A numerical method to assess the Gaussian Variational Method in disordered elastic systems — case study of the 1D interface

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Abstract

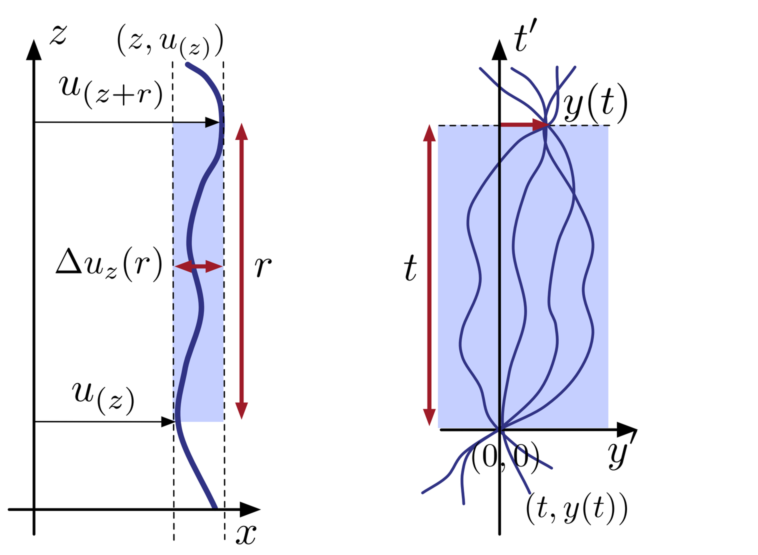
While several analytical arguments support power-law scaling behaviours in disordered elastic systems, those are often restricted to special dimensionalities and/or classes of disorder. The **Gaussian Variational Method** (GVM) offers a simplification that consists in finding the "best" quadratic Hamiltonian representing the initial problem (after introducing replicæ and integrating over disorder). It provides an approximation allowing one to determine correlation functions and their scalings — at the price of solving a *variational equation*.

The GVM can present two sorts of issues: (i) a technical one: solving the variational equation can be difficult and (ii) a physical one: the scaling exponents can be wrong. As a benchmark study, we consider here the fluctuations of the directed polymer in 1+1 dimensions in a Gaussian random environment with a finite correlation length and at finite temperature (whose scaling exponents belong to the KPZ universality class and are known exactly).

We unveil the crucial role played by two 'cut-off' lengths: the disorder correlation length and the system size. We focus on a numerical algorithm to solve the variational equation, based on a fixed-point approach. Results support the idea that correctly taking into account the finiteness of the mentioned cut-offs allows one to capture correct scaling exponents through GVM.

Based on: E Agoritsas and V Lecomte, J. Phys. A: Math. Theor. **50** 104001 (2017)

Interfaces in the Directed Polymer language



Geometrical parametrization:

- ⋆ longitudinal coordinate z
- ⋆ *univalued* transverse coordinate $u(z)$
- ⋆ no bubbles, no overhangs

Directed Polymer (DP) parametrization:

- ⋆ longitudinal coordinate: DP growing time $\boxed{t=z}$
- ⋆ transverse coordinate: DP endpoint $\boxed{y(t)=u(z)}$
- ⋆ working at fixed time t $\iff$ integration of fluctuations at scales smaller than t

Model & questions

- Competing ingredients in the total energy $\mathcal{H}_V[y(\cdot),t]=\mathcal{H}^{\text{el}}[y(\cdot),t]+\mathcal{H}^{\text{dis}}[y(\cdot),t]$:

  ⋆ elastic energy (*flattens* the interface) **vs** disorder potential (*deforms* the interface)

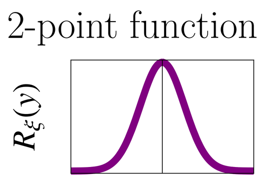
$$\mathcal{H}^{\text{el}}[y(\cdot),t]=\frac{c}{2}\int_0^t dt'\,\left[\partial_{t'}y(t')\right]^2 \qquad \mathcal{H}^{\text{dis}}_V[y(\cdot),t]=\int_0^t dt'\,V\big(t',y(t')\big)$$

