LECTURE 10

Widom-Rowlinson model for disks in the plane:
Mesoscopic fluctuations of the critical droplet

§ PREVIEW

The goal of Lecture 10 is to sketch the main ideas behind the proof of the main theorems in Lecture 9, subject to three technical conditions that will be addressed in Lecture 11.

The analysis carried out below relies on an identification of the large deviation and moderate deviation properties of the volume and the surface of the critical droplet.

The idea is to approximate, in the limit as $\beta \to \infty$, a high-dimensional volume integral by a low-dimensional surface integral. This reduction requires several steps, which we sketch without proof.

- In Lecture 10 we analyse the mesoscopic fluctuations of the surface of the critical droplet.
- In Lecture 11 we analyse the microscopic fluctuations of the locations of the disks in the boundary layer of the critical droplet.

Both are needed to obtain the sharp asymptotics for the metastable crossover time stated in Lecture 9.

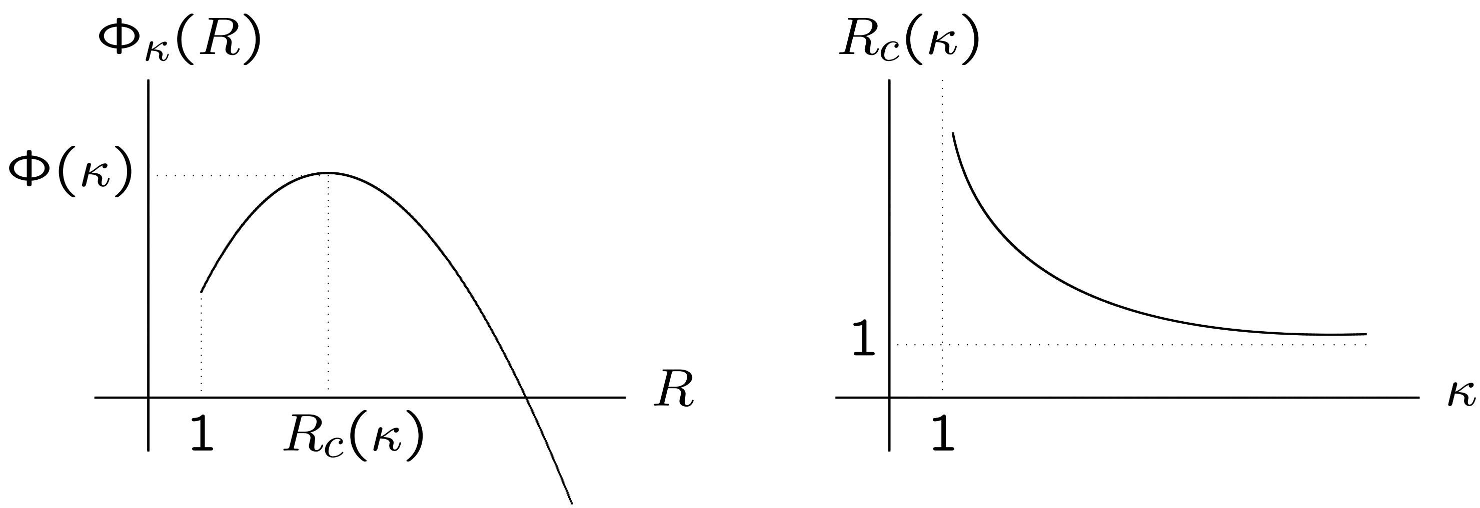
The results to be described provide a rigorous foundation for what in physics literature are called capillary waves.

Stillinger, Weeks 1995

§ FLUCTUATIONS OF THE CRITICAL DROPLET

For $\kappa \in (1,\infty)$, abbreviate

$$\Phi_\kappa(R) = \pi R^2 - \kappa\pi(R-1)^2, \quad R \in [1,\infty), \quad R_c(\kappa) = \frac{\kappa}{\kappa-1}.$$



Picture of $R \mapsto \Phi_\kappa(R)$ for fixed $\kappa \in (1,\infty)$, and of $\kappa \mapsto R_c(\kappa)$.

