PHASE TRANSITIONS FOR DILUTE PARTICLE SYSTEMS WITH LENNARD-JONES POTENTIAL

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Abstract: We consider a classical dilute particle system in a large box with pair-interaction given by a Lennard-Jones-type potential. The inverse temperature is picked proportionally to the logarithm of the particle density. We identify the free energy per particle in terms of a variational formula and show that this formula exhibits a cascade of phase transitions as the temperature parameter ranges from zero to infinity. Loosely speaking, the particle system separates into spatially distant components in such a way that within each phase all components are of the same size, which is the larger the lower the temperature. The main tool in our proof is a new large deviation principle for sparse point configurations.

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1. Introduction

1.1 Motivation

One of the basic themes of equilibrium statistical mechanics is the study of interacting many-body systems in the thermodynamic limit. A major problem in this area, which has not been mathematically solved so far, is to understand the transition between the gaseous and the solid phase at positive temperature and particle density. In the present paper we discuss the simpler situation when these two quantities vanish asymptotically with the relation between them fixed on the critical scale. We investigate a classical dilute system interacting via a pair potential of Lennard-Jones type, which includes attraction as well as repulsion. In this model we obtain that the temperature-density plane can be divided into separate phases, corresponding to the formation of clusters of different sizes. Within each phase all clusters have the same size. On the lines separating the phases, we encounter nondifferentiability of the free energy of the system, so that we may speak of *first-order phase transitions*.

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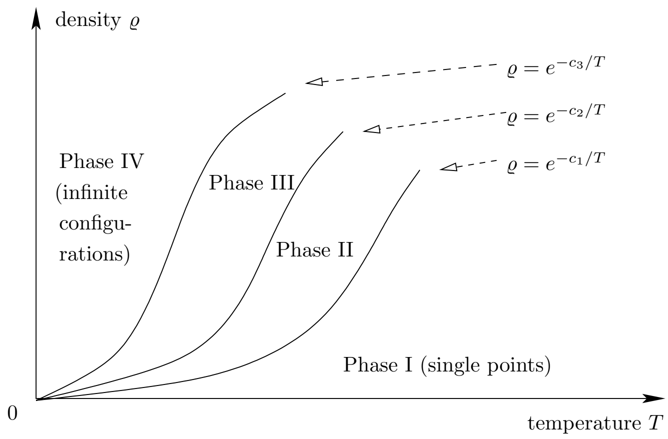


FIGURE 1. Blow-up near the origin in the temperature-density plane. The schematic phase diagram is for the case of three phase transitions, $\eta = 3$: Phase I (single points), Phase II (finite clusters with more than one point), Phase III (larger finite clusters), Phase IV (infinite clusters). Phases I-III are gaseous phases, Phase IV may be interpreted as a fluid or solid phase.

At fixed positive temperature, in a dilute system, the minimal inter-particle distance diverges and the system does not feel the interaction. At zero temperature, however, the minimisation of energy leads to the emergence of a macroscopic rigid crystalline structure, see [Th06]. We study the transition between these two scenarios by letting the temperature depend on the particle density in a critical way and thus zooming into the crucial region near the origin in the temperature-density plane.

We now turn to a detailed description of the model. We consider the following pair-interaction energy of N-point configurations in $\mathbb{R}^d$,

$$V_N(x_1, \dots, x_N) = \sum_{\substack{i,j=1 \\ i \neq j}}^{N} v\big(|x_i - x_j|\big), \qquad \text{for } x_1, \dots, x_N \in \mathbb{R}^d. \tag{1.1}$$

Here the *pair-interaction potential* $v\colon [0, \infty) \to (-\infty, \infty]$ is assumed to be of *Lennard-Jones type*, by which we mean that it explodes close to zero, has a nondegenerate negative part and vanishes at infinity. Additionally, we always assume that v has compact support. We allow the possibility that $v = \infty$ in some interval $[0, \nu_0]$ to represent hard core interaction. Assumption (V) below also ensures that the potential is *stable*, i.e., the energy V_N is of order N, see Lemma 1.1 below.

We consider N particles in a centred cube $\Lambda \subset \mathbb{R}^d$, such that the particle density is $\varrho := \frac{N}{|\Lambda|}$, where $|\Lambda|$ is the Lebesgue measure of Λ. The main object of our study is the partition function

$$Z_N(\beta, \varrho) := \frac{1}{N!} \int_{\Lambda^N} \mathrm{d}x_1 \dots \mathrm{d}x_N \, \exp\Big\{ - \beta V_N(x_1, \dots, x_N) \Big\}, \text{ for } \beta, \varrho \in (0, \infty), N \in \mathbb{N}. \tag{1.2}$$

We derive a variational characterisation of the limiting free energy per particle,

$$\Xi(c) := - \lim_{N \to \infty} \frac{1}{\beta_N N} \log Z_N(\beta_N, \varrho_N), \tag{1.3}$$

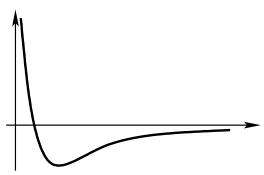
for $\beta_N \to \infty, \varrho_N \to 0$ such that $-\frac{1}{\beta_N} \log \varrho_N = c$ is constant. This relation implies that the energetic and entropic contributions to the partition function are on the same scale, and their competition determines the behaviour of the system.

1.2 The free energy

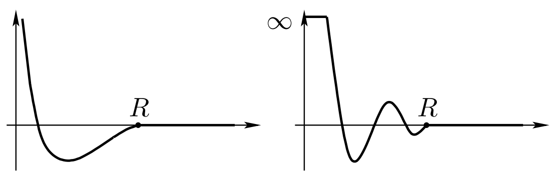
We now state our precise assumptions on the potential v. For each $r > 0$, denote by $s(r)$ the minimal number of balls of radius r required to cover a ball of radius one, and let $s^\star = \sup_{r\in(0,1]} s(r)r^d \in (0,\infty)$. Observe that $s^\star$ depends only on the dimension d.

Assumption (V). We suppose that the pair potential $v\colon [0,\infty) \to (-\infty,\infty]$ satisfies the following conditions:

(1) There is $\nu_0 \geq 0$ such that $v = \infty$ on $[0,\nu_0]$ and $v < \infty$ on (ν_0,∞);
(2) v is continuous on $[0,\infty)$;
(3) there is $R > 0$ such that $v = 0$ on $[R,\infty)$;
(4) there is $\nu_1 > 0$ such that $v < 0$ on $(R-\nu_1, R)$;
(5) there is $\nu_2 > 0$ such that $\min\limits_{[0,\nu_2]} v \geq -\nu_2^{-d}(2R)^d s^\star \min\limits_{[0,\infty)} v$.



Lennard-Jones potential
$v(r) = r^{-12} - r^{-6}$



Examples of potentials
satisfying Assumption (V)

In particular, v has a finite and strictly negative minimum, and $0 \leq \nu_0 \leq \nu_2 < R - \nu_1 < R$. We define the minimal energy of an N-particle configuration as

$$\varphi(N) = \inf_{x_1,\dots,x_N\in\mathbb{R}^d} V_N(x_1,\dots,x_N), \qquad \text{for } N \in \mathbb{N}. \tag{1.4}$$

Condition (5) will guarantee that $-\varphi(N)$ grows not faster than linearly, which is known as stability in statistical mechanics. Observe that (5) is always satisfied if $\nu_0 > 0$, as one can take $\nu_2 = \nu_0$.

Lemma 1.1 (Asymptotics of $\varphi(N)$)**.** *Let the pair-potential v satisfy Assumption (V), then the limit*

$$\tilde{\varphi} = \lim_{N\to\infty} \frac{\varphi(N)}{N} = \inf_{N\in\mathbb{N}} \frac{\varphi(N)}{N} \in (-\infty,0), \tag{1.5}$$

exists and is finite.

The existence of the limit relies on subadditivity, the finiteness on Assumption (V) (5), and the negativeness is provided by the presence of negative interactions according to Assumption (V) (4).

Remark 1.2. *The point configurations that minimise the energy $\varphi(N)$ received attention in the literature. In* [GR79, Th06] *crystallisation is proved for $d = 1$, resp. $d = 2$. This is the phenomenon that the minimising particle configuration approaches, as $N \to \infty$, a certain regular lattice which is unique up to translation and rotation. See also* [AFS09] *for more recent results. Physically speaking, these results are about zero temperature.*

By Lemma 1.1, the extended sequence $(\theta_\kappa\colon \kappa \in \mathbb{N}\cup\{\infty\})$ given by

$$\theta_\kappa = \begin{cases} \frac{\varphi(\kappa)}{\kappa}, & \text{if } \kappa \in \mathbb{N}, \\ \tilde{\varphi}, & \text{if } \kappa = \infty, \end{cases} \tag{1.6}$$

is a continuous map from $\mathbb{N}\cup\{\infty\}$ to $\mathbb{R}$.

Now we identify the logarithmic asymptotics of the partition function $Z_N(\beta_N, \varrho_N)$:

Theorem 1.3 (Free energy)**.** *Suppose the pair-potential v satisfies Assumption (V). Let $\Lambda_N \subset \mathbb{R}^d$ be a centred cube and $\beta_N \to \infty$ such that, for some $c \in (0,\infty)$, the particle density $\varrho_N = N/|\Lambda_N|$ satisfies $\varrho_N = \mathrm{e}^{-c\beta_N}$. Then the free energy per particle,*

$$\Xi(c) = -\lim_{N\to\infty} \frac{1}{N\beta_N} \log Z_N(\beta_N, \varrho_N), \tag{1.7}$$

exists and is given by

$$\Xi(c) = \inf\Big\{ \sum_{\kappa\in\mathbb{N}\cup\{\infty\}} q_\kappa\theta_\kappa - c\sum_{\kappa\in\mathbb{N}} \frac{q_\kappa}{\kappa} : q \in [0,1]^{\mathbb{N}\cup\{\infty\}}, \sum_{\kappa\in\mathbb{N}\cup\{\infty\}} q_\kappa = 1\Big\}. \tag{1.8}$$

Remark 1.4. *In the case of positive particle density at fixed positive temperature, the existence of the free energy per particle and of a close-packing phase transition when the potential is infinite in a neighbourhood of zero, is a classical fact, see e.g.* [Ru99, Theorem 3.4.4].

The probability sequence $q = (q_\kappa)_{\kappa\in\mathbb{N}\cup\{\infty\}}$ appearing in (1.8) has an interpretation, which we informally describe now. Since the support of v is bounded, any point configuration $\{x_1,\dots,x_N\}$ in the integral on the right of (1.2) can be decomposed into connected components such that no particles of different components interact with each other. The quantity q_κ characterises the relative frequency of components of cardinality κ among all these components, more precisely the configuration $\{x_1,\dots,x_N\}$ consists of Nq_κ/κ components of cardinality κ for each $\kappa \in \mathbb{N}$. In the case $\kappa = \infty$, one should speak of components whose cardinalities tend to infinity as some function of N. Each component of cardinality κ is chosen optimally, i.e., as a minimiser of the right-hand side in the definition (1.4) of $\varphi(\kappa)$. Then the term $\sum_{\kappa\in\mathbb{N}\cup\{\infty\}} q_\kappa\theta_\kappa$ expresses the energy coming from such a configuration, and the term $\sum_{\kappa\in\mathbb{N}} q_\kappa/\kappa$ describes its entropy.

Now the logarithmic asymptotics of the partition function $Z_N(\beta_N,\varrho_N)$ is determined by optimal configurations, i.e., by those configurations whose component structure follows the frequency distribution of any minimiser q of the right hand side of (1.8). By a straightforward, but technical, extension of the proof of the upper bound in (1.7), one could see that configurations with cluster frequencies different from the optimal q do not contribute to the limiting free energy, but we do not carry out details here. Neither information about the locations of the components relative to each other, nor about their shape is present in (1.8). The optimal shapes of cardinality κ are precisely those that minimize the right-hand side in the definition (1.4) of $\varphi(\kappa)$, but it goes far beyond the scope of the present paper to give more specific information about them.

