})}{q^2 - k^2}
\end{cases}$$

We also have the normalization $a\tilde{a} + b\tilde{b} = 1$, this is universal.
The inverse scattering is solvable by the means of Fredholm determinant: define the Fourier transform of the reflection coefficients

\[
A_t(x) = \int_{\mathbb{R}} \frac{dk}{2\pi} r(k)e^{ikx-k^2t}, \quad B_t(x) = \int_{\mathbb{R}} \frac{dk}{2\pi} \tilde{r}(k)e^{k^2t-ikx}
\]

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

\[
\mathcal{A}_{xt}(v, v') = A_t(x + v + v'), \quad \mathcal{B}_{xt}(v, v') = B_t(x + v + v')
\]

**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 \(\langle \delta | O | \delta \rangle = O(0, 0)\) for any operator \(O\) (~ selecting a matrix element).

The Fredholm determinant is hidden as: \(-zPQ = \partial_x^2 \log \det(I - z\mathcal{B}_{xt}\mathcal{A}_{xt})\).
But where is the large deviation function?

We don’t want to calculate

\[ \Phi(H) = z^2 \int_0^1 dt \int_{\mathbb{R}} dx \, P(x, t)^2 Q(x, t)^2 \]

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

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

Result (Infinite amount of conserved quantities)

The ZS system has conserved quantities

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

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

$$\log a(k) = \sum_{n \geq 1} \frac{C_n(x, t)}{(ik)^n}, \quad C_n = z \int_{\mathbb{R}} dx \, P(x, t) \Gamma_n(x, t)$$

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

\[
-i\int_{\mathbb{R}} \frac{dq}{2\pi} \frac{k \log(1 + ze^{-q^2})}{q^2 - k^2} = -i\varphi(k) = \sum_{n\geq 1} \frac{C_n(g)}{(ik)^n}
\]

The first one reads

\[
C_1 = \frac{1}{\sqrt{4\pi}} \text{Li}_{\frac{3}{2}}(-z)
\]

On the other side

\[
C_1 = -z \int_{\mathbb{R}} dx \ P(x, t = 1) Q(x, t = 1) = -ze^H
\]

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)**

\[
\Psi(z) = -\frac{1}{\sqrt{4\pi}} \text{Li}_{5/2}(-z)
\]
Are we done yet?

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

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

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

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

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

A continuation is required...!
Are we done yet?

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

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

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

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

and extending to \( z > -1 \) allows to obtain \( \Phi(H) \) for \( H < H_c \).
An analytic continuation required...

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

\[
\varphi(k) = \int_{\mathbb{R}} \frac{dq}{2\pi} \frac{k \log(1 + ze^{-q^2})}{q^2 - k^2},
\]

\[e^{q_0^2} = -z, \quad q_0 = i\kappa_0 \in i\mathbb{R}\]

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

**Result (Continuation of the conserved quantities)**

The conserved quantities are continued as

\[
C_n \mapsto C_n + \Delta C_n, \quad \Delta C_n = \frac{2}{n} \kappa_0^n
\]

This implies

\[
\Psi(z) \mapsto \Psi(z) + \Delta(z)
\]
Solitonic interpretation of the continuation

Recall the \( \{P, Q\} \) system

\[
\begin{align*}
\partial_t Q &= \partial_x^2 Q - 2zPQ^2 \\
-\partial_t P &= \partial_x^2 P - 2zP^2 Q
\end{align*}
\]

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 \(\kappa_0\) (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).

\[ h(x, t) \]

\[ Q(x, t) \]

\[ g_{\text{ext}} = 0.1, H = 3.42 \]

\[ H = 11.01 \]
Direct outlooks and extensions

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.

- Extension to the flat and Brownian initial condition in full-space ✓
- 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?
Practically, this modifies the reflection coefficients as

\[
A_t(x) = \int_{\mathbb{R}} \frac{dk}{2\pi} e^{ikx-k^2t+i\varphi(k)} \frac{1}{\sqrt{1 + z e^{-k^2}}}
\]

\[
A_t(x) = \int_{\mathbb{R}} \frac{dk}{2\pi} e^{ikx-k^2t+i\varphi(k)} \frac{1}{\sqrt{1 + z e^{-k^2}}} \frac{k + i\kappa_0}{k - i\kappa_0} + 2\kappa_0 e^{-\kappa_0 x + \kappa_0^2 t + i\varphi(i\kappa_0)}
\]

**Fredholm interpretation**

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