Fix $C \in (0,\infty)$, abbreviate $\delta(\beta) = \beta^{-2/3}$, and define

$$
\begin{aligned}
&I(\kappa,\beta;C)\\
&= \Xi\,\mu\Big(|V(\gamma) - \pi R_c(\kappa)^2| \le C\delta(\beta)\Big)\\
&= \int_\Gamma \mathbb{Q}(\mathrm{d}\gamma)\,(\kappa\beta)^{N(\gamma)}\,\mathrm{e}^{-\beta V(\gamma)}\,\mathbb{1}_{\{|V(\gamma)-\pi R_c(\kappa)^2|\le C\delta(\beta)\}}.
\end{aligned}
$$

As mentioned in Lecture 9, this integral is a very sharp approximation of $\Xi\mathrm{cap}(\square,\blacksquare)$, which is the minimum of Ξ times the Dirichlet form of the dynamic version of the Widom-Rowlinson model.

The harmonic function $h_{\square,\blacksquare}$, which is the minimiser of the Dirchlet form, is approximated by the test function

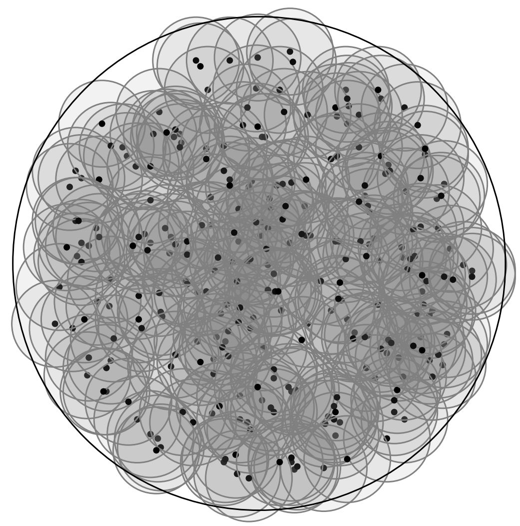
$$f(\gamma) = \begin{cases} 1, & V(\gamma) < \pi R_c(\kappa)^2 - C\delta(\beta), \\ f^*(\gamma), & |V(\gamma) - \pi R_c(\kappa)^2| \leq C\delta(\beta), \\ 0, & V(\gamma) > \pi R_c(\kappa)^2 + C\delta(\beta), \end{cases}$$

where the first and the last line do not contribute to the Dirichlet form, and in the second line the precise choice of f^* will turn out to vanish into an error term.

The special role played by the critical disk $B_{R_c(\kappa)}$ becomes apparent through the fact that the set

$$\{\gamma \in \Gamma\colon\ |V(\gamma) - \pi R_c(\kappa)^2| \leq C\delta(\beta)\}$$

is the gate for the metastable transition from the vapour phase (in which $\mathbb{T}$ is empty) to the liquid phase (in which $\mathbb{T}$ is full).



The critical droplet is close to a disc of radius $R_c(\kappa)$ and has a random boundary that fluctuates within a narrow annulus whose width shrinks to zero like $\beta^{-2/3}$ as $\beta \to \infty$. Order β discs lie inside, order $\beta^{1/3}$ disks touch the boundary.

§ TARGET

Throughout the sequel, $\kappa \in (1, \infty)$ is fixed. Define

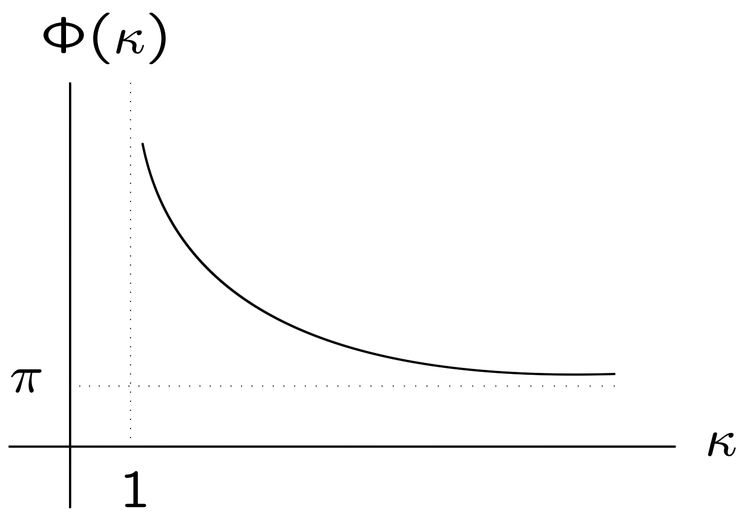
$$\Phi(\kappa) = \Phi_\kappa(R_c(\kappa)) = \frac{\pi\kappa}{\kappa - 1}, \quad \Psi(\kappa) = \frac{s^* \kappa^{2/3}}{\kappa - 1}, \quad s \in \mathbb{R},$$