  ⋆ no disordered potential $V(t,y)$: *diffusive* behaviour (typically, $y\sim t^{1/2}$), **Edwards-Wilkinson** (EW)

  ⋆ disordered potential $V(t,y)$: *super-diffusive* behaviour (—, $y\sim t^{2/3}$), **Kardar-Parisi-Zhang** (KPZ)

- Nature of the disordered potential $V(t,y)$: "**Random-Bond**", *i.e.*

  centered, Gaussian distributed, of 2-point function $\overline{V(t,y)V(t',y')}=D\delta(t'-t)R_\xi(y'-y)$

  disorder correlator: smoothed delta  scaling as $R_\xi(y)=\frac{1}{\xi}R_{\xi=1}(y/\xi)$

- What is the distribution of the (quenched) polymer end-point **free-energy**, encoding its *fluctuations*?

  partition function: $Z_V(t,y)=\int_{y(0)=0}^{y(t)=y}\mathcal{D}y(t')e^{-\frac{1}{T}\mathcal{H}_V[y(t'),t]}$ $\qquad$ $\boxed{\text{free energy: } F_V(t,y)=-\frac{1}{T}\log Z_V(t,y)}$

- What is the variance of the polymer endpoint at scale t?

  encoded in the $\boxed{\text{roughness}\quad B(t)=\overline{\langle y(t)^2\rangle}=\overline{\frac{\int dy\,y^2 Z_V(t,y)}{\int dy\,Z_V(t,y)}}}$ $\underbrace{\overset{?}{\sim}\ \text{const}\times t^{2\zeta}}_{\text{at large scale } t\to\infty}$

- Summary of parameters:

elastic constant c	disorder strength D	temperature T	disorder correlation length ξ

Evolution equations & Symmetries

- **Stochastic Heat Equation** for the partition function $Z_V(t,y)$

$$\partial_t Z_V=\Big[\frac{T}{2c}\partial_y^2-\frac{1}{T}V(t,y)\Big]Z_V(t,y)\qquad\textbf{(SHE)}$$

Linear, multiplicative noise, $Z_V(0,y)=\delta(y)$

- **Kardar-Parisi-Zhang** equation for the free-energy $F_V(t,y)$

$$\boxed{\partial_t F_V=\frac{T}{2c}\partial_y^2 F_V-\frac{1}{2c}\big[\partial_y F_V\big]^2+V(t,y)}\qquad\textbf{(KPZ)}$$

Non-linear, additive noise, $F_V(0,y)$: "sharp wedge" initial condition

- **Statistical Tilt Symmetry**:

$$F_V(t,y)=\underbrace{c\frac{y^2}{2t}+\frac{T}{2}\log\frac{2\pi Tt}{c}}_{\text{elastic contribution}}+\underbrace{\bar F_V(t,y)}_{\text{disorder contribution}}$$

$\bar F_V(t,y)$ *invariant by translat° in distribution*

- Implies $B(t)=B_{\text{th}}(t)+B_{\text{dis}}(t)$ with

$$B_{\text{th}}(t)=\frac{Tt}{c}\quad\text{and}\quad B_{\text{dis}}(t)=\overline{\langle y(t)\rangle^2}$$

- **Tilted** KPZ equation for the disorder free-energy $\bar F_V(t,y)$

$$\partial_t\bar F_V+\frac{y}{t}\partial_y\bar F_V=\frac{T}{2c}\partial_y^2\bar F_V-\frac{1}{2c}\big[\partial_y\bar F_V\big]^2+V(t,y)$$

Simple initial condition $\bar F_V(0,y)=0$

Replicæ

$$\overline{\langle\mathcal{O}\left[y(t_{\text{f}})\right]\rangle}=\int\mathcal{D}V\,\bar{\mathcal{P}}\left[V\right]\frac{\int_{y(0)=0}\mathcal{D}y(t)\,\mathcal{O}\left[y(t_{\text{f}})\right]\,e^{-\frac{1}{T}\mathcal{H}[y(\cdot),V;t_{\text{f}}]}}{\int_{y(0)=0}\mathcal{D}y(t)\,e^{-\frac{1}{T}\mathcal{H}[y(\cdot),V;t_{\text{f}}]}}$$

