Exercise: Lectures 9 + 10

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1 Exercise 1: Equivalence of one-species and two-species model

In this exercise you will prove that the Widom-Rowlinson model allows for an equivalent formulation in terms of a binary gas of hard discs with radius $\frac{1}{2}$, as shown in the original paper by Widom and Rowlinson [5].

1.1 Notation

Let $\mathbb{T} \subset \mathbb{R}^2$ be a torus of fixed size. Consider a particle configuration made up of two type of particles, say, *red* and *blue* particles. The set of finite particle configurations in $\mathbb{T}$ is

$$\tilde{\Gamma} = \big\{(\gamma^{\mathrm{red}}, \gamma^{\mathrm{blue}})\colon\ \gamma^{\mathrm{red}}, \gamma^{\mathrm{blue}} \subset \mathbb{T},\ N(\gamma^{\mathrm{red}}), N(\gamma^{\mathrm{blue}}) \in \mathbb{N}_0\big\}, \tag{1.1}$$

where $N(\gamma)$ denotes the cardinality of γ.

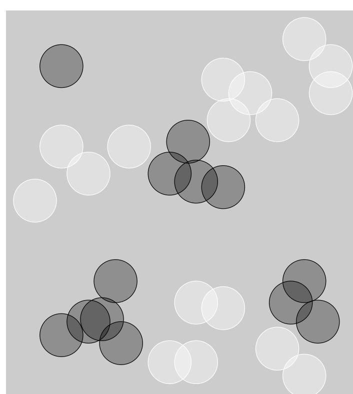

Figure 1: Picture of a two-species particle configuration, where particles of different type cannot overlap. The particles are discs of radius $\frac{1}{2}$.

The *grand-canonical Gibbs measure* is the probability measure on $\tilde{\Gamma}$ given by

$$\mathrm{d}\tilde{\mu}(\gamma^{\mathrm{red}}, \gamma^{\mathrm{blue}}) = \frac{1}{\Xi}\, \chi(\gamma^{\mathrm{red}}, \gamma^{\mathrm{blue}})\, z_{\mathrm{red}}^{N(\gamma^{\mathrm{red}})}\, z_{\mathrm{blue}}^{N(\gamma^{\mathrm{blue}})} \mathrm{d}\mathbb{Q}(\gamma^{\mathrm{red}})\, \mathrm{d}\mathbb{Q}(\gamma^{\mathrm{blue}}), \tag{1.2}$$

where $z_i = \mathrm{e}^{\beta\lambda_i}$ is the activity of type $i \in \{\mathrm{red}, \mathrm{blue}\}$, $\mathbb{Q}$ is the Poisson point process on $\mathbb{T}$ with intensity 1, and $\chi(\gamma^{\mathrm{red}}, \gamma^{\mathrm{blue}})$ is the indicator variable

$$\chi(\gamma_1, \gamma_2) = \begin{cases} 1, & \text{if} \quad d(\gamma_1, \gamma_2) \geq 1, \\ 0, & \text{otherwise}, \end{cases} \tag{1.3}$$

where $d(\gamma_1, \gamma_2)$ means the minimal distance between points in the sets γ_1 and γ_2. Particles can be viewed as discs of radius $\frac{1}{2}$ (as in Fig. 1). The indicator $\chi(\gamma^{\mathrm{red}}, \gamma^{\mathrm{blue}})$ means that discs of the *same* type can overlap while discs of *different* type cannot overlap. The normalising partition function is

$$\tilde{\Xi} = \int_{\tilde{\Gamma}} \chi(\gamma^{\text{red}}, \gamma^{\text{blue}})\, z_{\text{red}}^{N(\gamma^{\text{red}})} z_{\text{blue}}^{N(\gamma^{\text{blue}})} \mathrm{d}\mathbb{Q}(\gamma^{\text{red}})\, \mathrm{d}\mathbb{Q}(\gamma^{\text{blue}}). \tag{1.4}$$

1.2 Exercise

Fix $z_{\text{red}}, z_{\text{blue}} > 0$. Let $\pi_{\text{blue}} \colon \tilde{\Gamma} \to \Gamma$ be the projection that maps $(\gamma^{\text{red}}, \gamma^{\text{blue}})$ to γ^{blue}. Define β, z by putting

$$(z_{\text{red}}, z_{\text{blue}}) = (\beta, z\, \mathrm{e}^{\beta\pi}), \tag{1.5}$$

and let $\mu = \mu_{\beta,z}$ be the associated one-species Gibbs measure, i.e.

$$\mathrm{d}\mu(\gamma) = \frac{1}{\Xi}\, z^{N(\gamma)}\, \mathrm{e}^{-\beta H(\gamma)} \mathrm{d}\mathbb{Q}(\gamma). \tag{1.6}$$