where s^* is a constant that will be identified below and that does not depend on κ.

The crucial ingredient is the following sharp asymptotics, which is the main target of Lecture 10.

TARGET: For C large enough and $\beta \to \infty$,

$$I(\kappa, \beta; C) = \mathrm{e}^{-\beta\,\Phi(\kappa) + \beta^{1/3}\Psi(\kappa) + o(\beta^{1/3})}.$$


Φ(κ)
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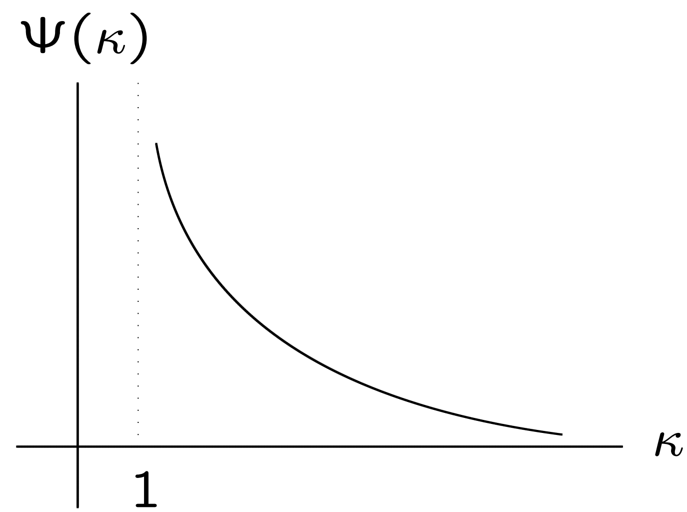
Ψ(κ)
1
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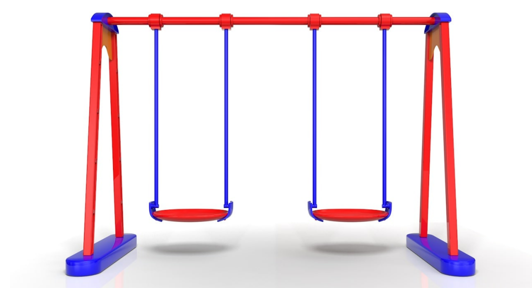
Below we formulate:

- Large deviation principles for the halo shape and the halo volume.
- Moderate deviations for the halo volume close to the critical droplet.

These ingredient serve as the main input for our analysis, and rely on certain key isoperimetric inequalities that play a crucial role in the conversion of probabilistic restrictions on the volume of the halo into geometric restrictions on the centers of the disks touching the boundary.

To describe the mesoscopic fluctuations of the surface of the critical droplet, we need to introduce auxiliary random processes, in particular, a certain constrained Brownian bridge that quantifies the cost of moderate deviations of the surface of the critical droplet.

The analysis relies on three technical conditions involving the microscopic fluctuations of the surface of the critical droplet that are the subject of Lecture 11.



§ LDPs AND ISOPERIMETRIC INEQUALITIES

▶ Admissible sets

Let $\mathcal{F}$ be the family of non-empty closed subsets of the torus $\mathbb{T}$. Equip $\mathcal{F}$ with the Hausdorff metric

$$d_{\mathrm{H}}(F_1, F_2) = \max\left\{\max_{x\in F_1} \mathrm{dist}(x, F_2), \max_{x\in F_2} \mathrm{dist}(x, F_1)\right\}, \quad F_1, F_2 \neq \emptyset,$$

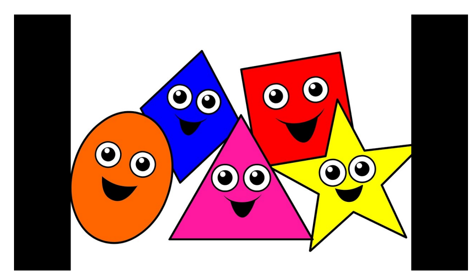
where $\mathrm{dist}(x, F) = \min_{y\in F} \mathrm{dist}(x, y)$. This turns $\mathcal{F}$ into a compact metric space.

