Self-interacting random walks, Polymers and Folding @ CIRM

Scaling limit of semiflexible polymers: a phase transition

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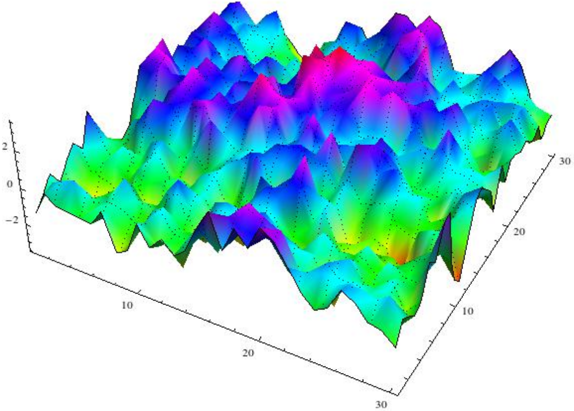

Figure: Discrete Gaussian Free Field on a 30x30 box

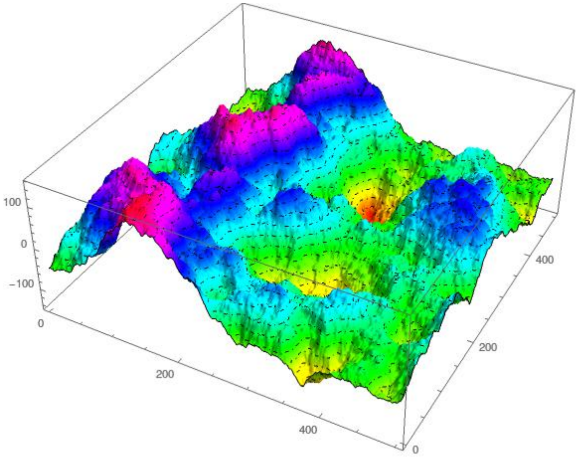

Figure: Membrane model on a 500x500 box

A random interface on $\Lambda \Subset \mathbb{Z}^d$ is a Gaussian process $(\varphi_x)_{x\in\mathbb{Z}^d}$ with the following properties:

- $\varphi_x = 0$ a.s., for all $x \in \mathbb{Z}^d \setminus \Lambda$

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- $(\varphi_x)_{x\in\Lambda} \sim \mathcal{N}(\mathbf{0},\ G_\Lambda)$ with

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- $G_\Lambda = \mathcal{L}_\Lambda^{-1}$.

Examples of interfaces

$$\Delta f(x) = \frac{1}{2d} \sum_{y:\|y-x\|=1} (f(y) - f(x)), \quad f : \mathbb{Z}^d \to \mathbb{R}\,.$$

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Discrete Gaussian Free Field

$$\mathcal{L} = -\Delta$$

Membrane model

$$\mathcal{L} = \Delta^2$$

$(\nabla + \Delta)$-model (mixed model)

$$\mathcal{L} = -\kappa_1 \Delta + \kappa_2 \Delta^2$$

A semiflexible polymer is a random interface with the following properties:

- $\varphi_x = 0$ a.s., for all $x \in \mathbb{Z}^d \setminus \Lambda$
- $(\varphi_x)_{x\in\Lambda} \sim \mathcal{N}(\mathbf{0},\ G_\Lambda)$ with
$$\mathbf{E}_\Lambda[\varphi_x \varphi_y] = G_\Lambda(x, y), \quad x, y \in \Lambda.$$
- For all $x \in \Lambda$
$$\begin{cases} \left(\kappa_1(-\Delta) + \kappa_2 \Delta^2\right) G_\Lambda(x, y) = \delta_x(y), & y \in \Lambda \\ G_\Lambda(x, y) = 0, & y \notin \Lambda. \end{cases}$$