(see slides of Lecture 9 for the notation of the one-species WR-model). Prove that

$$\boxed{\tilde{\mu} \circ \pi_{\text{blue}}^{-1} = \mu} \tag{1.7}$$

1.3 Guidelines for solving the exercise

- **Step 1:** Fix the centers of the blue discs and integrate over the centers of the red discs. Prove that

$$\frac{1}{\tilde{\Xi}} \int_{\Gamma} \mathbb{Q}(\mathrm{d}\gamma^{\text{red}})\, z_{\text{red}}^{N(\gamma^{\text{red}})} z_{\text{blue}}^{N(\gamma^{\text{blue}})} \chi(\gamma^{\text{red}}, \gamma^{\text{blue}}) = \frac{1}{\tilde{\Xi}}\, \mathrm{e}^{(\beta-1)|\mathbb{T}|} \big(z\, \mathrm{e}^{\beta\pi}\big)^{N(\gamma^{\text{blue}})}\, \mathrm{e}^{-\beta V(\gamma^{\text{blue}})}, \tag{1.8}$$

  where $V(\gamma)$ is the volume of the halo $h(\gamma)$ of γ.

  [Hint: Use that the union of the blue discs is impenetrable for the red discs, so that the halo of the blue discs is a "forbidden area" for the centres of the red discs.]

- **Step 2:** Explain why

$$\frac{1}{\Xi} = \frac{\mathrm{e}^{(\beta-1)|\mathbb{T}|}}{\tilde{\Xi}} \tag{1.9}$$

  and use this to conclude the proof.

2 Exercise 2: LDP for the Widom-Rowlinson model

In this exercise you will prove a Large Deviation Principle (LDP) for the equilibrium measure μ_β of the WR-model, as shown in den Hollander, Jansen, Kotecký and Pulvirenti [2].

2.1 Notation and LDP setting

To make the exercise self contained, we recall the definition of the Large Deviation Principle (see e.g. den Hollander [1, Chapter 3]).

Definition 2.1. *A sequence of probability measures $(P_n)_{n\in\mathbb{N}}$ on a Polish space $\mathcal{X}$ is said to satisfy the large deviation principle (LDP) with rate n and with rate function $I\colon \mathcal{X} \to [0,\infty]$ if*

- *I has compact level sets and $I \not\equiv \infty$,*
- $\liminf_{n\to\infty} \frac{1}{n} \log P_n(O) \geq -I(O)$, *for all $O \subset \mathcal{X}$ open,*
- $\limsup_{n\to\infty} \frac{1}{n} \log P_n(C) \leq -I(C)$, *for all $C \subset \mathcal{X}$ closed,*

where $I(A) = \inf_{x \in A} I(x)$.

Informally, the LDP says that if $B_\delta(x)$ is the open ball of radius $\delta > 0$ centred at $x \in \mathcal{X}$, then

$$P_n(B_\delta(x)) = \mathrm{e}^{-[1+o(1)]\, n\, I(x)} \tag{2.1}$$

when $n \to \infty$ followed by $\delta \downarrow 0$.

We also recall the following version of Varadhan's lemma (see e.g. den Hollander [1, Theorem 3.17]).

Theorem 2.2 (Tilted LDP)**.** *Let* $(P_n)_{n\in\mathbb{N}}$ *satisfy the LDP on* $\mathcal{X}$ *with rate* n *and rate function* I*. Let* $F \in C_b(\mathcal{X})$*, the space of bounded continuous functions on* $\mathcal{X}$*. Define*

$$J_n(S) = \int_S \mathrm{e}^{nF(x)} P_n(\mathrm{d}x), \qquad S \subset \mathcal{X} \text{ Borel.} \tag{2.2}$$

Then $(P_n^F)_{n\in\mathbb{N}}$ *defined by*

$$P_n^F(S) = \frac{J_n(S)}{J_n(\mathcal{X})}, \qquad S \subset \mathcal{X} \text{ Borel,} \tag{2.3}$$

satisfies the LDP on $\mathcal{X}$ *with rate* n *and rate function*

$$I^F(x) = \sup_{y\in\mathcal{X}} [F(y) - I(y)] - [F(x) - I(x)]\,. \tag{2.4}$$

Let $\mathcal{F}$ be the family of non-empty closed (and hence compact) subsets of the torus $\mathbb{T}$. By equipping $\mathcal{F}$ with the Hausdorff metric, we turn it into a compact metric space. The halo of any $F \in \mathcal{F}$ is given by the Minkowski addition, i.e.,

$$F^+ = F + B(0) = \bigcup_{x\in B(0)} (F + x) = h(F), \tag{2.5}$$

where $B(0)$ is the ball of radius 1 centered at $x = 0$.