Let $\mathcal{S} \subset \mathcal{F}$ be the collection of sets that are admissible, i.e.,

$$\mathcal{S} = \{S \subset \mathbb{T} \colon \exists F \text{ such that } h(F) = S\},$$

where $h(F) = \cup_{x \in F} B(x)$ is the halo of F. We will see that there is a unique maximal F such that $h(F) = S$, which we denote by S^- and which equals $S^- = \{x \in S \colon B(x) \subset S\}$, the 1-interior of S.

REMARK: Not every closed set is admissible. For example, when we form 1-halos we round off corners, and so a shape with sharp corners cannot be in $\mathcal{S}$. Also note that $S^- \neq \emptyset$ whenever S is admissible: S necessarily contains at least one disk $B(x)$ with $x \in S$.



▶ Two large deviation principles

Define

$$J(S) = |S| - \kappa|S^-|, \qquad S \in \mathcal{S},$$

and

$$I(S) = J(S) - \inf_{\mathcal{S}} J.$$

We view the halo $h(\gamma)$ of the random configuration γ as a random variable taking values in the space $\mathcal{S}$. Note that

$$\inf_{\mathcal{S}} J = (1-\kappa)|\mathbb{T}|$$

because $\kappa \in (1,\infty)$.

Since κ is fixed and $\beta \to \infty$, we henceforth write $\mu = \mu_\beta$ for the grand-canonical Gibbs measure and its partition sum $\Xi = \Xi_\beta$ introduced in Lecture 9.

THEOREM 10.1 LDP for the halo shape

The family of probability measures

$$\Big(\mu_\beta(h(\gamma) \in \cdot\,)\Big)_{\beta \geq 1}$$

satisfies the LDP on $\mathcal{S}$ with rate β and with good rate function I.

Informally, Theorem 10.1 says that

$$\mu_\beta\big(h(\gamma) \approx S\big) \approx \exp\big(-\beta I(S)\big), \qquad \beta \to \infty.$$

The contraction principle suggests that an LDP also holds for the halo volume. To formulate this LDP, we first state a minimisation problem for $J(S)$. Write $\mathbb{T} = [-\frac{1}{2}L, \frac{1}{2}L)^2$.

THEOREM 10.2 Minimisers of rate function for halo volume

(1) *For every* $R \in (1, (\frac{L}{\pi} + \frac{1}{2}) \wedge \frac{L}{2})$*,*

$$\min\Big\{|S| - \kappa|S^-| \colon\ S \in \mathcal{S}, |S| = |B_R|\Big\} = |B_R| - \kappa|B_R^-|$$

and the minimisers are the disks of radius R*.*

(2) *The minimisers are stable in the following sense: There exists an* $\varepsilon_0 > 0$ *such that if* $R - 1 \geq \varepsilon_0$ *and* S *satisfies*

$$\Big(|S| - \kappa|S^-|\Big) - \Big(|B_R| - \kappa|B_R^-|\Big) \leq \pi\kappa\varepsilon$$
with $|S| = |B_R|$ and $\varepsilon \in (0, \varepsilon_0)$,

then S^- *and* $\mathbb{T} \setminus S^-$ *are connected, and*

$$d_{\mathrm{H}}(\partial S, \partial B_R) \leq \sqrt{5R\varepsilon}.$$

Theorem 10.2 is a powerful tool because it shows that the near-minimers of the rate function for the halo shape are close to a disk and have no holes inside. In particular, it tells us that

$$I(B_R) = \Phi_\kappa(R) - (1-\kappa)|\mathbb{T}|,$$

and allows us, via the contraction principle, to deduce the LDP for the halo volume, which we state next.