$$=\lim_{n\to0}\int_{y_1(0)=0}\mathcal{D}y_1(t)\,(\dots)\int_{y_n(0)=0}\mathcal{D}y_n(t)\,\mathcal{O}\left[y_1(t_{\text{f}})\right]\,e^{-\frac{1}{T}\widetilde{\mathcal{H}}[y_1(\cdot),\dots,y_n(\cdot);t_{\text{f}}]}$$

$$\widetilde{\mathcal{H}}\left[y_1(\cdot),\dots,y_n(\cdot);t_{\text{f}}\right]=\int_0^{t_{\text{f}}}dt\,\left[\frac{c}{2}\sum_{a=1}^{n}(\partial_t y_a(t))^2-\frac{D}{T}\sum_{a,b=1}^{n}R_\xi(y_a(t)-y_b(t))\right]$$

GVM for an infinite system ($t_{\text{f}}\to\infty$)

Trial Hamiltonian:

$$\widetilde{\mathcal{H}}_0[\mathbf{y}]=\frac{1}{2}\int_{\mathbb{R}}\bar{d}q\sum_{a,b=1}^{n}y_a(-q)G^{-1}_{ab}(q)y_b(q)\qquad(\text{with } \bar{d}q\equiv\tfrac{dq}{2\pi})$$

Parametrization:

$$G^{-1}_{ab}(q)=cq^2\delta_{ab}-\sigma_{ab}\qquad\text{with } \sigma_{ab} \text{ described by a function } \sigma(u)\quad[0\le u\le1]$$

Re-parametrization:

$$\left[\sigma\right](u)=u\,\sigma(u)-\int_0^u dv\,\sigma(v)\qquad(\star)$$

Variational equations (for a Gaussian correlator function):

$$\sigma(u)=\frac{2}{\sqrt{\pi}}\beta^{\frac32}\left[\xi^2+\beta^{-1}\int_{\mathbb{R}}\bar{d}q\,\left[G(q)-G(q,u)\right]\right]^{-\frac32}\qquad(\star\star)$$

$$\int_{\mathbb{R}}\bar{d}q\,\left[\tilde G(q)-\ G(q,u)\right]=\frac{1}{u}\frac{1}{\sqrt{[\sigma](u)}}-\int_u^1\frac{dv}{v^2}\frac{1}{\sqrt{[\sigma](v)}}\qquad(\star\star\star)$$

A fixed-point algorithm to solve the GVM variational equation

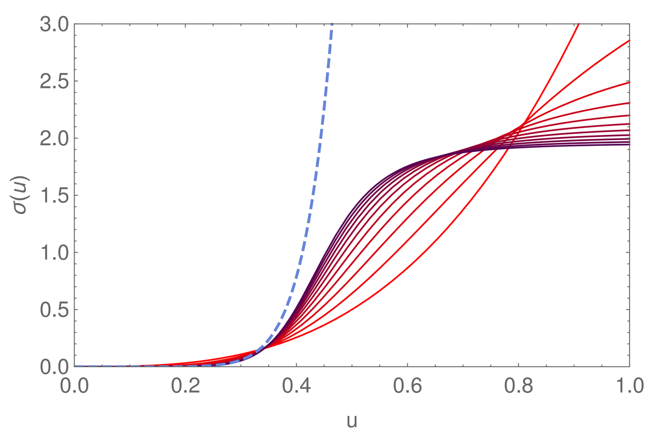
Start from an 'initial' $\sigma_0(u)$. To evaluate $\sigma_{k+1}(u)$ from $\sigma_k(u)$, iterate the following procedure:

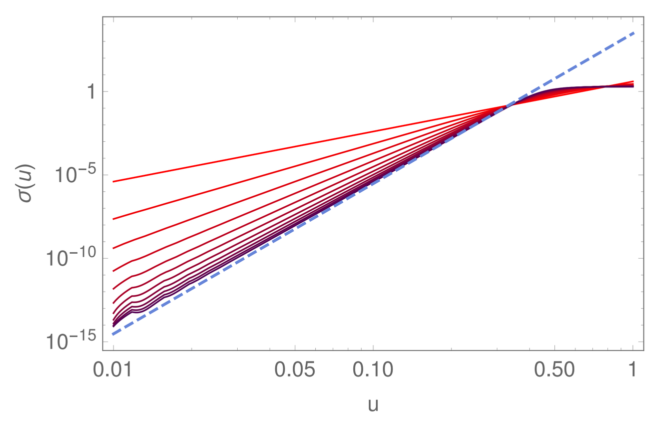
- determine $[\sigma_k](u)$ from $\sigma_k(u)$, using $(\star)$
- determine the corresponding $\int_{\mathbb{R}}\bar{d}q\,\left[\tilde G_k(q)-\ G_k(q,u)\right]$, using $(\star\star)$
- determine the next iteration $\sigma_{k+1}(u)$ as follows [see $(\star\star\star)$]:

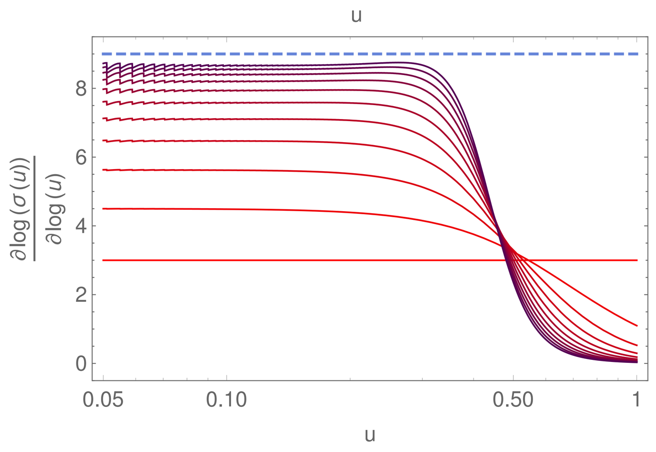
$$\sigma_{k+1}(u)=\frac{2}{\sqrt{\pi}}\beta^{\frac32}\left[\xi^2+\beta^{-1}\int_{\mathbb{R}}\bar{d}q\,\left[\tilde G_k(q)-G_k(q,u)\right]\right]^{-\frac32}$$

If $\sigma_k(u)\to\sigma_\infty(u)$ as $k\to\infty$, one expects a **fixed point** $\sigma_\infty(u)$ [**stable solution** of $(\star\star-\star\star\star)$]

Numerical test: GVM for an infinite system







Iterations increase from red to dark purple.
Compatible with the analytical solution (dashed blue)

$$\sigma(u)=\begin{cases}A\,u^9 & \text{if } u<u_{\text{c}}\\ [\sigma](u_{\text{c}}) & \text{if } u>u_{\text{c}}\end{cases}$$

(yielding a wrong roughness exponent $\zeta=\zeta_{\text{Flory}}=\frac35$)

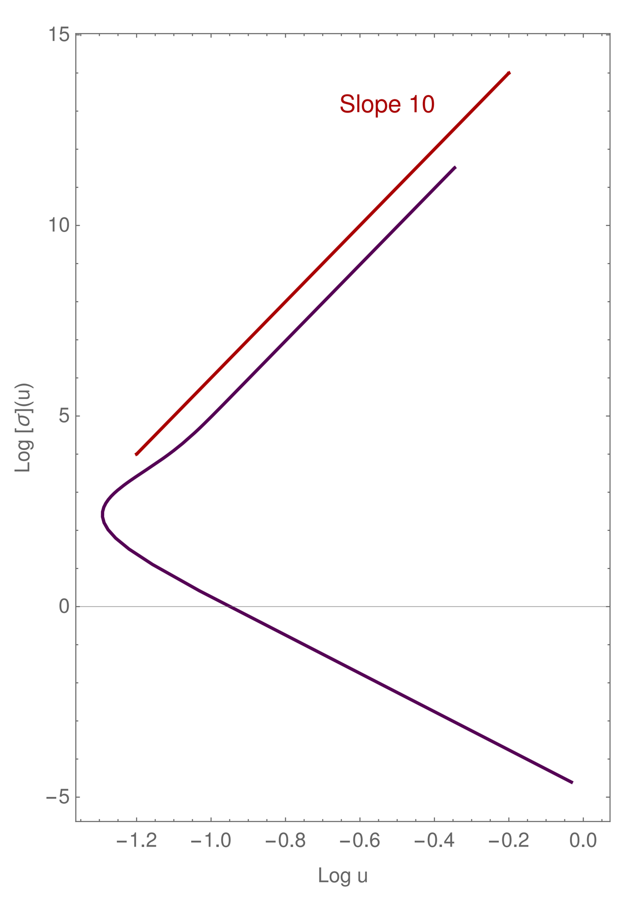
GVM for a *finite* system ($t_{\text{f}}<\infty$)