Now recall the formula for the equilibrium Gibbs measure of the WR-model at inverse temperature β and activity $z = \kappa z_c(\beta) = \kappa\beta\mathrm{e}^{-\beta\pi}$ given on the slides,

$$\mu_\beta(\mathrm{d}\gamma) = \frac{1}{\Xi}\,(\kappa\beta)^{N(\gamma)}\,\mathrm{e}^{-\beta V(\gamma)}\,\mathbb{Q}(\mathrm{d}\gamma), \qquad \gamma \in \Gamma, \tag{2.6}$$

where $V(\gamma) = |h(\gamma)|$ and Ξ is the normalising partition function. This is a probability measure on the space $\Gamma \subset \mathcal{F}$ of particle configurations. We identify μ_β on Γ with the measure on $\mathcal{F}$ supported on Γ.

2.2 Exercise

Prove that the family of probability measures $(\mu_\beta)_{\beta\geq 1}$ on $\mathcal{F}$, supported on $\Gamma \subset \mathcal{F}$, satisfies the LDP with rate β and rate function I^{WR} given by

$$I^{\mathrm{WR}} = J^{\mathrm{WR}} - \inf_{\mathcal{F}} J^{\mathrm{WR}}, \quad J^{\mathrm{WR}}(F) = |F^+| - \kappa|F|, \quad F \in \mathcal{F}. \tag{2.7}$$

2.3 Guidelines for solving the exercise

- **Step 1:** Let $\Pi_{\kappa\beta}$ be the homogeneous Poisson point process on $\mathbb{T}$ with intensity $\kappa\beta$. Denote its law by $\mathsf{P}_{\kappa\beta}$. Show that μ_β is absolutely continuous with respect to $\mathsf{P}_{\kappa\beta}$, with Radon-Nikodym derivative

$$\frac{\mathrm{d}\mu_\beta}{\mathrm{d}\mathsf{P}_{\kappa\beta}}(\gamma) = \frac{\exp(-\beta|h(\gamma)|)}{\int_\Gamma \exp(-\beta|h|)\,\mathrm{d}\mathsf{P}_{\kappa\beta}}, \qquad \gamma \in \Gamma. \tag{2.8}$$

- **Step 2:** Use the following fact (Schreiber [3], [4, Theorem 1]): the family $(\mathsf{P}_{\kappa\beta})_{\beta\geq 1}$ satisfies the LDP with rate β and with rate function $I(F) = \kappa|\mathbb{T} \setminus F|$, $F \in \mathcal{F}$.

  Note that, by the properties of the Poisson point process, $\mathbb{P}(\Pi_{\kappa\beta} \subset F) = \mathbb{P}(\Pi_{\kappa\beta} \cap (\mathbb{T}\setminus F) = \emptyset) = \mathrm{e}^{-\beta I(F)}$, $F \in \mathcal{F}$.

- **Step 3:** Now apply Theorem 2.2 to the family $(\mu_\beta)_{\beta\geq 1}$, where $\mu_\beta(\mathcal{C}) = \mathcal{J}_\beta(\mathcal{C})/\mathcal{J}_\beta(\Gamma)$, $\forall\,\mathcal{C}\subset\mathcal{F}$ Borel, with
$$\mathcal{J}_\beta(\mathcal{C}) = \int_{\mathcal{C}} \exp(-\beta|h(\gamma)|)\,\mathrm{d}\mathsf{P}_{\kappa\beta}(\gamma). \tag{2.9}$$
[Hint: Use that the map $F \mapsto |F^+| = |h(F)|$ is continuous with respect to the Hausdorff metric.]

3 Exercise 3: LDP for the halo shape and the halo volume

In this exercise you will see how to obtain the leading order term of the average metastable crossover time via two Large Deviation Principles and an isoperimetric inequality, as shown in den Hollander, Jansen, Kotecký and Pulvirenti [2]. Even though this exercise uses the outcome of Exercise 2, you may try to solve it even when you did not manage to solve Exercise 2.

3.1 Notation and useful results

Let $\mathcal{S}\subset\mathcal{F}$ be the collection of all sets that are *admissible*, i.e.,
$$\mathcal{S} = \{S\subset\mathbb{T}\colon\ \exists\, F \text{ such that } h(F)=S\}. \tag{3.1}$$
There is a unique maximal F such that $h(F)=S$, which we denote by S^- and which equals $S^- = \{x\in S\colon\ B(x)\subset S\}$. We can view the halo $h(\gamma)$ as a random variable taking values in the space $\mathcal{S}$, endowed with the Hausdorff distance.

We recall the following corner stone from large deviation theory (see e.g. den Hollander [1, Theorem 3.20]).