THEOREM 10.3 LDP for the halo volume

The family of probability measures

$$(\mu_\beta(V(\gamma) \in \cdot\,))_{\beta \geq 1}$$

satisfies the LDP on $[0,\infty)$ *with rate* β *and with good rate function* I^* *given by*

$$I^*(A) = \inf\{I(S)\colon\ |S| = A\}, \qquad A \in [0,\infty).$$

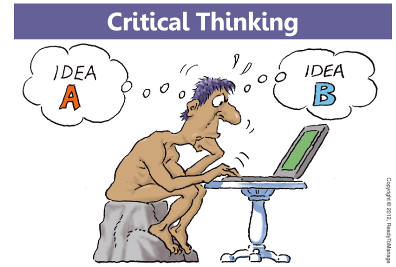
Informally, Theorem 10.3 says that

$$\mu_\beta\big(V(\gamma) \approx A\big) \approx \exp\big(-\beta I^*(A)\big), \qquad \beta \to \infty.$$

For every $R \in (1, (\frac{L}{\pi} + \frac{1}{2}) \wedge \frac{L}{2})$, we have

$$I^*(\pi R^2) = I(B_R).$$

§ NEAR THE CRITICAL DROPLET: MODERATE DEVIATIONS



▶ Fluctuations of the halo volume

The function $R \mapsto I(B_R)$ is maximal at

$$R_c = R_c(\kappa) = \frac{\kappa}{\kappa - 1}.$$

Next, zoom in on a neighbourhood of the critical droplet. The LDP tells us that

$$\mu_\beta\Big(|V(\gamma) - \pi R_c^2| \leq \varepsilon\Big) = \exp\Big(-\beta \min_{\substack{A\in[0,\infty):\\ |A-\pi R_c^2|\leq\varepsilon}} I^*(A) + o(\beta)\Big)$$

for $\beta \to \infty$ and $\varepsilon > 0$ fixed. We would like to take $\varepsilon = \varepsilon(\beta) \downarrow 0$, for which we need a stronger property.

CONJECTURE 10.4

Weak moderate deviations for the halo volume

There exists a function $\Psi_R\colon \mathbb{R} \to \mathbb{R}$ *such that*

$$\limsup_{\beta\to\infty} \frac{1}{\beta^{1/3}} \log\left\{ e^{\beta I(B_R)} \mu_\beta\left(\beta^{2/3}\left[V(\gamma) - \pi R^2\right] \in K \right)\right\}$$

$$\leq \sup_{u\in K} \Psi_R(u) \quad \forall\, K \subset \mathbb{R} \text{ compact},$$

$$\liminf_{\beta\to\infty} \frac{1}{\beta^{1/3}} \log\left\{ e^{\beta I(B_R)} \mu_\beta\left(\beta^{2/3}\left[V(\gamma) - \pi R^2\right] \in O \right)\right\}$$

$$\geq \sup_{u\in O} \Psi_R(u) \quad \forall\, O \subset \mathbb{R} \text{ open}.$$

Conjecture 10.4 has the flavor of a weak LDP on scale $\beta^{-2/3}$ with rate $\beta^{1/3}$. For $R = R_c$ we expect the function Ψ_{R_c} to be constant.

Below we establish a version of Conjecture 10.4 with

$$\Psi_{R_c}(u) = \Psi(\kappa) \qquad \forall\, u \in \mathbb{R},$$

the surface free energy encountered before. This version will settle the target asymptotics for $I(\kappa, \beta; C)$, the integral that approximates $\Xi_\beta \text{cap}(\square, \blacksquare)$.

To do so we rely on three technical conditions involving an effective interface model. This model is of independent interest, and will be analysed in Lecture 11.