1.3 The phase transitions

Now we analyse the minimisers q on the right-hand side of (1.8). It turns out that, as the temperature parameter c decreases from infinity to zero, the minimiser q jumps between Dirac sequences on increasing component sizes, beginning with the size one. This means that, for sufficiently large c, the interparticle distance diverges, and that for smaller values of c all components of the system have the same finite size, which depends on the phase. The number of phases may be finite or infinite (depending on the interaction potential v). If it is finite then there is a phase with components of unbounded size. We interpret the phases with finite component sizes as the gaseous phases of the system. It remains open whether the phase with infinite component size is a fluid or solid phase.

Let us turn to the details. Consider the sequence of points $(1/\kappa,\theta_\kappa)$ with $\kappa\in\mathbb{N}\cup\{\infty\}$, and extend them to the graph of a piecewise linear function $[0,1]\to(-\infty,0]$. Pick those of them which determine the largest convex minorant of this function. In formulas, let $\kappa_1 = 1$ and, for $n\in\mathbb{N}$,

$$\kappa_{n+1} = \max\Big\{ i\in\mathbb{N}\cup\{\infty\} : i > \kappa_n \text{ and } \frac{\theta_{\kappa_n}-\theta_i}{1/\kappa_n - 1/i} = \max_{j>\kappa_n} \frac{\theta_{\kappa_n}-\theta_j}{1/\kappa_n - 1/j}\Big\}, \tag{1.9}$$

if $\kappa_n \neq \infty$. Observe that the maximum in (1.9) exists since the set $\{j \in \mathbb{N} \cup \{\infty\} : j > \kappa_n\}$ is compact and the mapping $j \mapsto \frac{\theta_{\kappa_n} - \theta_j}{1/\kappa_n - 1/j}$ is continuous.

Hence, the sequence $(\kappa_1, \kappa_2, \dots)$ either terminates at $\kappa_{\eta+1} = \infty$ for some $\eta \in \mathbb{N}$ or continues infinitely, in which case we put $\eta = \infty$. We thus have

$$\eta = \sup\{n : \kappa_n < \infty\} \in \mathbb{N} \cup \{\infty\}.$$

By

$$c_n = \frac{\theta_{\kappa_n} - \theta_{\kappa_{n+1}}}{1/\kappa_n - 1/\kappa_{n+1}}, \qquad \text{for } 1 \leq n < \eta + 1, \tag{1.10}$$

we denote the slope of the convex minorant in the n-th interval. If $\eta = \infty$ define $c_\infty = \inf_{n \in \mathbb{N}} c_n$.

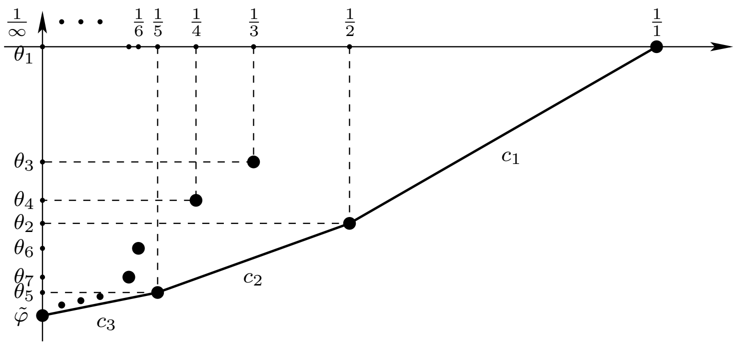


FIGURE 2. Example with $\eta = 3$ phase transitions and $\kappa_1 = 1, \kappa_2 = 2, \kappa_3 = 5$.

For $1 \leq n < \eta + 1$, let

$$I^{(n)} = \big\{\kappa_n \leq i \leq \kappa_{n+1} : (1/i, \theta_i) \text{ lies on the straight line passing through } (1/\kappa_n, \theta_{\kappa_n}) \text{ and } (1/\kappa_{n+1}, \theta_{\kappa_{n+1}})\big\}.$$

For $\kappa \in \mathbb{N} \cup \{\infty\}$, we denote by $\mathfrak{q}^{(\kappa)}$ the Dirac sequence that has a one in the κ-th entry and zeros everywhere else; we use the conventions $1/\infty = 0$ and $1/0 = \infty$. Let $\mathfrak{Q}^{(n)}$ be the convex hull of all $\mathfrak{q}^{(i)}$ with $i \in I^{(n)}$, i.e.,

$$\mathfrak{Q}^{(n)} = \Big\{ \sum_{i \in I^{(n)}} \lambda_i \mathfrak{q}^{(i)} : \sum_{i \in I^{(n)}} \lambda_i = 1, \lambda_i \geq 0 \text{ for all } i \in I^{(n)} \Big\}.$$

Now we can identify the free energy introduced in Theorem 1.3. It turns out that there are precisely η phase transitions, and they occur at the critical values c_n with $1 \leq n < \eta + 1$ (with one more phase transition at c_∞ in the case when $\eta = \infty$ and $c_\infty > 0$). In particular, the function $c \mapsto \Xi(c)$ is continuous and is linear between c_n and c_{n-1}, with slope equal to $-1/\kappa_n$, which is strictly decreasing in n.

Theorem 1.5 (Analysis of the variational formula)**.** *Let Ξ be as in Theorem 1.3. Then*

(i) *The sequence $(c_n)_{1 \leq n < \eta+1}$ is positive, finite and strictly decreasing.*

(ii)

$$\Xi(c) = \begin{cases} \tilde{\varphi} & \text{if } c \in (0, c_\eta], \\ \frac{\varphi(\kappa_n)}{\kappa_n} - \frac{c}{\kappa_n} & \text{if } c \in (c_n, c_{n-1}] \text{ for some } 2 \leq n < \eta + 1, \\ -c, & \text{if } c \in (c_1, \infty). \end{cases} \tag{1.11}$$

(iii) *If* $c \in (0,\infty) \setminus \{c_n : 1 \le n < \eta+1\}$, *then the minimiser* q *of* (1.8) *is unique:*

- *for* $c \in (0, c_\eta)$ *it is equal to* $\mathfrak{q}^{(\infty)}$,
- *for* $c = c_\infty$ *it is equal to* $\mathfrak{q}^{(\infty)}$ *(this is only applicable if* $\eta = \infty$ *and* $c_\infty > 0$*),*
- *for* $c \in (c_n, c_{n-1})$, *with some* $2 \le n < \eta + 1$, *it is equal to* $\mathfrak{q}^{(\kappa_n)}$,
- *for* $c \in (c_1, \infty)$ *it is equal to* $\mathfrak{q}^{(\kappa_1)} = \mathfrak{q}^{(1)}$.

(iv) *If* $c = c_n$ *for some* $1 \le n < \eta+1$, *then the set of the minimisers of* (1.8) *is equal to* $\mathfrak{Q}^{(n)}$.

Note that $\eta \ge 1$, that is, there is at least one phase transition. In particular, the high temperature phase corresponding to the last case in (1.11) is always present. In this phase the relevant configurations $\{x_1, \dots, x_N\}$ on the right-hand side of (1.2) consist of single points, i.e., there is no interaction between any of the particles of the configuration and we are in an entropy dominated regime. The first case in (1.11) is the low-temperature phase, where the relevant configurations consist of components whose cardinalities tend to infinity as $N \to \infty$. This case is empty if $\eta = \infty$ and $c_\eta = c_\infty = 0$. The second case in (1.11) is the case of intermediate temperatures; here those configurations dominate whose connected components have a finite cardinality ≥ 2. If $\eta = 1$, then the second case is empty, that is, only one-point configurations appear for c above the critical point $c_1 = -\tilde\varphi$ and infinitely large ones for c below that point. This happens if and only if neither of the points $(1/\kappa, \theta_\kappa)$ with $1 < \kappa < \infty$ lies below the line connecting $(1, \theta_1) = (1, 0)$ and $(0, \theta_\infty) = (0, \tilde\varphi)$, that is, if and only if $\frac{\varphi(\kappa)}{\kappa - 1} \ge \tilde\varphi$.

We do not offer any criterion under which the value of η is determined. See Section 6 for an example of a potential v for which there are two phase transitions.

1.4 Outline of the proof of Theorem 1.3

As $v(x) = 0$ for $x \ge R$, points do not interact if the distance between them is larger than R. We therefore introduce a graph structure on point configurations, connecting two points by an edge if the distance between them is at most R. A finite or countable set $C \subset \mathbb{R}^d$ is called *connected* if for any two elements $a, b \in C$ there exist $k \in \mathbb{N}$ and $a_0, \dots, a_k \in C$ such that $a_0 = a$, $a_k = b$ and $|a_i - a_{i-1}| \le R$ for $i \in \{1, \dots, k\}$.

For a configuration $x = (x_1, \dots, x_N)$ of points in Λ_N, we define Θ_i to be the largest subset of $\{1, \dots, N\}$ containing i such that the set $\{x_j : j \in \Theta_i\}$ is connected. Now the i-th connected cloud is defined by

$$[x_i] := \sum_{j \in \Theta_i} \delta_{x_j},$$

and the shifted i-th connected cloud by

$$[x_i] - x_i := \sum_{j \in \Theta_i} \delta_{x_j - x_i},$$

where δ_y denotes the Dirac measure at $y \in \mathbb{R}^d$. If $[x_i](\{a\}) \neq 0$ we say that $a \in [x_i]$ and denote $\#[x_i] = [x_i](\mathbb{R}^d)$, which is equal to the number of points in the i-th connected cloud. The main object of our analysis is the empirical measure on the connected components of the graph induced by the configuration, translated such that any of its points is at the origin with equal measure,

$$Y_N^{(x)} = \frac{1}{N} \sum_{i=1}^N \delta_{[x_i] - x_i}. \tag{1.12}$$

Observe that the energy of the configuration may be written as

$$V_N(x) = \sum_{\substack{i,j=1\\ i \neq j}}^N v\big(|x_i - x_j|\big) = \sum_{i=1}^N \sum_{\substack{j \neq i\\ x_j \in [x_i]}} v\big(|x_i - x_j|\big) = \sum_{i=1}^N \frac{1}{\#[x_i]} \sum_{\substack{x, y \in [x_i]\\ x \neq y}} v\big(|x - y|\big) = N\, \Psi\big(Y_N^{(x)}\big),$$

where, for a suitable class of probability measures Y on configurations, we define

$$\Psi(Y) = \int Y(\mathrm{d}A)\, \frac{1}{\#A} \sum_{\substack{x,y\in A\\ x\neq y}} v(|x-y|).$$

Let X be a vector of independent random variables $X_1^{(N)}, X_2^{(N)}, \dots, X_N^{(N)}$ uniformly distributed on Λ_N, and write $Y_N = Y_N^{(X)}$. Hence we can represent the partition function as

$$Z_N\big(\beta_N, \mathrm{e}^{-c\beta_N}\big) = \frac{|\Lambda_N|^N}{N!} \mathbb{E}_{\Lambda_N}\Big[\exp\big\{ -N\beta_N \Psi(Y_N)\big\}\Big], \tag{1.13}$$

where $\mathbb{E}_{\Lambda_N}$ and $\mathbb{P}_{\Lambda_N}$ denote the expectation and probability with respect to X. The main step, formulated as Proposition 2.2, is a large deviation principle for Y_N in the weak topology with speed $N\log(1/\varrho_N)$ and a rate function

$$J(Y) = 1 - \int Y(\mathrm{d}A)\, \frac{1}{\#A}.$$

By definition, this means that

$$\frac{1}{N\log(1/\varrho_N)}\, \log \mathbb{P}_{\Lambda_N}\big(Y_N \in \,\cdot\,\big) \Longrightarrow -\inf_{Y\in\,\cdot} J(Y)\,,$$

where $\Rightarrow$ denotes weak convergence. Large deviation principles for particle systems with interactions were also considered in [Ge94], though in the non-dilute case which is significantly different.