Consider $\Lambda = \Lambda_N = [0,\ 1] \cap {}^1\!/\!_N\,\mathbb{Z}$.
The limit of the $(\nabla + \Delta)$-model turns out to have continuous paths.
For $0 \leq t \leq 1$,

$$\widehat{\varphi}_N(t) = \varphi_{\lfloor Nt \rfloor} + (Nt - \lfloor Nt \rfloor)\left(\varphi_{\lfloor Nt \rfloor + 1} - \varphi_{\lfloor Nt \rfloor}\right).$$

Theorem (DGFF & Mixed; C., Dan, Hazra (2018))

On $C[0,1]$*,*

$$(N^{-1/2}\widehat{\varphi}_N(t))_{t\in[0,1]} \Rightarrow (B^\circ_t)_{t\in[0,1]}$$

where $(B^\circ_t)_{t\in[0,1]}$ *is the Brownian Bridge.*

THEOREM (DGFF & MIXED; C., DAN, HAZRA (2018))

On $C[0,1]$,

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where $(B_t^\circ)_{t\in[0,1]}$ is the Brownian Bridge.

THEOREM (MEMBRANE; CARAVENNA, DEUSCHEL (2009))

On $C[0,1]$,

$$(N^{-3/2}\widehat{\varphi}_N(t))_{t\in[0,1]} \Rightarrow (\widehat{I}_t)_{t\in[0,1]}$$

where

$$(\widehat{I}_t)_{t\in[0,1]} = \text{“}\left(\int_0^t B_s ds \,\Big|\, \int_0^1 B_s ds = 0\right)_{0\le t\le 1}\text{”}.$$

A phase transition picture

Let $\kappa_1 = 1$ and $\kappa_2 = \kappa_N$. Can one see a phase transition in κ_N?

$\kappa_N \ll N^2$

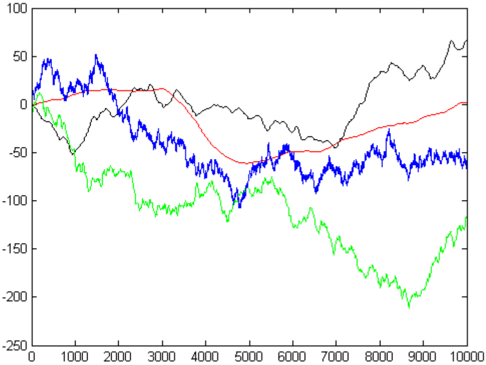

FIGURE: Trajectories with $N = 10^4$ and $\kappa_N = 0$, $\kappa_N = 2 \times 10^2$, $\kappa_N = 2 \times 10^4$, $\kappa_N = 2 \times 10^6$.

$\kappa_N \gg N^2$

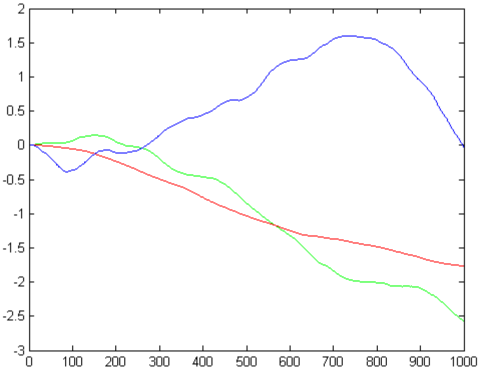

FIGURE: Trajectories with $N = 10^3$ and $\kappa_N = 2 \times 10^{6.5}$, $\kappa_N = 2 \times 10^7$, $\kappa_N = 2 \times 10^8$.