▶ Boundary points

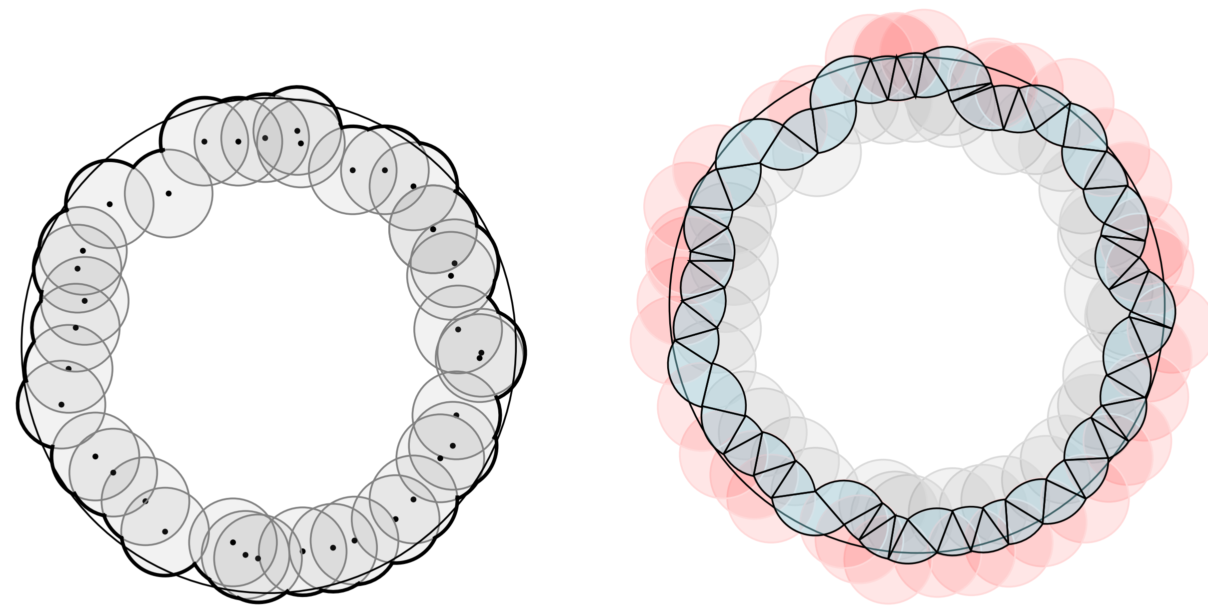
Let $S = h(\gamma)$ be the halo of some configuration γ. The boundary of S consists of a union of arcs of unit circles that are disjoint except for their endpoints. We call the centres

$$z_1, \ldots, z_n, \qquad n = n(\gamma),$$

of these circles the boundary points of S, and we say that

$$z(\gamma) = (z_1, \ldots, z_n)$$

is a connected outer contour if there exists a halo S with a simply connected 1-interior S^- having precisely these points as boundary points.



Left: The set $z(\gamma)$ of boundary points of the configuration γ. The thick black curve is the boundary $\partial h(\gamma)$ of the halo $h(\gamma)$.

Right: The boundary layer is drawn in light blue: the outer boundary is $\partial h(\gamma)$, while the inner boundary $\partial h(\gamma)^{-}$ consists of a union of arcs of unit circles with centres at the cusps of the outer boundary.

Let

$$\mathcal{O} = \text{ set of connected outer contours.}$$

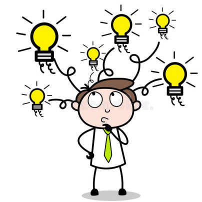
It will be expedient to parametrise the boundary points $z_1, \ldots, z_n$ of an approximately disk-shaped droplet in polar coordinates.

We will see that we may think of:

- the angular coordinates $t_1, \ldots, t_n$ as the points of an angular point process;
- the radii $r_1, \ldots, r_n$ as the values of a Gaussian process evaluated at the random angles.

To make this picture more precise, we need to introduce auxiliary processes.

§ AUXILIARY PROCESSES



1. Let $(W_t)_{t\geq 0}$ be standard Brownian motion starting in 0, and let

$$(\widetilde{W}_t)_{t\in[0,2\pi]}, \qquad \widetilde{W}_t = W_t - \frac{t}{2\pi} W_{2\pi},$$

be standard Brownian bridge on $[0, 2\pi]$. The process

$$(B_t)_{t\in[0,2\pi]}, \qquad B_t = \widetilde{W}_t - \frac{1}{2\pi}\int_0^{2\pi} \widetilde{W}_s \mathrm{d}s,$$

is called the mean-centred Brownian bridge.