By our assumption $N\log(1/\varrho_N) = cN\beta_N$ and hence an informal application of Varadhan's lemma (whose direct application is impossible by the lack of continuity of the functional Ψ) to (1.13) implies that

$$\lim_{N\to\infty} \frac{1}{N\beta_N}\, \log \mathbb{E}_{\Lambda_N}\Big[\exp\big\{ -N\beta_N\Psi(Y_N)\big\}\Big] = -\inf_{Y} \big\{\Psi(Y) + c\, J(Y)\big\}\,.$$

Using (1.13) and

$$\frac{|\Lambda_N|^N}{N!} = \exp\big\{N\log \tfrac{1}{\varrho_n}\big\}\, e^{O(N)} = \exp\{cN\beta_N\}\, e^{o(N\beta_N)}, \tag{1.14}$$

it is easily seen that this gives Theorem 1.3.

The remainder of this paper is organised as follows. In Section 2, we analyse the distribution of $Y_N^{(X)}$ and prove a large deviation principle. In Section 3 we analyse $\varphi(N)$ and its asymptotics and prove in particular Lemma 1.1. The proofs of Theorems 1.3 and 1.5 are in Sections 4 and 5. Finally, an example of a potential v that admits several phase transitions is described in Section 6.

2. Large deviations for Y_N

In this section we analyse the distribution of the empirical measure Y_N introduced in (1.12) asymptotically as $N\to\infty$. In particular, we state and prove one of our main tools, the large deviation principle. In Section 2.1 we introduce the topological framework. The principle is formulated in Section 2.2 and proved in Sections 2.3 and 2.4.

2.1 Topological framework

A measure A on $\mathbb{R}^d$ is called a *configuration* or a *point measure* if $A = \sum_{i\in I}\delta_{a_i}$ for some finite or countable collection $(a_i\colon i\in I)$ of (not necessarily distinct) points of $\mathbb{R}^d$ such that $A(K) < \infty$ for any compact set $K\subset\mathbb{R}^d$. For any configuration A, we denote $\#A = A(\mathbb{R}^d)$ and, for $a\in\mathbb{R}^d$, we write $a\in A$ if $A(\{a\})\geq 1$. We call a point a a *multiple point* of a configuration A if $A(\{a\})\geq 2$.

Denote by $\mathcal{N}$ the space of all configurations on $\mathbb{R}^d$. We equip $\mathcal{N}$ with the vague topology, that is, A_n converges to A if $\limsup_{n\to\infty} A_n(K) \le A(K)$ and $\liminf_{n\to\infty} A_n(O) \ge A(O)$, for any compact set $K \subset \mathbb{R}^d$ and open set $O \subset \mathbb{R}^d$. The vague convergence is metrisable and $\mathcal{N}$ is a Polish space, cf. [Res87, Prop. 3.17].

A configuration $A = \sum_{i\in I} \delta_{a_i} \in \mathcal{N}$ is called *connected* if the set $\{a_i \colon i \in I\}$ is connected in the sense explained in Section 1.4. We denote by $\mathcal{N}_R^{(0)}$ the set of all configurations $A \in \mathcal{N}$ which are connected and such that $0 \in A$. It is easy to see from [Res87, Prop. 3.13] that the set $\mathcal{N}_R^{(0)}$ is closed in $\mathcal{N}$. Hence $\mathcal{N}_R^{(0)}$ is a Polish space. We equip $\mathcal{N}$ with the Borel σ-algebra and denote by $\mathcal{M}_1 = \mathcal{M}_1(\mathcal{N}_R^{(0)})$ the set of all probability measures on $\mathcal{N}_R^{(0)}$. We equip $\mathcal{M}_1$ with the weak topology and observe that it is Polish as so is $\mathcal{N}_R^{(0)}$ (see [Bil68, App. III]).

In the sequel, it will often be more convenient to work with atomic measures in $\mathcal{M}_1$ that are concentrated on finitely many finite configurations without multiple points and without points at the critical distance R. Observe that the clouds $[X_i^{(N)}]$ have this property with probability one; the shifted clouds have this property too, and they additionally contain zero. Denote by $\mathcal{N}_{R,\star}^{(0)}$ the set of all finite configurations $A \in \mathcal{N}_R^{(0)}$ which satisfy $A(\{x\}) = 1$, for any $x \in A$, and $|x-y| \neq R$, for any $x, y \in A$. Let

$$\mathcal{M}_{1,\star} := \Big\{ Y = \sum_{i=1}^m p_i \delta_{A_i} \colon m \in \mathbb{N}, \sum_{i=1}^m p_i = 1, \text{ and } p_i > 0, A_i \in \mathcal{N}_{R,\star}^{(0)} \text{ for all } i \Big\}$$

denote the set of all convex combinations of finitely many Dirac measures configurations in $\mathcal{N}_{R,\star}^{(0)}$. Observe that Y_N belongs to the space $\mathcal{M}_{1,\star}$ with probability one but it additionally has a lot of symmetries. Namely, for each $A \in \mathcal{N}_R^{(0)}$ and $a \in A$ one has $Y_N(\{A-a\}) = Y_N(\{A\})$.. Hence, with probability one, Y_N is element of

$$\mathcal{M}_{1,\star}^{(0)} := \Big\{ Y \in \mathcal{M}_{1,\star} \colon Y(\{A-a\}) = Y(\{A\}) \text{ for each } A \in \mathcal{N}_R^{(0)} \text{ and } a \in A \Big\}.$$

Let us denote by $\mathcal{M}_1^{(0)}$ the closure of $\mathcal{M}_{1,\star}^{(0)}$ in $\mathcal{M}_1$. It will be the main state space for our analysis.

Finally, for $\nu > 0$ and $n \in \mathbb{N}$, denote

$$\mathcal{N}_{R,n,\nu}^{(0)} := \big\{ A \in \mathcal{N}_{R,\star}^{(0)} \colon \#A \le n, |x-y| > \nu \text{ for any distinct } x, y \in A \big\}. \tag{2.1}$$

Our last preparation is the following continuity property.

Lemma 2.1. *The map $A \mapsto \#A$ from $\mathcal{N}_R^{(0)}$ to $\mathbb{N} \cup \{\infty\}$ is continuous in the vague topology.*

Proof. Let $\{A_n \colon n \in \mathbb{N}\}$ be a sequence in $\mathcal{N}_R^{(0)}$ converging to some $A \in \mathcal{N}_R^{(0)}$. Since $\mathbb{R}^d$ is open we have $\liminf_{n\to\infty} \#A_n = \liminf_{n\to\infty} A_n(\mathbb{R}^d) \ge A(\mathbb{R}^d) = \#A$. If $\#A = \infty$ we are done. If $\#A < \infty$ we need to prove that $\limsup_{n\to\infty} \#A_n \le \#A$. If this is not the case then $\#A_n \ge \#A + 1$ for infinitely many n and, for those n, $A_n(K) \ge \#A + 1$, where K is a closed ball of radius $R(\#A+1)$ centred at zero. Then $\limsup_{n\to\infty} A_n(K) \ge \#A + 1 > A(\mathbb{R}^d) \ge A(K)$ which is a contradiction. □

2.2 The large deviation principle

Now we formulate the main result of this section, the large deviation principle for the empirical measures Y_N introduced in (1.12). Let $L, J \colon \mathcal{M}_1 \to [0,\infty)$ be defined by

$$L(Y) := \int_{\mathcal{N}_R^{(0)}} Y(\mathrm{d}A) \frac{1}{\#A} \qquad \text{and} \qquad J(Y) := 1 - L(Y), \tag{2.2}$$

where we recall our conventions $1/\infty = 0$ and $1/0 = \infty$.

Proposition 2.2 (Large deviation principle for Y_N)**.**

(*i*) *The sequence* $(Y_N)_{N\in\mathbb{N}}$ *satisfies a large deviation principle on the space* $\mathcal{M}_1^{(0)}$ *with speed* $N\log(1/\varrho_N)$ *and rate function* J*, that is, the following holds. For any open set* $O\subset\mathcal{M}_1^{(0)}$*,*

$$\liminf_{N\to\infty}\frac{1}{N\log(1/\varrho_N)}\log\mathbb{P}_{\Lambda_N}(Y_N\in O)\geq-\inf_{Y\in O}J(Y), \tag{2.3}$$

and for any closed set $C\subset\mathcal{M}_1^{(0)}$*,*

$$\limsup_{N\to\infty}\frac{1}{N\log(1/\varrho_N)}\log\mathbb{P}_{\Lambda_N}(Y_N\in C)\leq-\inf_{Y\in C}J(Y). \tag{2.4}$$

Furthermore, J *is continuous.*

(*ii*) *Let* $O\subset\mathcal{M}_1^{(0)}$ *be an open set and* $Y\in\mathcal{M}_{1,\star}^{(0)}\cap O$*. Denote*

$$n(Y)=\max\big\{\#A\colon Y(\{A\})>0\big\}$$

and pick $\nu<\nu(Y)$*, where*

$$\nu(Y)=\min\big\{\,|x-y|\colon x,y\in A \textit{ for some } A \textit{ with } Y(\{A\})>0 \textit{ and } x\neq y\big\}.$$

Then

$$\liminf_{N\to\infty}\frac{1}{N\log(1/\varrho_N)}\log\mathbb{P}_{\Lambda_N}\Big(Y_N\in O,\,Y_N\big(\mathcal{N}^{(0)}_{R,n(Y),\nu}\big)=1\Big)\geq-J(Y).$$

Proposition 2.2 shows that the distribution of Y_N depends, on the exponential scale $N\log(1/\varrho_N)$, only on the distribution of the component sizes, i.e., on the distribution of the mapping $\hat{q}=(\hat{q}_\kappa)_{\kappa\in\mathbb{N}}\colon\mathcal{M}_1\to[0,1]^{\mathbb{N}}$ defined by its coordinates

$$\hat{q}_\kappa(Y)=Y(\{A\colon\#A=\kappa\}),\qquad\text{for }\kappa\in\mathbb{N}. \tag{2.5}$$

This can be understood as follows. Given q, the probability that the configuration $\{X_1,\dots,X_N\}$ has about Nq_κ/κ components of size κ for each $\kappa\in\mathbb{N}$, is determined by the probability to place, for any $\kappa\in\mathbb{N}$, Nq_κ/κ points somehow into Λ_N and to control the combinatorics coming from the possible choices of the indices $1,\dots,N$. The excluded-volume effect requiring that these points are sufficiently distant from each other may be ignored when deriving upper bounds and has a negligible effect because of the diluteness. Placing the remaining points in such a way that components of the required sizes arise has an effect on the scale $\mathrm{e}^{-O(N)}$, which is negligible. This explains why the large-deviation rate function is only a function of the numbers $\hat{q}_\kappa(Y)$.

We refer to (2.3) and (2.4) as to the lower bound for open sets and the upper bound for closed sets, respectively. The version of the large deviation lower bound in Proposition 2.2 (ii) is used in Section 4.2, where we apply Varadhan's lemma to a functional without sufficient continuity properties.

Observe that the continuity of J follows from the continuity of L, which itself immediately follows from Lemma 2.1. In Section 2.3 we prove (ii) and in Section 2.4 we prove the upper bound for closed sets. Observe that the lower bound for open sets immediately follows from (ii) by the continuity of J, since $\mathcal{M}_{1,\star}^{(0)}$ is dense in $\mathcal{M}_1^{(0)}$. By $B_r(x)$ we denote the Euclidean ball of radius $r>0$ around $x\in\mathbb{R}^d$.