Heuristics for $\kappa_1 = 1$ and $\kappa_2 = \kappa_N$

$$\gamma = \left(\frac{1 + \kappa_N - \sqrt{1 + 2\kappa_N}}{1 + \kappa_N + \sqrt{1 + 2\kappa_N}} \right)^{\frac{1}{2}}, \quad \sigma^2 = \frac{2}{(1 + \kappa_N + \sqrt{1 + 2\kappa_N})}, \quad (\varepsilon_i)_{i \in \mathbb{Z}^+} \overset{iid}{\sim} \mathcal{N}(0, \sigma^2).$$

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$$Y_N = \gamma^{N-1}\varepsilon_1 + \ldots + \gamma^0 \varepsilon_N, \quad W_N = \frac{1}{1-\gamma} \sum_{i=1}^{N} Y_i$$

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Theorem (Borecki (2010), Borecki, Caravenna (2010))

Let $\mathbf{P}_N$ be the law of the semi-flexible membrane on $[1, N-1]$, then

$$\mathbf{P}_N(\cdot) = \mathbf{P}\left((W_1, \cdots, W_{N-1}) \in \cdot \,|\, W_N = W_{N+1} = 0\right)$$

Process W_N

$$W_N = \underbrace{\frac{1}{1-\gamma}(\varepsilon_1 + \cdots + \varepsilon_N)}_{S_N} - \underbrace{\frac{1}{1-\gamma}(\gamma^N \varepsilon_1 + \gamma^{N-1}\varepsilon_2 + \cdots + \gamma\varepsilon_N)}_{U_N}.$$

$$\sigma^2 \sim \frac{1}{\kappa_N} \text{ and } (1-\gamma) \sim \frac{1}{\sqrt{\kappa_N}}.$$

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- $\kappa_N \sim N^2$: the contribution from S_N and U_N is similar $\Rightarrow$ mixed model.

THEOREM (C., DAN, HAZRA (2019))

- $\kappa_N \ll N^{\frac{1}{2}}$

$$(N^{-1/2}\widehat{\varphi}_N(t))_{t\in[0,1]} \Rightarrow (B_t^{\circ})_{t\in[0,1]} \quad in\ C([0,1])$$

Scaling limit in $d = 1$

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- $\kappa_N \gg N^2$

$$(\sqrt{\kappa_N}N^{-3/2}\widehat{\varphi}_N(t))_{t\in[0,1]} \Rightarrow (\Psi^{\Delta^2}_t)_{t\in[0,1]} \quad \textit{in } C([0,1]).$$

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$$(\sqrt{\kappa_N}N^{-3/2}\widehat{\varphi}_N(t))_{t\in[0,1]} \Rightarrow (\Psi_t^{\Delta^2})_{t\in[0,1]} \quad in\ C([0,1]).$$

- $\kappa_N \sim N^2$

$$(N^{-1/2}\widehat{\varphi}_N(t))_{t\in[0,1]} \Rightarrow (\Psi_t^{\Delta+\Delta^2})_{t\in[0,1]} \quad in\ C([0,1])$$

The limiting processes: $\Psi_t^{\Delta^2}$

$(\Psi_t^{\Delta^2})_{t\in[0,1]^d}$ is a centered Gaussian process with continuous paths and

$$\mathbf{E}[\Psi_t^{\Delta^2}\Psi_s^{\Delta^2}] = G_D(t,s)$$

and G_D is the Green's function on $\overline{D} = [0,1]^d$ satisfying the following Dirichlet problem:

$$\begin{cases} \Delta^2 G_D(x,y) = \delta_x(y), & y \in D \\ G_D(x,y) = 0, & y \in \partial D \\ \mathbf{D} G_D(x,y) = 0, & y \in \partial D. \end{cases}$$

The definition and results are valid in $d = 2, 3$ also.

$\Psi_t^{\Delta+\Delta^2}$ is a centered continuous Gaussian process on $\overline{D}$ with covariance G_D, where G_D is the Green's function for the problem

$$\begin{cases} -\frac{\mathrm{d}^2}{\mathrm{d}\,x^2}u(x) + \frac{\mathrm{d}^4}{\mathrm{d}\,x^4}u(x) = \delta_y(x) & x \in D \\ u(x) = \frac{\mathrm{d}}{\mathrm{d}\,x}u(x) = 0 & x \in \partial D. \end{cases}$$