Theorem 3.1 (Contraction principle)**.** *Let $(P_n)_{n\in\mathbb{N}}$ satisfy the LDP on $\mathcal{X}$ with rate n and with rate function $\mathcal{I}$. Let $\mathcal{Y}$ be a second Polish space, and $T\colon\ \mathcal{X}\to\mathcal{Y}$ a continuous map. Then $(Q_n)_{n\in\mathbb{N}}$ on $\mathcal{Y}$ defined by $Q_n = P_n\circ T^{-1}$ satisfies the LDP on $\mathcal{Y}$ with rate n and with rate function $\mathcal{J}$ given by*
$$\mathcal{J}(y) = \inf_{x\in\mathcal{X}\colon\ T(x)=y} \mathcal{I}(x). \tag{3.2}$$

Finally, for completeness we write down the following result that you have seen in Lecture 3 (see also den Hollander, Jansen, Kotecký and Pulvirenti [2, Theorem 2.2]).

Theorem 3.2 (Minimisers of rate function for halo volume)**.** *For every $R\in(1,\frac{L}{\pi}+\frac{1}{2})$,*
$$\min\left\{|S|-\kappa|S^-|\colon\ S\in\mathcal{S}, |S|=\pi R^2\right\} = \pi R^2 - \kappa\pi(R-1)^2, \tag{3.3}$$
and the minimisers are the discs of radius R.

(We refer to [2] for a statement about the *stability* of the minimisers under small perturbations. Since this statement is not needed for the exercise, we omitted it.)

3.2 Exercise

(i) Prove that the family of probability measures $(\mu_\beta(h(\gamma)\in\cdot))_{\beta\geq 1}$ satisfies the LDP on $\mathcal{S}$ with rate β and rate function I given by
$$I(S) = |S| - \kappa|S^-| - (1-\kappa)|\mathbb{T}|, \qquad S\in\mathcal{S}. \tag{3.4}$$

(ii) Prove that 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 rate function I^* given by
$$I^*(A) = \inf\{I(S)\colon\ S\in\mathcal{S},\ |S|=A\}. \tag{3.5}$$

(iii) Explain the following (informal) statement, for $\beta\to\infty$,
$$\mu_\beta(V(\gamma)\approx\pi R^2) \approx \exp\left[-\beta\left(\pi R^2-\kappa\pi(R-1)^2\right)+(1-\kappa)\beta|\mathbb{T}|\right]. \tag{3.6}$$

3.3 Guidelines for solving the exercise

- **Step 1:** Use the contraction principle, i.e., Theorem 3.1, and Exercise 2, i.e., (2.7), to prove that the family $(\mu_\beta(h(\gamma) \in \cdot))_{\beta \geq 1}$ satisfies the LDP with rate β and with rate function

$$I = J - \inf_{\mathcal{F}} J, \quad J(S) = \inf\left\{|F^+| - \kappa|F| \colon F \in \mathcal{F}, F^+ = S\right\}, \quad S \in \mathcal{S}. \tag{3.7}$$

  [Hint: Use that the map $\mathcal{F} \to \mathcal{S}$ defined by $F \mapsto S = F^+$ is continuous with respect to the Hausdorff metric.]

- **Step 2:** Show that $J(S) = |S| - \kappa|S^-|$ via upper and lower bounds.

  [Hint: Use that if $F^+ = S$, then $F \subset S^-$. If $F = S^-$, then for S to be an admissible set it must be that $F^+ = (S^-)^+ = S$.]

- **Step 3:** Use again the contraction principle, i.e., Theorem 3.1, and the previous steps, to prove that the family $(\mu_\beta(V(\gamma) \in \cdot))_{\beta \geq 1}$ satisfies the LDP with rate β and with rate function I^* given by the difference of two infima.

  [Hint: Use that the map $F \mapsto |F^+| = |h(F)|$ is continuous.]

- **Step 4:** Compute the two infima in I^*. First set $A = \pi R^2$ and use Theorem 3.2. Afterwards show that $\inf_{\mathcal{S}} J = (1-\kappa)|\mathbb{T}|$ because $\kappa \in (1, \infty)$. Conclude by explaining in words what the asymptotic expression (3.6) means.

References

[1] F. den Hollander, *Large Deviations*, Fields Institute Monographs 14, American Mathematical Society, Providence RI, 2000.

[2] 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].

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[4] T. Schreiber, Asymptotic geometry of high-density smooth-grained Boolean models in bounded domains, Adv. Appl. Prob. (SGSA) 35 (2003) 913–936.

[5] B. Widom and J.S. Rowlinson, New model for the study of liquid-vapor phase transitions, J. Chem. Phys. 52 (1970) 1670–1684.