2.3 Proof of Proposition 2.2 (ii)

Let $O\subset\mathcal{M}_1^{(0)}$ be an open set, and let $Y\in\mathcal{M}_{1,\star}^{(0)}\cap O$. Let us write Y in the form

$$Y=\sum_{i=1}^m p_i\delta_{A_i},$$

where $m\in\mathbb{N}$, $p_1,\dots,p_m>0$ add up to one, and the configurations $A_i\in\mathcal{N}_{R,\star}^{(0)}$ are pairwise distinct. The symmetries of Y as a member of the space $\mathcal{M}_{1,\star}^{(0)}$ imply that any two atoms of Y that are shifts of each other appear with the same probability. This allows us to introduce an equivalence relation on the integers $\{1,\dots,m\}$: we say that $i\sim j$ if there is $x\in A_i$ such that $A_j=A_i-x$. It is easy to see that this is indeed an equivalence relation: $i\sim i$ as $0\in A_i$; if $i\sim j$ then $j\sim i$ since $0\in A_i$ and so $-x\in A_j$; if $i\sim j$ and $j\sim k$ then $A_j=A_i-x$ for some $x\in A_i$ and $A_k=A_j-y$ for some $y\in A_j$, which implies $A_k=A_i-x-y$, and it suffices to notice that $x+y\in A_i$ since $y=z-x$ for some $z\in A_i$. For each configuration $A\in\mathcal{N}^{(0)}_{R,\star}$ we denote by $b(A)=\frac{1}{\#A}\sum_{a\in A}a$ its barycentre. If $i\sim j$ then $\#A_i=\#A_j$, $A_i-b(A_i)=A_j-b(A_j)$ and $p_i=p_j$. Denote the set of equivalence classes by $\mathcal{C}$ and, for any $c\in\mathcal{C}$, define $E_c=A_i-b(A_i)$ and $q_c=p_i$ for some $i\in c$. For technical reasons, we extend the set $\mathcal{C}$ by one extra element $c^\star$ and write $\mathcal{C}^\star=\mathcal{C}\cup\{c^\star\}$. Finally, we denote $E_{c^\star}=\{0\}$ and $q_{c^\star}=0$. Hence, we may write

$$Y=\sum_{c\in\mathcal{C}}q_c\sum_{e\in E_c}\delta_{E_c-e}. \tag{2.6}$$

For any N, let $k_c^{(N)}=\lfloor Nq_c\rfloor$ if $c\in\mathcal{C}$ and $k_{c^\star}^{(N)}=N-\sum_{c\in\mathcal{C}}k_c^{(N)}\#E_c$, also put $k^{(N)}=\sum_{c\in\mathcal{C}^\star}k_c^{(N)}$.

Below we prescribe certain ways to place N points $x_1,\dots,x_N$ into Λ_N such that, for large N, the resulting measure $Y_N^{(x)}$ lies in O and $Y_N^{(x)}(\mathcal{N}^{(0)}_{R,n(Y),\nu})=1$.

Roughly speaking, we pick, for any $c\in\mathcal{C}^\star$, precisely $k_c^{(N)}$ places in Λ_N at which we put slightly perturbed copies of the set E_c; let $\{x_1,\dots,x_N\}$ be the union of these copies. If all these places are not too close to each other, then these copies are its connected components, and $Y_N^{(x)}\approx Y$. Afterwards, we give a lower bound for the total mass of the choices of these places and the choices of the perturbed copies under the N-fold product of the uniform distribution on Λ_N. Using elementary combinatorics, we show that the exponential rate of this probability is bounded from below by $-J(Y)$.

The role of $c^\star$ is the following. Having taken care of the components that appear with positive probability in Y, we have distributed only $\sum_{c\in\mathcal{C}}k_c^{(N)}\#E_c$ points; the remaining $k_{c^\star}^{(N)}$ points will be placed by default at the origin.

Let us turn to the details. Denote

$$r=\max\big\{\,|x-y|\colon x,y\in A_i\text{ for some }i\big\}\in[0,\infty),$$
$$\rho^\star=\max\big\{\,|x-y|\colon x,y\in A_i\text{ for some }i\text{ and }|x-y|<R\big\}\in[0,R).$$

Observe that $\rho^\star<R$ since $Y\in\mathcal{M}^{(0)}_{1,\star}$, and that $|e|\le r$ for any $e\in E_c$ for any $c\in\mathcal{C}^\star$. Let $\Delta=2r+2R+1$ and define the grid

$$\mathcal{D}_N:=\big\{x\in\Delta\mathbb{Z}^d\cap\Lambda_N\colon \mathrm{dist}(x,\partial\Lambda_N)>r+R\big\}$$

and observe that $\#\mathcal{D}_N\ge\Delta^{-d}|\Lambda_N|\,(1+o(1))$. Let

$$Z^{(N)}:=\big\{z=(z_{c,i}\colon c\in\mathcal{C}^\star,i\le k_c^{(N)})\in(\mathcal{D}_N)^{k^{(N)}}\colon z_{c,i}\neq z_{c',i'}\text{ for }(c,i)\neq(c',i')\big\},$$

the set of vectors of places where the perturbed copies of the E_c will be located. Note that, for any $z\in Z^{(N)}$, for $(c,i)\neq(c',i')$, the distance between $z_{c,i}$ and $z_{c',i'}$ is larger than $2r+2R$. Observe that, as $N\uparrow\infty$,

$$\begin{aligned}\#Z^{(N)}&=\prod_{j=1}^{k^{(N)}}\big[\#\mathcal{D}_N-j+1\big]\ge(\#\mathcal{D}_N)^{k^{(N)}}\Big(1-\frac{k^{(N)}}{\#\mathcal{D}_N}\Big)^{k^{(N)}}\\&\ge|\Lambda_N|^{k^{(N)}}\,\mathrm{e}^{O(N)}\,\exp\Big\{-\frac{(k^{(N)})^2}{|\Lambda_N|}\,O(1)\Big\}=|\Lambda_N|^{k^{(N)}}\,\mathrm{e}^{o(N\log(1/\varrho_N))}.\end{aligned}\tag{2.7}$$

For each $z\in Z^{(N)}$, denote

$$\sigma_z^{(N)}=\bigcup_{c\in\mathcal{C}^\star}\bigcup_{i=1}^{k_c^{(N)}}\big(z_{c,i}+\mathrm{supp}(E_c)\big)\qquad\text{and}\qquad S_z^{(N)}=\sum_{x\in\sigma_z^{(N)}}\delta_x\in\mathcal{N}.$$

Since all E_c do not have multiple points, and due to our choice of $Z^{(N)}$, the configuration $S_z^{(N)}$ consists of N distinct points of mass 1 belonging to Λ_N, which form $k_c^{(N)}$ connected components of size $\#E_c$ for each $c \in \mathcal{C}^\star$. Later we will introduce a perturbation of the set $\sigma_z^{(N)}$ to obtain the set $\{x_1, \dots, x_N\}$ mentioned in the rough explanation below (2.6).

Fix $0 < \rho < \min\{\nu(Y) - \nu, R - \rho^\star\}$. Observe that the $\rho/2$-balls around the points of $S_z^{(N)}$ lie in Λ_N and have distance larger than ν to each other. The former follows from $\rho/2 + r < r + R$ and the latter from $\rho + \nu < \nu(Y)$ for balls centred at points belonging to the same cloud and from $\rho + 2r + \nu < 2r + 2R$ (provided by the conditions $\nu < R$ and $\rho < R$) for balls centred at points belonging to different clouds. Further, if $y_1, y_2 \in S_z^{(N)}$ are such that $|y_1 - y_2| < R$ then the same is true for any $\widetilde{y}_1 \in B_{\rho/2}(y_1)$, $\widetilde{y}_2 \in B_{\rho/2}(y_2)$. Indeed, $|y_1 - y_2| < R$ implies $|y_1 - y_2| \leq \rho^\star$ and $|\widetilde{y}_1 - \widetilde{y}_2| < R$ follows from $\rho^\star + \rho < R$. On the other hand, if $y_1, y_2 \in S_z^{(N)}$ lie in different clouds, then $|y_1 - y_2| \geq (2r + 2R) - 2r = 2R$. Since $\rho < R$ we obtain $|\widetilde{y}_1 - \widetilde{y}_2| \geq 2R - \rho > R$ for any $\widetilde{y}_1 \in B_{\rho/2}(y_1)$, $\widetilde{y}_2 \in B_{\rho/2}(y_2)$ and also $\widetilde{y}_1$ and $\widetilde{y}_2$ lie in different clouds. Finally, the case $|\widetilde{y}_1 - \widetilde{y}_2| = R$ is impossible since Y is concentrated on configurations in $\mathcal{N}_{R,\star}^{(0)}$.

For any $A = \sum_{i \in I} \delta_{x_i} \in \mathcal{N}$ and any $\varepsilon > 0$, we denote

$$A(\varepsilon) = \Big\{ \sum_{i \in I} \delta_{\widetilde{x}_i} : |\widetilde{x}_i - x_i| < \varepsilon \text{ for all } i \in I \Big\}.$$

The preceding arguments imply that any configuration $S \in S_z^{(N)}(\rho/2)$, like $S_z^{(N)}$ itself, consists of N points which form $k_c^{(N)}$ clouds of size $\#E_c$ for each $c \in \mathcal{C}^\star$. In particular, S does not contain clouds of size larger than $n(Y)$ since $\#E_c \leq n(Y)$ for all c. Moreover, S has no multiple points, and any two distinct points of S have distance larger than ν to each other. Finally, any two points of S belonging to the same cloud have distance smaller than R to each other. We write $\{x_1, \dots, x_N\}$ for the support of S. This is the set mentioned in the rough explanation below (2.6). Recall that the measure $Y_N^{(x)}$ is defined in (1.12). Summarising, we have that $Y_N^{(x)}$ is concentrated on the set $\mathcal{N}_{R,n(Y),\nu}^{(0)}$.

Observe that $Y_N^{(x)}$ can be written as

$$Y_N^{(x)} = \frac{1}{N} \sum_{c \in \mathcal{C}^*} \sum_{i=1}^{k_c^{(N)}} \sum_{e \in E_c} \delta_{E_{c,i} - \widetilde{e}(e,c,i)},$$

where $E_{c,i} \in E_c(\rho/2)$ and $\widetilde{e}(e,c,i) \in E_{c,i}$ is uniquely determined by the condition $|\widetilde{e}(e,c,i) - e| < \rho/2$.