Plan

Facts about eigenfunctions

There exist eigenfunctions $u_1, u_2, \ldots$ of $(-\Delta_c)^m$ with corresponding eigenvalues $0 < \lambda_1 \leq \lambda_2 \leq \ldots \to \infty$ such that

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3. $\lambda_j \sim c j^{2m/d}$ (Weyl's asymptotics, Beals (1967))

Existence of the limit field

Let $f \in C_c^\infty(D)$, define

$$\|f\|_s^2 = \sum_{j \geq 1} \lambda_j^{s/m} \left\langle f, u_j \right\rangle_{L^2}^2, \quad \mathcal{H}_m^s = \overline{C_c^\infty(D)}^{\|\cdot\|_s}.$$

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Let λ_j be the eigenvalues of $(-\Delta_c)^m$ and u_j be the corresponding eigenfunctions. Define

$$\Psi_D^m = \sum_{j \geq 1} \frac{X_j u_j}{\sqrt{\lambda_j}}, \quad X_j \overset{iid}{\sim} \mathcal{N}(0, 1).$$

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Theorem (C., Dan, Hazra (2018))

For $m = 1, 2$ and $s > \frac{d-2m}{2}$, Ψ_D^m exists in

$$\mathcal{H}_m^{-s} := \mathcal{H}_m^s(D)^*.$$

Main results: GFF scaling

Theorem (C., Dan, Hazra (2019))

Let $\kappa_N \ll N^{\frac{1}{2}}$. Let $d \geq 2$. Define Ψ_N by

$$(\Psi_N, f) := (2d)^{-\frac{1}{2}} N^{-\frac{d+2}{2}} \sum_{x \in \frac{1}{N}\Lambda_N} \varphi_{Nx} f(x), \quad f \in \mathcal{H}_1^s(D).$$

$$\Psi_N \Rightarrow \Psi_D^{-\Delta} \text{ on } \mathcal{H}_1^{-s}(D) \text{ for all } s > s_0.$$

$\Psi_D^{-\Delta}$ is the Gaussian Free Field, arising out of $-\Delta$.

Theorem (C., Dan, Hazra (2019))

Let $\kappa_N \sim N^2$. Let $d \geq 2$. Define Ψ_N by

$$(\Psi_N, f) := (2d)^{-\frac{1}{2}} N^{-\frac{d+2}{2}} \sum_{x \in \frac{1}{N}\Lambda_N} \varphi_{Nx} f(x), \quad f \in \mathcal{H}_2^s(D)$$

$$\Psi_N \to \Psi^{\Delta+\Delta^2} \text{ on } \mathcal{H}_2^{-s}(D) \text{ for all } s > s_0.$$

$\Psi^{\Delta+\Delta^2}$ is the mixed field, arising out of $-\Delta + \Delta^2$.

THEOREM (C., DAN, HAZRA (2019))

Let $\kappa_N \gg N^2$. Let $d \geq 2$. Define Ψ_N by

$$(\Psi_N, f) := (2d)^{-1}\sqrt{\kappa_N} N^{-\frac{d+4}{2}} \sum_{x \in \frac{1}{N}\Lambda_N} \varphi_{Nx} f(x), \quad f \in \mathcal{H}_2^s(D).$$

$$\Psi_N \Rightarrow \Psi_D^{\Delta^2} \text{ on } \mathcal{H}_2^{-s}(D) \text{ for all } s > s_0 \text{ for some } s_0 > 0.$$

$\Psi_D^{\Delta^2}$ is the (continuum) Membrane model, arising out of Δ^2.