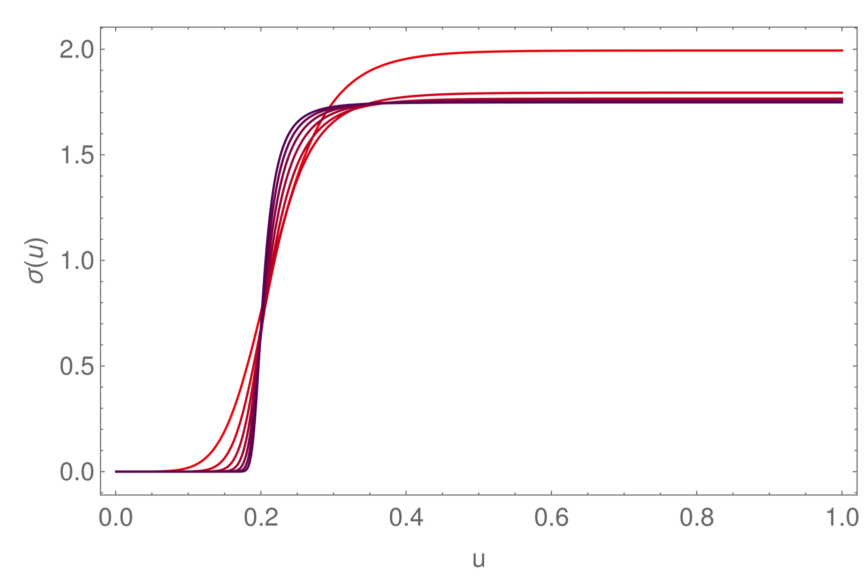
Rescalings chosen such that : $\mathring{\xi}(t_{\text{f}})=\dfrac{\xi}{t_{\text{f}}^{\zeta}\big(\frac{D}{cT}\big)^{\frac13}}$ and $\hat\beta(t_{\text{f}})=\left[\dfrac{t_{\text{f}}}{\frac{T^5}{cD^2}}\right]^{\frac13}$ with $\zeta=\zeta_{\text{KPZ}}=\frac23$.

Variational equations, now with discrete Fourier modes $\omega\in2\pi\mathbb{Z}/t_{\text{f}}$:

$$\sigma(u)=\frac{2}{\sqrt{\pi}}\hat\beta^{\frac32}\Big\{\hat\beta\mathring{\xi}^2+\sum_\omega\left[\tilde G(\omega)-G(\omega,u)\right]\Big\}^{-\frac32}\qquad(\star\star)'$$

$$\sum_\omega\left[\tilde G(\omega)-G(\omega,u)\right]=\frac{1}{u}\frac{\coth\left(\frac12\sqrt{[\sigma](u)}\right)}{2\sqrt{[\sigma](u)}}-\int_u^1\frac{dv}{v^2}\frac{\coth\left(\frac12\sqrt{[\sigma](v)}\right)}{2\sqrt{[\sigma](v)}}\qquad(\star\star\star)'$$





(**Left**) Solution of $(\star\star)'$, $(\star\star\star)'$ when $\sigma'(u)\neq0$.
(**Top**) Numerical procedure for small ξ (iterations increase from red to dark purple).

- Compatible with a $\sigma(u)$ behaving as: plateau+full RSB+plateau
- Effective 1-step solution $\Rightarrow$ **correct** $\zeta=\zeta_{\text{KPZ}}=\frac23$

Open questions: full solution in 1D ; extensions to other dimensions, disorder, elasticity.