Let us show that $Y_N^{(x)} \in O$ for any support $x = \{x_1, \dots, x_N\}$ of an $S \in S_z^{(N)}(\rho/2)$ with $z \in Z^{(N)}$. There is an open set $U_Y \subset O$ of the form

$$U_Y = \bigcap_{j=1}^{n} \Big\{ \widetilde{Y} \in \mathcal{M}_1^{(0)} : \Big| \int \widetilde{Y}(\mathrm{d}A)\, F_j(A) - \int Y(\mathrm{d}A)\, F_j(A) \Big| < \eta \Big\},$$

where $\eta > 0$, $n \in \mathbb{N}$ and $F_1, \dots, F_n : \mathcal{N}_R^{(0)} \to \mathbb{R}$ are continuous and bounded. Let M be such that $|F_j(A)| \leq M$ for all A and all $j \in \{1, 2, \dots, n\}$. Denote $q = \min\{q_c : c \in \mathcal{C}\}$. We have, for $N \geq 1/q$,

$$\Big| \int Y_N^{(x)}(\mathrm{d}A)\, F_j(A) - \int Y(\mathrm{d}A)\, F_j(A) \Big| = \Big| \frac{1}{N} \sum_{c \in \mathcal{C}^\star} \sum_{i=1}^{k_c^{(N)}} \sum_{e \in E_c} F_j\big(E_{c,i} - \widetilde{e}(e,c,i)\big) - \sum_{c \in \mathcal{C}^\star} \sum_{e \in E} q_c F_j(E_c - e) \Big|$$

$$\leq \sum_{c \in \mathcal{C}} \sum_{e \in E_c} \sum_{i=1}^{k_c^{(N)}} \Big| \frac{1}{N} F_j\big(E_{c,i} - \widetilde{e}(e,c,i)\big) - \frac{q_c}{k_c^{(N)}} F_j(E_c - e) \Big| + \frac{1}{N} \sum_{i=1}^{k_{c^\star}^{(N)}} \big| F_j(E_{c^\star,i} - \widetilde{e}(0, c^\star, i)) \big|.$$

Observe that $E_{c,i} - \widetilde{e}(e,c,i) \in (E_c - e)(\rho) = A_l(\rho)$ for some $l \leq m$. Since the functions $F_1, \dots, F_n$ are continuous and since the configurations $A_1, \dots, A_m$ are finite, there is $\varepsilon > 0$ such that $A \in A_i(\varepsilon)$

implies $|F_j(A) - F_j(A_i)| < \eta/2$ for all i, j. We further require that $\rho < \varepsilon$, then we have

$$|F_j\big(E_{c,i} - \widetilde{e}(e,c,i)\big) - F_j(E_c - e)| < \frac{\eta}{2}$$

for all j, c, i, e. Further, notice that

$$\Big|\frac{1}{N} - \frac{q_c}{k_c^{(N)}}\Big| = \frac{q_c}{\lfloor Nq_c \rfloor} - \frac{1}{N} \le \frac{q_c}{Nq_c - 1} - \frac{1}{N} \le \frac{1}{N(Nq-1)}.$$

Using the boundedness of all F_j by M we obtain

$$\begin{aligned}
&\Big|\int Y_N^{(x)}(\mathrm{d}A)\, F_j(A) - \int Y(\mathrm{d}A)\, F_j(A)\Big| \\
&\le \sum_{c\in\mathcal{C}} \sum_{e\in E_c} \sum_{i=1}^{k_c^{(N)}} \Big[\frac{1}{N}\big|F_j\big(E_{c,i} - \widetilde{e}(e,c,i)\big) - F_j(E_c - e)\big| + \Big|\frac{1}{N} - \frac{q_c}{k_c^{(N)}}\Big|\big|F_j(E_c - e)\big|\Big] + \frac{k_{c^\star}^{(N)} M}{N} \\
&\le \frac{1}{N} \sum_{c\in\mathcal{C}} \sum_{e\in E_c} \sum_{i=1}^{k_c^{(N)}} \Big[\frac{\eta}{2} + \frac{M}{Nq-1}\Big] + \frac{k_{c^\star}^{(N)} M}{N} = \frac{\eta}{2} + \frac{M}{Nq-1} + \frac{k_{c^\star}^{(N)} M}{N}.
\end{aligned}$$

Observe that

$$k_{c^\star}^{(N)} = N - \sum_{c\in C} k_c^{(N)} \# E_c = N - \sum_{c\in C} \lfloor Nq_c \rfloor \# E_c \le \sum_{c\in C} \# E_c, \tag{2.8}$$

which implies that $\frac{k_{c^\star}^{(N)} M}{N} \to 0$, since the right hand side of (2.8) does not depend on N. Since $\frac{M}{Nq-1} \to 0$ as well, there is N_0 such that for all $N \ge N_0$

$$\Big|\int Y_N^{(x)}(\mathrm{d}A)\, F_j(A) - \int Y(\mathrm{d}A)\, F_j(A)\Big| < \eta$$

for all $j \le n$. This proves that, for $N \ge N_0$, $Y_N^{(x)} \in O$ for any $S \in S_z^{(N)}(\rho/2)$, $z \in Z^{(N)}$.

Recall that $X_1^{(N)}, \dots, X_N^{(N)}$ under $\mathbb{P}_{\Lambda_N}$ are independent and chosen uniformly from the set Λ_N. For $N \ge N_0$, we have

$$\mathbb{P}_{\Lambda_N}\Big(Y_N^{(X)} \in O, Y_N^{(X)}\big(\mathcal{N}_{R,n(Y),\nu}^{(0)}\big) = 1\Big) \ge \mathbb{P}_{\Lambda_N}\Big(\bigcup_{z\in Z^{(N)}} \Omega_z^{(N)}\Big), \tag{2.9}$$

where

$$\Omega_z^{(N)} := \Big\{\sum_{i=1}^{N} \delta_{X_i^{(N)}} \in S_z^{(N)}(\rho/2)\Big\}.$$

For a fixed z, $\Omega_z^{(N)}$ is the event that each of N fixed non-intersecting balls of radius $\rho/2$ contains exactly one of the points $X_1^{(N)}, \dots, X_N^{(N)}$. Therefore

$$\mathbb{P}_{\Lambda_N}\big(\Omega_z^{(N)}\big) = N!\Big(\frac{|B_{\rho/2}(0)|}{|\Lambda_N|}\Big)^N.$$

Two events $\Omega_z^{(N)}$ and $\Omega_{z'}^{(N)}$ are either equal or disjoint. Equality holds if and only if $\{z_{c,i} \colon i \le k_c^{(N)}\} = \{z'_{c,i} \colon i \le k_c^{(N)}\}$ for all $c \in \mathcal{C}$ with $\#E_c > 1$ and additionally $\{z_{c,i} \colon i \le k_c^{(N)}, \#E_c = 1\} = \{z'_{c,i} \colon i \le k_c^{(N)}, \#E_c = 1\}$. Hence we can pick a subset of $Z^{(N)}$ consisting of

$$\frac{\# Z^{(N)}}{\Big(\prod_{\substack{c\in\mathcal{C} \\ \#E_c>1}} k_c^{(N)}!\Big)\Big(\sum_{\substack{c\in\mathcal{C}^\star \\ \#E_c=1}} k_c^{(N)}\Big)!} \ge |\Lambda_n|^{k^{(N)}} \exp\Big\{-N\log N \sum_{c\in\mathcal{C}} q_c\Big\}\, \mathrm{e}^{o(N\log(1/\varrho_N))}$$

elements such that the corresponding events $\Omega_z^{(N)}$ are pairwise disjoint. For the lower bound we used (2.7). Together with (2.9) we obtain, for $N \geq N_0$,

$$\begin{aligned}
&\mathbb{P}_{\Lambda_N}\Big(Y_N^{(X)} \in O, Y_N^{(X)}\big(\mathcal{N}^{(0)}_{R,n(Y),\nu}\big) = 1\Big) \\
&\quad \geq |\Lambda_n|^{k^{(N)}} \exp\Big\{ - N\log N \sum_{c\in\mathcal{C}} q_c\Big\} \, \mathrm{e}^{o(N\log(1/\varrho_N))}\, N!\, \frac{|B_{\rho/2}(0)|^N}{|\Lambda_N|^N} \\
&\quad = \exp\Big\{k^{(N)}\log|\Lambda_N| - N\log N\sum_{c\in\mathcal{C}} q_c + N\log N - N\log|\Lambda_N| + o(N\log(1/\varrho_N))\Big\}.
\end{aligned}$$

Recall that

$$\sum_{c\in\mathcal{C}} q_c = \sum_{i=1}^m \frac{p_i}{\# A_i} = L(Y)$$

and hence $k^{(N)} = NL(Y) + O(1)$. This gives

$$\begin{aligned}
k^{(N)}\log|\Lambda_N| &- N\log N\sum_{c\in\mathcal{C}} q_c + N\log N - N\log|\Lambda_N| \\
&= (L(Y)-1)\big(N\log|\Lambda_N| - N\log N\big) + O(\log|\Lambda_N|) \\
&= -J(Y)N\log\frac{1}{\varrho_N} + O(\log\tfrac{N}{\varrho_N}).
\end{aligned}$$

Obviously $O(\log\frac{N}{\varrho_N})$ is also $o(N\log(1/\varrho_N))$. Hence

$$\liminf_{N\to\infty} \frac{1}{N\log(1/\varrho_N)} \log\mathbb{P}_{\Lambda_N}\Big(Y_N \in O, Y_N\big(\mathcal{N}^{(0)}_{R,n(Y),\nu}\big) = 1\Big) \geq -J(Y),$$

which finishes the proof of Proposition 2.2 (ii).

2.4 Proof of Proposition 2.2 (i), upper bound

Now we show the upper bound for closed sets. As a preliminary step, we estimate the probability $\mathbb{P}_{\Lambda_N}(\hat q(Y_N^{(X)}) = q)$ from above for any $q \in [0,1]^{\mathbb{N}}$, where $\hat q$ is as defined in (2.5). By the discrete nature of $Y_N^{(X)}$, this probability is nonzero only when q lies in the set

$$\mathcal{Q}^{(N)} = \Big\{q \in [0,1]^{\mathbb{N}} \colon \sum_{i=1}^N q_i = 1, \frac{Nq_i}{i} \in \mathbb{N}\cup\{0\} \text{ for all } i \leq N, q_i = 0 \text{ for all } i > N\Big\}.$$

Substituting $k_i = Nq_i/i$ and noting that $k_i \leq N/i$, the cardinality of this set can be estimated by

$$\#\mathcal{Q}^{(N)} = \#\Big\{(k_1,\dots,k_N) \in \mathbb{N}_0^N \colon \sum_{i=1}^N ik_i = N\Big\} \leq \prod_{i=1}^N \Big(\frac{N}{i}+1\Big) \leq \frac{(2N)^N}{N!} \leq \mathrm{e}^{2N}. \tag{2.10}$$

Fix $q \in \mathcal{Q}^{(N)}$. On the event $\{\hat q(Y_N) = q\}$, the points $X_1^{(N)},\dots,X_N^{(N)}$ form $k_i = Nq_i/i$ connected components of size i, for each $i \leq N$, and no connected components of size larger than N. The number of ways to decompose $\{1,\dots,N\}$ into $\sum_{i=1}^N k_i$ sets such that there are k_i sets of cardinality i, for any i, is equal to

$$\frac{N!}{(\prod_i k_i!)(\prod_i i!^{k_i})}.$$

We bound the probability that such a decomposition represents the connected components of $\{X_1^{(N)},\dots,X_N^{(N)}\}$ by the probability that each partition set is just connected. Therefore, using independence, we obtain

$$\mathbb{P}_{\Lambda_N}\big(\hat q(Y_N^{(X)}) = q\big) \leq \frac{N!}{(\prod_i k_i!)(\prod_i i!^{k_i})} \prod_{i=1}^N \mathbb{P}_{\Lambda_N}\big(\{X_1^{(N)},\dots,X_i^{(N)}\} \text{ is connected}\big)^{k_i}.$$

If $\{X_1^{(N)},\dots,X_i^{(N)}\}$ is connected, there exists a labelled tree on $\{1,\dots,i\}$ with root in 1, such that for every edge (j,k) in the tree, we have

$$X_k^{(N)}\in B_R(X_j^{(N)}).$$

By Cayley's theorem, see [AZ98, pp. 141–146], the number of labelled trees with i vertices is i^{i-2}, and therefore we can estimate

$$\begin{aligned}\mathbb{P}_{\Lambda_N}\big(\hat q(Y_N^{(X)})=q\big)&\le N!\prod_{i=1}^N\Big[\frac{1}{k_i!(i!)^{k_i}}\Big(\frac{i|B_R(0)|}{|\Lambda_N|}\Big)^{(i-1)k_i}\Big]\\&\le \varrho_N^N\exp\Big\{-\sum_i k_i\log\frac{k_i}{|\Lambda_N|}+O(N)\Big\},\end{aligned}$$

uniformly in $q\in\mathcal{Q}^{(N)}$, using the convention $0\log 0=0$ and that $\sum_{i=1}^N ik_i=N$.