Plan

Idea of the proof

We denote

$$G_{\frac{1}{N}}(x, y) := \mathbf{E}_{\Lambda_N}[\varphi_{Nx}\varphi_{Ny}], \quad x, y \in \frac{1}{N}\mathbb{Z}^d.$$

Idea of the proof

We denote

$$G_{\frac{1}{N}}(x,\,y) := \mathbf{E}_{\Lambda_N}[\varphi_{Nx}\varphi_{Ny}], \quad x,\,y \in \frac{1}{N}\mathbb{Z}^d.$$

For f smooth

$$H_N(x) := c_N \sum_{y\in\frac{1}{N}\Lambda_N} G_{\frac{1}{N}}(x,y)f(y)$$

BVP for H_N

- $\kappa_N \gg N^2$

$$\begin{cases} \left(-\frac{2dN^2}{\kappa_N}\Delta_{\frac{1}{N}} + \Delta^2_{\frac{1}{N}}\right) H_N(x) = f(x), & x \in \frac{1}{N}\Lambda_N \\ H_N(x) = 0, & x \notin \frac{1}{N}\Lambda_N. \end{cases}$$

- $\kappa_N \sim N^2$, $\kappa_N \ll N^{1/2}$

$$\begin{cases} \left(-\Delta_{\frac{1}{N}} + \frac{\kappa}{2dN^2}\Delta^2_{\frac{1}{N}}\right) H_N(x) = f(x) & x \in \frac{1}{N}\Lambda_N \\ H_N(x) = 0 & x \notin \frac{1}{N}\Lambda_N. \end{cases}$$

Idea of the proof

Let L denote one of the following three elliptic operators:

$$L = \begin{cases} -\Delta \\ \Delta^2 \\ -\Delta + \Delta^2 \end{cases}$$

We consider the following continuum Dirichlet problem:

$$\begin{cases} Lu(x) = f(x) & x \in D \\ D^\alpha u(x) = 0 & |\alpha| \leq m - 1,\ x \in \partial D. \end{cases}$$

Idea of proof

- Difference between continuum and discrete Dirichlet problem solutions:

$$e_N(x) := u(x) - H_N(x)$$

- Using results by Thomée (1964) for approximation of solutions of PDE we have

$$\|e_N\|_{\ell^2} \to 0.$$

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Idea of the proof

Open questions

- We expect that for $\kappa_N \ll N^2$ one should scale to Brownian bridge/GFF.

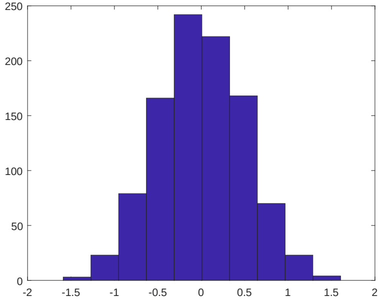

FIGURE: Histogram of the interpolated field in $d = 1$ at the point $1/2$ with $N = 100$, $\kappa_N = 2 \times 100^{3/2}$ and 10^3 iterations. The variance is about 0.2485 (vs. theoretical value of 0.25, the variance of the Brownian bridge at the point $1/2$).

Open questions

- Extremes: $\max_{x\in\Lambda}\varphi_x$ of the $(\nabla+\Delta)$ model is open in $d\geq 2$.

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- Extremes: $\max_{x\in\Lambda}\varphi_x$ of the $(\nabla+\Delta)$ model is open in $d\geq 2$.

- Let $\varepsilon \geq 0$ and consider the following pinned measure on $\mathbb{R}^{\Lambda_N}$:

$$\mathbf{P}_{\varepsilon,N} = \frac{1}{Z_{\varepsilon,N}} \mathrm{e}^{-\frac{\|(\nabla+\Delta)\varphi\|^2}{2}} \prod_{x\in\Lambda_N} (\varepsilon\delta_0(\mathrm{d}\varphi_x) + \mathrm{d}\phi_x) \prod_{x\in\mathbb{Z}^d\setminus\Lambda_N} \delta_0(\mathrm{d}\varphi_x)$$

  Let $F(\varepsilon)$ be the free energy of the above system, namely,

$$F(\varepsilon) = \lim_{N\to\infty} \frac{1}{N} \log \frac{Z_{\varepsilon,N}}{Z_{0,N}}.$$

  For which $\varepsilon > 0$ and κ_1, κ_2 is $F(\varepsilon) > 0$?

Thank you!