2. Set

$$\lambda(\beta) = G_\kappa \beta^{1/3}, \quad G_\kappa = \frac{(2\kappa)^{2/3}}{\kappa - 1},$$

and let

$\mathcal{T}$ = Poisson point process on $[0, 2\pi)$ with intensity $\lambda(\beta)$.

Note that $N = |\mathcal{T}|$ is a Poisson random variable with mean $2\pi\lambda(\beta) = 2\pi G_\kappa \beta^{1/3}$.

Conditional on the event $\{N = n\}$, we may write

$$\mathcal{T} = \{T_i\}_{i=1}^n, \qquad 0 \le T_1 < \cdots < T_n < 2\pi,$$

and define

$$\Theta_i = T_{i+1} - T_i,\ 1 \le i \le n, \qquad \Theta_n = (T_1 + 2\pi) - T_n.$$

Note that

$$\Theta_i \ge 0, \quad 1 \le i \le n, \qquad \sum_{i=1}^n \Theta_i = 2\pi.$$

3. Assume that $(B_t)_{t\in[0,2\pi]}$ and $\mathcal{T}$ are defined on a common probability space $(\Omega, \mathscr{F}, \mathbb{P})$ and that they are independent.

4. For $m \in \mathbb{R}$, set

$$Z^{(m)} = \{Z_i^{(m)}\}_{i=1}^N$$

with

$$Z_i^{(m)} = \left(r_i^{(m)} \cos T_i, r_i^{(m)} \sin T_i\right),$$
$$r_i^{(m)} = (R_c - 1) + \frac{m + B_{T_i}}{\sqrt{(\kappa - 1)\beta}}, \qquad 1 \le i \le N.$$

This formula constitutes a convenient representation of the probability measure for the boundary points in terms of the auxiliary processes.

REMARK: The parameter m plays the role of a dilation, and will turn out to be insignificant. Think of $m = 0$.

5. Set

$$\widehat{Y}_0 = \frac{1}{2}\sum_{i=1}^{N} \log\Big(2\pi\beta^{1/3}G_\kappa\Theta_i\Big), \qquad \widehat{Y}_1 = \frac{1}{24}\sum_{i=1}^{N}\Big(\beta^{1/3}G_\kappa\Theta_i\Big)^3,$$

and consider the tilted probability measure $\widehat{\mathbb{P}}$ on $(\Omega, \mathscr{F}, \mathbb{P})$ defined by

$$\widehat{\mathbb{P}}(A) = \frac{\mathbb{E}[\exp(\widehat{Y}_0 - \widehat{Y}_1)\mathbb{1}_A]}{\mathbb{E}[\exp(\widehat{Y}_0 - \widehat{Y}_1)]}, \qquad A \subset \Omega \text{ measurable.}$$

The somewhat baroque quantities $\widehat{Y}_0$ and $\widehat{Y}_1$ arise from a Taylor expansion of the difference between the volume of the halo and the volume of the critical disk.

6. Let $\tau_* \in \mathbb{R}$ be the unique solution of the equation

$$\int_0^\infty \sqrt{2\pi u}\,\mathrm{exp}\Big(-\tau_* u - \frac{u^3}{24}\Big)\,\mathrm{d}u = 1.$$

The observation that

$$\int_0^\infty s^{-1/2}\mathrm{e}^{-s}\mathrm{d}s = \Gamma\Big(\frac{1}{2}\Big) = \sqrt{\pi},$$

combined with the change of variable $s = u^3/24$, yields

$$\int_0^\infty \sqrt{2\pi u}\,\mathrm{exp}\left(-\frac{u^3}{24}\right)\,\mathrm{d}u = \frac{4\pi}{\sqrt{3}} > 1,$$

and so $\tau_* > 0$.

▶ Three technical conditions

The main theorems in Lecture 9 are proved subject to the following conditions:

(C1) The limit

$$-c_{**} = \lim_{\beta\to\infty} \frac{1}{\beta^{1/3}} \log \widehat{\mathbb{P}}(Z^{(0)} \in \mathcal{O})$$

exists and is of the form

$$c_{**} = 2\pi G_\kappa \tau_{**}$$

for some $\tau_{**} > 0$ that does not depend on κ, to be identified in Lecture 11.