Let $t\in(0,1)$. Observe from (2.5) and (2.2) that $L(Y_N)=\sum_{i=1}^\infty\frac{q_i}{i}$ on the event $\{\hat q(Y_N)=q\}$. Hence

$$\begin{aligned}\log\mathbb{P}_{\Lambda_N}(L(Y_N)\le t)&=\log\sum_{\substack{q\in\mathcal{Q}^{(N)}\\ \sum_i q_i/i\le t}}\mathbb{P}_{\Lambda_N}(\hat q(Y_N)=q)\\&\le\log\Big[\big(\#\mathcal{Q}^{(N)}\big)\max\Big\{\mathbb{P}_{\Lambda_N}\big(\hat q(Y_N)=q\big)\colon q\in\mathcal{Q}^{(N)},\sum_{i=1}^\infty\frac{q_i}{i}\le t\Big\}\Big]\\&\le N\log\varrho_N-\inf_{k\in D_N}\sum_{i=1}^N k_i\log\frac{k_i}{|\Lambda_N|}+O(N),\end{aligned}\tag{2.11}$$

where we introduced

$$D_N=\Big\{k\in[0,\infty)^N\colon\sum_{i=1}^N ik_i=N,\sum_{i=1}^N k_i\le tN\Big\}.$$

We show that

$$\inf_{k\in D_N}\sum_{i=1}^N k_i\log\frac{k_i}{|\Lambda_N|}\ge tN\log\varrho_N+o\big(N\log\tfrac{1}{\varrho_N}\big),\qquad\text{for }N\to\infty.\tag{2.12}$$

Indeed, substituting $r_i=k_i/N$, it suffices to show that

$$\sum_{i=1}^N r_i\log(\varrho_N r_i)\ge t\log\varrho_N+o\big(\log\tfrac{1}{\varrho_N}\big),$$

whenever $r_1,\dots,r_N\ge 0$ satisfy $\sum_{i=1}^N ir_i=1$ and $\sum_{i=1}^N r_i\le t$. Distinguishing the alternatives $\log(1/r_i)\le i$ and $r_i<\mathrm{e}^{-i}$ and using that $x\mapsto x\log(1/x)$ is increasing near the origin, we get

$$\sum_{i=1}^N r_i\log(1/r_i)\le\sum_{i=1}^N ir_i+\sum_{i=1}^N i\mathrm{e}^{-i}\le 1+\sum_{i=1}^\infty i\mathrm{e}^{-i}.$$

Therefore $\sum_{i=1}^N r_i\log r_i$ is bounded from $-\infty$, which proves (2.12).

Inserting (2.12) into (2.11) implies that

$$\log\mathbb{P}_{\Lambda_N}(L(Y_N)\le t)\le-(1-t)N\log\frac{1}{\varrho_N}+o\big(N\log\tfrac{1}{\varrho_N}\big),\qquad\text{for }N\to\infty.\tag{2.13}$$

Now let $C\subset\mathcal{M}_1^{(0)}$ be a closed set. Let $s=\inf_C J\in[0,1]$. If $s=1$ then C contains only infinite configurations and so $\mathbb{P}_{\Lambda_N}(Y_N\in C)=0$. If $s=0$ then the upper bound is obviously satisfied. Assume that $s \in (0,1)$. We have

$$\log \mathbb{P}_{\Lambda_N}(Y_N \in C) \le \log \mathbb{P}_{\Lambda_N}(J(Y_N) \ge s) = \log \mathbb{P}_{\Lambda_N}\big(L(Y_N) \le 1-s\big)$$
$$\le -sN \log \frac{1}{\varrho_N} + o\big(N \log \tfrac{1}{\varrho_N}\big) = -N \log \frac{1}{\varrho_N}\Big(\inf_C J + o(1)\Big), \qquad \text{for } N \to \infty.$$

This finishes the proof of the upper bound for closed sets.

3. Analysis of $\varphi(n)$

In this section we prove Lemma 1.1 and provide some properties of $\varphi(n)$ introduced in Section 1.4. Recall that $\nu_0 = \inf\{x > 0 \colon v(x) < \infty\}$ and $v(\nu_0) = \infty$. For $n \ge 1$, denote

$$\mathcal{D}_n = \big\{x = (x_1, \dots, x_n) \in (\mathbb{R}^d)^n \colon |x_i - x_j| > \nu_0 \text{ for all } i \ne j\big\},$$

so that $\varphi(n) = \inf_{x \in \mathcal{D}_n} V_n(x)$. Further recall the definition of $\mathcal{N}^{(0)}_{R,n,\nu_0}$ from (2.1).

Lemma 3.1.

(i) *For each n, there is a minimiser $x^{(n)} \in \mathcal{D}_n$ such that $V_n(x^{(n)}) = \varphi(n)$.*

(ii) $\lim\limits_{n\to\infty} \frac{\varphi(n)}{n} = \tilde\varphi \in (-\infty, 0)$ *and* $\frac{\varphi(n)}{n} > \tilde\varphi$ *for all $n \in \mathbb{N}$.*

(iii) *For each n, there is a sequence $(x^{(n,m)} \colon m \in \mathbb{N})$ in $\mathcal{D}_n$ such that $V_n(x^{(n,m)}) \to \varphi(n)$ as $m \to \infty$, and*

$$\sum_{i=1}^n \delta_{x_i^{(n,m)}} \in \mathcal{N}^{(0)}_{R,n,\nu_0}, \qquad \textit{for all } m \in \mathbb{N}.$$

Proof. (i) Denote $\mathcal{D}'_n = \{x \in \mathcal{D}_n \colon x_1 = 0 \text{ and } |x_i| \le nR \text{ for all } i\}$. Observe that $\varphi(n) = \inf_{x \in \mathcal{D}'_n} V_n(x)$. Indeed, V_n is invariant under parallel translations, which allows to fix the first variable to be zero. Further, since v is strictly negative on $(R - \nu_1, R)$ and the system is invariant under rotations and translations, only the points x with connected configurations $\sum_{i=1}^n \delta_{x_i}$ contribute to the infimum. Indeed, if the configuration has more than one connected component then two of them can be rotated and translated in such a way that exactly one new negative interaction (at distance close to R) occurs.

The set $\mathcal{D}'_n$ is bounded and, by Assumption (V) (2), the function V_n is continuous on $\mathcal{D}'_n$. As $\partial\mathcal{D}'_n \setminus \mathcal{D}'_n$ has components of distance precisely ν_0 we infer from Assumption (V) (1) that $V_n(x) \to \infty$ as $x \to y \in \partial\mathcal{D}'_n \setminus \mathcal{D}'_n$. Hence V_n has a minimum $x^{(n)}$ on $\mathcal{D}'_n$, which is also a minimum on $\mathcal{D}_n$.

(ii) We first show subadditivity of the sequence $(\varphi(n) \colon n \in \mathbb{N})$.. Fix $n, m \in \mathbb{N}$. If $y^{(n)}$ and $y^{(m)}$ denote any two configurations of n resp. m points in $\mathbb{R}^d$, then we obtain a configuration $y^{(n+m)}$ of $n+m$ points by putting the two configurations at distance R to each other, such that they do not interact. Then $V_{n+m}(y^{(n+m)}) = V_n(y^{(n)}) + V_m(y^{(m)})$. Passing to the infimum of V_n resp. V_m over $y^{(n)}$ and $y^{(m)}$ yields that $\varphi(n+m) \le \varphi(n) + \varphi(m)$. Hence $(\varphi(n) \colon n \in \mathbb{N})$ is subadditive and so $\tilde\varphi = \lim_{n\to\infty} \frac{\varphi(n)}{n}$ exists and satisfies $\tilde\varphi \le \frac{\varphi(n)}{n}$, for all $n \in \mathbb{N}$.

Now suppose that for some n we have $\frac{\varphi(n)}{n} = \tilde\varphi$.. Let $y^{(n)}$ be a translated and rotated copy of $x^{(n)}$ such that there is exactly one pair (i,j) with $R > |x_i^{(n)} - y_j^{(n)}| > R - \nu_1$. Then, by Assumption (V) (4),

$$\varphi(2n) \le V_{2n}(x^{(n)}, y^{(n)}) < V_n(x^{(n)}) + V_n(x^{(n)}) = 2\varphi(n) = 2n\tilde\varphi$$

and so $\frac{\varphi(2n)}{2n} < \tilde\varphi$, which contradicts the fact that $\tilde\varphi = \inf_n \frac{\varphi(n)}{n}$. Further, $\tilde\varphi \le \varphi(2)/2 = \frac{1}{2}\min_{[0,\infty)} v < 0$ and so it remains to prove that $\tilde\varphi > -\infty$. This is easy in the case $\nu_0 > 0$, since all the points $x_i^{(n)}$ have distance $\ge \nu_0$ to each other, and, by a comparison of volume, each of these points interacts only with a number of other particles that is bounded in n. Hence, the total number of interactions is of order n, and $\varphi(n)$ is of order n as well, resulting in $\tilde\varphi > -\infty$.

Now suppose $\nu_0 = 0$. Let $I_{n,i}\colon \mathcal{D}_n \to \mathbb{R}$ be defined by

$$I_{n,i}(x) = \sum_{\substack{j=1\\ j\neq i}}^{n} v(|x_i - x_j|)$$

for $1 \le i \le n$. Then $V_n(x) = \sum_{i=1}^n I_{n,i}(x)$. For each n, let

$$I_n = \max_{1\le i\le n} I_{n,i}(x^{(n)}). \tag{3.1}$$

The main step of the proof is to show that the sequence $(I_n\colon n \in \mathbb{N})$ is bounded from below.

For each n, choose $i(n) \in \{1, \dots, n\}$ in such a way that the ball $B_{\nu_2}\big(x^{(n)}_{i(n)}\big)$ contains the maximal number, $k(n)$, of points $x^{(n)}_1, \dots, x^{(n)}_n$. In particular, no ball of radius $\nu_2/2$ contains more than $k(n)$ of the points $x^{(n)}_1, \dots, x^{(n)}_n$. Introduce $\nu_3 = \inf\{x > 0\colon v(x) = 0\}$ and denote by $m(n)$ the number of points $x^{(n)}_1, \dots, x^{(n)}_n$ that interact with $x^{(n)}_{i(n)}$, but have distance $\ge \nu_3$ to this point. Since v is nonnegative on $[\nu_2, \nu_3]$, we obtain

$$I_n \ge I_{n,i(n)}(x^{(n)}) \ge (k(n) - 1) \min_{[0,\nu_2]} v + m(n) \min_{[0,\infty)} v.$$

Hence

$$m(n) \ge \frac{I_n - (k(n) - 1) \min_{[0,\nu_2]} v}{\min_{[0,\infty)} v}.$$

Recall the function s defined in Section 1.2. By scaling, for any $r > 0$, $s(r/R)$ is the minimal number of balls of radius r required to cover a ball of radius R. By definition of $s^\star$, we have $(r/R)^d s(r/R) \le s^\star$. Cover the ball $B_R(x^{(n)}_{i(n)})$ with a least number of balls of radius $\nu_2/2$. By choice of $k(n)$, each of these balls contains at most $k(n)$ of the points $x^{(n)}_1, \dots, x^{(n)}_n$. Hence the total number of points $x^{(n)}_j$ in $B_R\big(x^{(n)}_{i(n)}\big)$ is bounded by $k(n)s(\nu_2/2R)$, which is not larger than $k(n)(2R/\nu_2)^d s^\star$. In particular,

$$\frac{I_n - (k(n) - 1) \min_{[0,\nu_2]} v}{\min_{[0,\infty)} v} \le m(n) \le k(n)(2R/\nu_2)^d s^\star$$

and so

$$I_n \ge k(n)\Big[\min_{[0,\nu_2]} v + \nu_2^{-d}(2R)^d s^\star \min_{[0,\infty)} v\Big] - \min_{[0,\nu_2]} v.$$

By Assumption (V) (5), the expression in brackets is nonnegative. Using that $k(n) \ge 1$ we obtain, for all n,

$$I_n \ge \nu_2^{-d}(2R)^d s^\star \min_{[0,\infty)} v =: c > -\infty.$$

For each n, let $j(n)$ be the index where the maximum in (3.1) is attained, then we have

$$\varphi(n) = V_{n-1}(x^{(n)}_1, \dots, \widehat{x^{(n)}_{j(n)}}, \dots, x^{(n)}_n) + 2I_n \ge \varphi(n-1) + 2c \ge \dots \ge 2c(n-1),$$

where the hat indicates the dropped component. Hence $\tilde\varphi \ge 2c > -\infty$.