(C2) The change from $Z^{(0)}$ to $Z^{(m)}$ does not affect (C1) when m is not too large:

$$\lim_{\beta\to\infty} \frac{1}{\beta^{1/3}} \sup_{|m|=O(\beta^{1/6})} \left| \log \frac{\widehat{\mathbb{P}}(Z^{(m)} \in \mathcal{O})}{\widehat{\mathbb{P}}(Z^{(0)} \in \mathcal{O})} \right| = 0.$$

(C3) With the notation

$$\overline{u_i} = \tfrac{1}{2}(u_i + u_{i+1}), \quad 1 \le i \le N,$$

let

$$D_1 = \frac{1}{\sqrt{\pi}} \sum_{i=1}^{N} \Theta_i \overline{B_{T_i} \cos T_i}, \quad D_1^* = \frac{1}{\sqrt{\pi}} \sum_{i=1}^{N} \Theta_i \overline{B_{T_i} \sin T_i},$$

and

$$\chi = \sum_{i=1}^{N} \Theta_i \overline{B_{T_i}}^2 - D_1^2 - D_1^{*2}.$$

Then, for $\delta > 0$ sufficiently small,

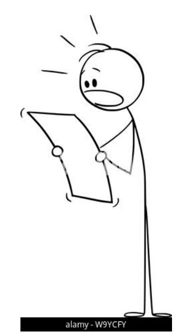
$$\limsup_{\beta \to \infty} \frac{1}{\beta^{1/3}} \log \frac{\widehat{\mathbb{E}}[\exp(\frac{1}{2}(1+\delta)\chi)\mathbb{1}_{\{Z^{(m)} \in \mathcal{O}\}}]}{\widehat{\mathbb{P}}(Z^{(m)} \in \mathcal{O})} = 0,$$

uniformly in $|m| = O(\beta^{1/6})$.

Condition (C1) comes from the fact that for each of the boundary points there is a constraint in terms of the two neighbouring boundary points that must be satisfied in order for the corresponding unit disk to touch the boundary of the critical droplet. The constant τ_{**} is related to the free energy of an effective interface model.

Condition (C2) says that the constraint imposed by Condition (C1) is not affected by small dilations of size m of the critical droplet, and implies that the free energy of the effective interface model is Lipschitz under small perturbations.

Condition (C3) says that the first Fourier coefficient χ of the surface of the critical droplet is small. In essence χ represents an energetic and entropic reward for the droplet boundary to fluctuate away from ∂B_{R_c}. The condition requires that this reward does not affect the microscopic free energy of the droplet.



§ MAIN THEOREM: SHARP ASYMPTOTICS

We are now ready to formulate our main theorem.

THEOREM 10.5 Moderate deviations

Suppose that Conditions (C1)–(C3) hold. Then, for all C large enough and $\beta \to \infty$,

$$\mu_\beta\Big(|V(\gamma) - \pi R_c^2| \le C\beta^{-2/3}\Big) = \mathrm{e}^{-\beta I(B_{R_c}) + \beta^{1/3}\Psi(\kappa) + o(\beta^{1/3})},$$

where

$$I(B_{R_c}) = \Phi(\kappa) - (1-\kappa)|\mathbb{T}|, \qquad \Psi(\kappa) = 2\pi G_\kappa(\tau_* - \tau_{**}).$$

Because

$$I(\kappa, \beta; C) = \Xi_\beta \, \mu_\beta\Big(|V(\gamma) - \pi R_c(\kappa)^2| \leq C\delta(\beta)\Big)$$

approximates the Dirichlet form for the dynamic Widom-Rowlinson model, we see that Theorem 10.5 settles the main theorems in Lecture 9, in particular, Theorem 9.1 and Theorem 9.3.

The factor $-(1-\kappa)|\mathbb{T}|$ *can be conveniently absorbed into the partition function* Ξ_β.

The proof of Theorem 10.5 is long and complicated. It uses a series of coarse-graining techniques, perturbation arguments, comparison couplings and a priori estimates that are beyond the scope of this lecture.

PAPER:

F. den Hollander, S. Jansen, R. Kotecký and E. Pulvirenti,
The Widom-Rowlinson model: Mesoscopic fluctuations
for the critical droplet.
Preprint 2019 [arXiv:1907.00453].