(iii) It has already been argued that there is a minimiser $x^{(n)} \in \mathcal{D}_n$ for which $\sum_{i=1}^n \delta_{x^{(n)}_i}$ is connected and contains zero. Obviously, it can be approximated by $x^{(n,m)} \in \mathcal{D}_n$ having both these properties and additionally having no points at distance R. Since V_n is continuous the statement follows. □

4. Asymptotics of Z_N

In this section we complete the proof of Theorem 1.3. Recall from (1.13) that the partition function $N!|\Lambda_N|^{-N}\, Z_N(\beta_n, \varrho_N)$ is the expectation of an exponential of $\Psi(Y_N)$, for $\Psi\colon \mathcal{M}_{1,\star}^{(0)} \to (0,\infty]$ defined by

$$\Psi(Y) := \int Y(\mathrm{d}A)\, W(A), \qquad \text{where } W(A) := \frac{1}{\#A} \sum_{\substack{x,y\in A\\ x\neq y}} v(|x-y|).$$

We would like to apply Varadhan's lemma for the large deviation principle for Y_N established in Proposition 2.2 and the function Ψ. However, for both bounds there are technical obstacles. For the upper bound, compactness of the level sets of the rate function J would be required, which is missing. For the lower bound, upper semicontinuity of Ψ would be required. But W is only defined on *finite* configurations and Ψ has no upper-semicontinuous extension to the whole space $\mathcal{M}_1^{(0)}$. In case of hard core interactions, a further problem is that $\Psi(Y)$ is infinity if Y gives positive weight to configurations A with points close to each other.

In Section 4.1 we prove the upper bound by estimating $\Psi(Y_N)$ from below by $\Phi(\hat{q}(Y_N))$, where Φ is a bounded and continuous function on a compact space and $\hat{q}(Y) = (Y(\{A\colon \#A = n\})\colon n\in\mathbb{N})$. By projection, we derive a large deviation principle for $\hat{q}(Y_N)$ from the large deviation principle for Y_N. We then apply Varadhan's lemma to the function Φ.

In Section 4.2 we prove the lower bound by first restricting the expectation to the event that the measure Y_N is concentrated on configurations with a bounded number of well-separated points. On this event Ψ coincides with a cut-off approximation, which is continuous and bounded on $\mathcal{M}_1^{(0)}$. Proposition 2.2 (ii) shows that the restriction of Y_N to this event satisfies the same large deviation lower bound. Hence we can apply the lower bound of Varadhan's lemma on this event, and we finish by showing that the restricted variational formula has the same value as the original one.

4.1 Proof of the upper bound

We endow $[0,1]^{\mathbb{N}}$ with the topology of pointwise convergence and recall that it is compact. Further denote

$$\mathcal{Q} = \Big\{ q\in[0,1]^{\mathbb{N}}\colon \sum_{i=1}^{\infty} q_i \leq 1\Big\},$$

and note that $\mathcal{Q}$ is closed, by Fatou's lemma, and therefore compact. Let $\Phi\colon \mathcal{Q}\to\mathbb{R}$ be defined by

$$\Phi(q) = \sum_{n=1}^{\infty} q_n \frac{\varphi(n)}{n} + \tilde{\varphi}\Big(1 - \sum_{n=1}^{\infty} q_n\Big) = \sum_{n=1}^{\infty} q_n \Big(\frac{\varphi(n)}{n} - \tilde{\varphi}\Big) + \tilde{\varphi}.$$

We recall from (2.5) the definition of the mapping $\hat{q}\colon \mathcal{M}_1 \to \mathcal{Q}$ given by $\hat{q}_n(Y) = Y(\{A\colon \#A = n\})$.

Lemma 4.1.

(*i*) *For any real sequence $(b_n\colon n\in\mathbb{N})$ converging to zero the mapping $q\mapsto \sum_{n=1}^{\infty} q_n b_n$ is continuous on $\mathcal{Q}$. In particular, Φ is continuous.*

(*ii*) *The sequence $(\hat{q}(Y_N)\colon N\in\mathbb{N})$ satisfies a large deviation principle on the space $\mathcal{Q}$ with speed $N\log(1/\varrho_N)$ and rate function $H\colon \mathcal{Q}\to[0,\infty)$ given by*

$$H(q) := 1 - \sum_{n=1}^{\infty} \frac{q_n}{n}.$$

The rate function H is continuous, and the level sets of H are compact.

Proof. (*i*) Let $q^{(i)} \to q$ in $\mathcal{Q}$ as $i \to \infty$. For any $\varepsilon > 0$ let n_0 be such that $|b_n| < \varepsilon/4$ for all $n \geq n_0$. There is i_0 such that $|q_n^{(i)} - q_n| < \varepsilon(2n_0(\max_k |b_k| + 1))^{-1}$ for all $i \geq i_0$ for all $n \leq n_0$. For all $i \geq i_0$ we obtain

$$\Big|\sum_{n=1}^{\infty} q_n^{(i)} b_n - \sum_{n=1}^{\infty} q_n b_n\Big| \leq \max_k |b_k| \sum_{n=1}^{n_0} |q_n^{(i)} - q_n| + \frac{\varepsilon}{4} \sum_{n>n_0} (q_n^{(i)} + q_n) < \varepsilon.$$

Therefore, Φ is continuous, as $\varphi(n)/n \to \tilde{\varphi}$ by Lemma 3.1.

(*ii*) For any $n \in \mathbb{N}$, let $C_n = \{A \in \mathcal{N}_R^{(0)} \colon \#A = n\}$, then the indicator function $1\!\!1_{C_n} \colon \mathcal{N}_R^{(0)} \to \{0,1\}$ is continuous since the mapping $A \mapsto \#A$ is continuous by Lemma 2.1. Since $\hat{q}_n(Y) = \int 1\!\!1_{C_n} \,\mathrm{d}Y$ for any Y, the map $\hat{q}_n$ is continuous. Hence $\hat{q}$ is continuous.

The statement of the lemma follows now from the contraction principle (see [DZ98, Theorem 4.2.1]) since, for any $q \in \mathcal{Q}$, J is constant on the set $\{Y \colon \hat{q}(Y) = q\}$ and equal to $H(q)$. The continuity of H follows from (i). The level sets of H are closed, and hence compact as $\mathcal{Q}$ is compact. □

Observe that if $\#A = n$ and $A(\{a\}) = 1$ for all $a \in A$ then $W(A) \geq \varphi(n)/n$. Because $Y_N \in \mathcal{M}_{1,\star}^{(0)}$ with probability 1 and $\sum_{n=1}^{\infty} \hat{q}_n(Y_N) = 1$, for all $N \in \mathbb{N}$, we obtain

$$\Psi(Y_N) \geq \sum_{n=1}^{\infty} \hat{q}_n(Y_N) \frac{\varphi(n)}{n} = \Phi(\hat{q}(Y_N)).$$

Therefore

$$Z_N(\beta_N, \varrho_N) \leq \frac{|\Lambda_N|^N}{N!} \, \mathbb{E}_{\Lambda_N}\big[\exp\big\{ - N\beta_N \, \Phi(\hat{q}(Y_N))\big\}\big].$$

Recall that $N\beta_N = \frac{1}{c} N \log(1/\varrho_N)$. Observe that $\inf_{\mathcal{Q}} \Phi \geq \tilde{\varphi} > -\infty$ by Lemma 3.1. Since Φ is continuous and nonnegative and $\hat{q}(Y_N)$ satisfies a large deviation principle with speed $N\log(1/\varrho_N)$ and rate function H (with compact level sets) by Lemma 4.1, we can use the upper bound in Varadhan's lemma, see [DZ98, Lemma 4.3.6], which implies

$$\limsup_{N\to\infty} \frac{1}{N\log(1/\varrho_N)} \log \mathbb{E}_{\Lambda_N}\big[\exp\big\{ - N\beta_N \, \Phi(\hat{q}(Y_N))\big\}\big] \leq - \inf_{\mathcal{Q}} \big\{ \tfrac{1}{c}\Phi + H\big\}.$$

Using (1.14) we get

$$\limsup_{N\to\infty} \frac{1}{N\beta_N} \log Z_N(\beta_N, \varrho_N) \leq - \inf_{\mathcal{Q}} \big\{\Phi + c(H-1)\big\}.$$

Let $q_\infty = 1 - \sum_{n=1}^{\infty} q_n$. Then we see that

$$\begin{aligned} \inf_{\mathcal{Q}} \big\{\Phi + c(H-1)\big\} &= \inf_{q\in\mathcal{Q}} \Big\{ \sum_{n\in\mathbb{N}} q_n \frac{\varphi(n)}{n} + \tilde{\varphi}\Big(1 - \sum_{n\in\mathbb{N}} q_n\Big) - c\sum_{n\in\mathbb{N}} \frac{q_n}{n}\Big\} \\ &= \inf\Big\{ \sum_{n\in\mathbb{N}\cup\{\infty\}} q_n\theta_n - c\sum_{n\in\mathbb{N}} \frac{q_n}{n} \colon q \in [0,1]^{\mathbb{N}\cup\{\infty\}}, \sum_{n\in\mathbb{N}\cup\{\infty\}} q_n = 1\Big\}, \end{aligned} \tag{4.1}$$

which is equal to the right hand side of (1.8).

4.2 Proof of the lower bound

Recall that v is continuous with a negative minimum and let $\nu_3 = \inf\{x > 0 \colon v(x) = 0\} \in (\nu_0, \nu_1)$. For any $\nu \in (\nu_0, \nu_3)$, denote $v_\nu(x) = \min\{v(x), v(\nu)\}$ for $x \geq 0$. For each such ν and $n \in \mathbb{N}$ consider $W_{n,\nu} \colon \mathcal{N}_R^{(0)} \to \mathbb{R}$ defined by

$$W_{n,\nu}(A) = \begin{cases} \dfrac{1}{\#A} \displaystyle\sum_{\substack{i,j=1 \\ i\neq j}}^{k} v_\nu(|x_i - x_j|) & \text{if } A = \displaystyle\sum_{i=1}^{k} \delta_{x_i} \text{ and } k \leq n, \\ 0 & \text{otherwise.} \end{cases}$$

and denote $\Psi_{n,\nu}\colon \mathcal{M}_1^{(0)} \to \mathbb{R}$ by

$$\Psi_{n,\nu}(Y) = \int Y(\mathrm{d}A)\, W_{n,\nu}(A).$$

Lemma 4.2. *For each $\nu \in (\nu_0, \nu_3)$ and n, $\Psi_{n,\nu}$ is well-defined and continuous.*

Proof. Observe that $-\infty < \min_{[0,\infty)} v \le v_\nu(x) \le \max_{[\nu,\nu_3]} v < \infty$ for all $x \ge 0$ and so, for each A,

$$n \min_{[0,\infty)} v \le W_{n,\nu}(A) \le n \max_{[\nu,\nu_3]} v.$$

Hence $\Psi_{n,\nu}$ is well-defined. To prove the continuity of $\Psi_{n,\nu}$ it suffices to show the continuity of $W_{n,\nu}$.

Let $A^{(i)} \to A$ in $\mathcal{N}_R^{(0)}$ as $i \to \infty$. If $\#A > n$ then $\#A^{(i)} > n$ eventually by Lemma 2.1 and so $W_{n,\nu}(A^{(i)}) = W_{n,\nu}(A) = 0$. If $\#A = k \le n$ then eventually $\#A^{(i)} = k$. It follows from [Res87, Prop. 3.13] that if $A = \sum_{j=1}^k \delta_{a_j}$ then eventually $A^{(i)} = \sum_{j=1}^k \delta_{a_{i,j}}$, where $a_{i,j} \to a_j$ as $i \to \infty$ for all $j \le k$. Now the continuity of $W_{n,\nu}$ obviously follows from the continuity of v_ν. □

Note that W and $W_{n,\nu}$ agree on $\mathcal{N}_{R,n,\nu}^{(0)}$, for each $n \in \mathbb{N}$ and $\nu \in (\nu_0, \nu_3)$. Using (1.13) we obtain, for each n and ν, that

$$Z_N(\beta_N, \varrho_N) \ge \frac{|\Lambda|^N}{N!}\, \mathbb{E}_{\Lambda_N}\Big[\exp\big\{-N\beta_N\, \Psi_{n,\nu}(Y_N)\big\} \mathbf{1}\big\{Y_N(\mathcal{N}_{R,n,\nu}^{(0)}) = 1\big\}\Big]. \tag{4.2}$$

Denote

$$\mathcal{M}_{1,\star,v}^{(0)} = \big\{\widetilde{Y} \in \mathcal{M}_{1,\star}^{(0)} \colon \nu(\widetilde{Y}) > \nu_0\big\},$$

where $\nu(Y)$ and $n(Y)$ have been defined in Proposition 2.2(ii). Let $\varepsilon > 0$ and $Y \in \mathcal{M}_{1,\star,v}^{(0)}$. Pick $\nu \in (\nu_0, \min\{\nu(Y), \nu_3\})$. Since $\Psi_{n(Y),\nu}$ is continuous at Y by Lemma 4.2, there is an open set $O \subset \mathcal{M}_1^{(0)}$ such that $Y \in O$ and $\Psi_{n(Y),\nu}(\widetilde{Y}) < \Psi_{n(Y),\nu}(Y) + \varepsilon$ for all $\widetilde{Y} \in O$. Recall that $\log(1/\varrho_N) = c\beta_N$. We obtain, using (4.2), (1.14) and Proposition 2.2(ii),

$$\begin{aligned}
&\liminf_{N\to\infty} \frac{1}{N\log(1/\varrho_N)} \log Z_N(\beta_N, \varrho_N)\\
&\quad\ge 1 + \liminf_{N\to\infty} \frac{1}{N\log(1/\varrho_N)} \log \mathbb{E}_{\Lambda_N}\Big[\exp\big\{-N\beta_N\, \Psi_{n(Y),\nu}(Y_N)\big\}\mathbf{1}\big\{Y_N \in O, Y_N\big(\mathcal{N}_{R,n(Y),\nu}^{(0)}\big) = 1\big\}\Big]\\
&\quad\ge 1 - \tfrac{1}{c}\big(\Psi_{n(Y),\nu}(Y) + \varepsilon\big) + \liminf_{N\to\infty} \frac{1}{N\log(1/\varrho_N)} \log \mathbb{P}_{\Lambda_N}\Big(Y_N \in O, Y_N\big(\mathcal{N}_{R,n(Y),\nu}^{(0)}\big) = 1\Big)\\
&\quad\ge -\tfrac{1}{c}\,\Psi_{n(Y),\nu}(Y) - \tfrac{\varepsilon}{c} + L(Y).
\end{aligned}$$

Observe that $\Psi_{n(Y),\nu}(Y) = \Psi(Y)$ for each Y, as it is concentrated on $\mathcal{N}_{R,n(Y),\nu}^{(0)}$. Since ε and Y are arbitrary, we get

$$\liminf_{N\to\infty} \frac{1}{N\beta_N} \log Z_N(\beta_N, \varrho_N) \ge -\inf_{Y \in \mathcal{M}_{1,\star,v}^{(0)}(\mathcal{N}_R^{(0)})} \big\{\Psi(Y) - cL(Y)\big\}. \tag{4.3}$$

Now we explicitly construct a sequence in $\mathcal{M}_{1,\star,v}^{(0)}(\mathcal{N}_R^{(0)})$ such that the values of $\Psi - cL$ along the sequence approach $\Xi(c)$. Let $\varepsilon > 0$. For each $n \in \mathbb{N}$, choose $m(n)$ in such a way that $V_n(x^{(n,m(n))}) - \varphi(n) < \varepsilon$, where $x^{(n,m)}$ has been defined in Lemma 3.1. Denote $y^{(n)} = x^{(n,m(n))}$ and $A^{(n)} = \sum_{j=1}^n \delta_{y_j^{(n)}}$, which is in $\mathcal{N}_R$, by Lemma 3.1. For each $k \in \mathbb{N}$ and $q \in \mathcal{Q}$, denote

$$p_n^{(k,q)} = \begin{cases} q_n & \text{if } n \le k,\\ 1 - \displaystyle\sum_{j=1}^k q_j & \text{if } n = 2^k,\\ 0 & \text{otherwise.}\end{cases}$$

Finally, denote

$$Y_{k,q} = \sum_{n=1}^{2^k} p_n^{(k,q)} \frac{1}{n} \sum_{j=1}^{n} \delta_{A^{(n)} - y_j^{(n)}}$$

and observe that $Y_{k,q} \in \mathcal{M}_{1,\star,v}^{(0)}(\mathcal{N}_R^{(0)})$ by Lemma 3.1. We have

$$L(Y_{k,q}) = \sum_{n=1}^{\infty} \frac{\hat{q}_n(Y_{k,q})}{n} = \sum_{n=1}^{\infty} \frac{p_n^{(k,q)}}{n} = \sum_{n=1}^{k} \frac{q_n}{n} + 2^{-k}\Big(1 - \sum_{n=1}^{k} q_n\Big).$$

Further,

$$\Psi(Y_{k,q}) = \sum_{n=1}^{\infty} \hat{q}_n(Y_{k,q})\, W(A^{(n)}) = \sum_{n=1}^{2^k} p_n^{(k,q)} \frac{V_n(y^{(n)})}{n} \le \sum_{n=1}^{k} q_n \frac{\varphi(n)}{n} + \frac{\varphi(2^k)}{2^k}\Big(1 - \sum_{n=1}^{k} q_n\Big) + \varepsilon.$$

We obtain

$$\begin{aligned} \inf_{Y \in \mathcal{M}_{1,\star,v}^{(0)}(\mathcal{N}_R^{(0)})} &\big\{\Psi(Y) - cL(Y)\big\} \le \Psi(Y_{k,q}) - cL(Y_{k,q}) \\ &= \sum_{n=1}^{k} q_n \frac{\varphi(n)}{n} + \frac{\varphi(2^k)}{2^k}\Big(1 - \sum_{n=1}^{k} q_n\Big) + \varepsilon - c \sum_{n=1}^{k} \frac{q_n}{n} - c\, 2^{-k}\Big(1 - \sum_{n=1}^{k} q_n\Big). \end{aligned}$$

This inequality is satisfied for all k and ε and hence we can take the limit as $k \to \infty$ and $\varepsilon \to 0$, which gives

$$\inf_{Y \in \mathcal{M}_{1,\star,v}^{(0)}(\mathcal{N}_R^{(0)})} \big\{\Psi(Y) - cL(Y)\big\} \le \sum_{n=1}^{\infty} q_n \frac{\varphi(n)}{n} + \tilde{\varphi}\Big(1 - \sum_{n=1}^{\infty} q_n\Big) - c \sum_{n=1}^{\infty} \frac{q_n}{n}.$$

Since this is true for all $q \in \mathcal{Q}$ we can take the infimum. Using (4.1) and recalling (4.3), we get the lower bound.

5. Analysis of the variational formula

In this section we prove Theorem 1.5. Recall that $\theta_\kappa = \varphi(\kappa)/\kappa$ for $\kappa \in \mathbb{N}$, $\theta_\infty = \tilde{\varphi}$, and denote by g the largest convex function $[0,1] \to [\tilde{\varphi}, 0]$ whose graph lies below the points $(1/\kappa, \theta_\kappa)$, see Figure 2. This graph changes its slope precisely in the points $(1/\kappa_n, \theta_{\kappa_n})$ with $1 \le n < \eta + 1$, but may contain more of these points. In particular, the sequence of slopes c_n with $1 \le n < \eta + 1$ is strictly decreasing in n. As $\theta_\kappa > \tilde{\varphi}$ by Lemma 3.1 (ii), all slopes c_n of g are strictly positive. We write

$$g(x) = \begin{cases} \theta_{\kappa_n} + c_n(x - 1/\kappa_n) & \text{if } x \in (1/\kappa_{n+1}, 1/\kappa_n] \text{ for some } 1 \le n < \eta + 1, \\ \tilde{\varphi} & \text{if } x = 0. \end{cases}$$

Using the convention $1/\infty = 0$, we can rewrite (1.8) as

$$\Xi(c) = \inf\Big\{ \sum_{\kappa \in \mathbb{N} \cup \{\infty\}} q_\kappa \Big(\theta_\kappa - \frac{c}{\kappa}\Big) : q \in [0,1]^{\mathbb{N} \cup \{\infty\}}, \sum_{\kappa \in \mathbb{N} \cup \{\infty\}} q_\kappa = 1 \Big\}. \tag{5.1}$$

For each c, denote by $I(c) \subset \mathbb{N} \cup \{\infty\}$ the set of points where the continuous mapping $\kappa \mapsto \theta_\kappa - c/\kappa$ from $\mathbb{N} \cup \{\infty\}$ to $\mathbb{R}$ attains its minimum.

Lemma 5.1.

$$\Xi(c) = \min_{\kappa \in \mathbb{N} \cup \{\infty\}} \Big(\theta_\kappa - \frac{c}{\kappa}\Big),$$

the infimum in (5.1) *is a minimum, and the set of minimisers is the convex hull of* $\mathfrak{q}^{(i)}$ *with* $i \in I(c)$.

Proof. Let $q \in [0,1]^{\mathbb{N}\cup\{\infty\}}$ be such that $\sum_{\kappa\in\mathbb{N}\cup\{\infty\}} q_\kappa = 1$. If $q_j > 0$ for some $j \notin I(c)$ then

$$\sum_{\kappa\in\mathbb{N}\cup\{\infty\}} q_\kappa\Big(\theta_\kappa - \frac{c}{\kappa}\Big) > \min_{\kappa\in\mathbb{N}\cup\{\infty\}} \Big(\theta_\kappa - \frac{c}{\kappa}\Big) \sum_{\kappa\in\mathbb{N}\cup\{\infty\}} q_\kappa = \min_{\kappa\in\mathbb{N}\cup\{\infty\}} \Big(\theta_\kappa - \frac{c}{\kappa}\Big),$$

otherwise equality holds. ☐

Lemma 5.2.

$$\min_{\kappa\in\mathbb{N}\cup\{\infty\}} \Big(\theta_\kappa - \frac{c}{\kappa}\Big) = \begin{cases} \tilde{\varphi} & \text{if } c \in (0, c_\eta], \\ -\frac{c}{\kappa_n} + \theta_{\kappa_n} & \text{if } c \in [c_n, c_{n-1}) \text{ for some } 2 \le n < \eta + 1, \\ -c & \text{if } c \in (c_1, \infty). \end{cases} \tag{5.2}$$

Further,

- *if* $c \in (0, c_\eta)$ *then* $I(c) = \{\infty\}$,
- *if* $c = c_\infty$ *then* $I(c) = \{\infty\}$; *this is only applicable if* $\eta = \infty$ *and* $c_\infty > 0$,
- *if* $c \in (c_n, c_{n-1})$, *with some* $2 \le n < \eta + 1$, *then* $I(c) = \{\kappa_n\}$,
- *if* $c \in (c_1, \infty)$ *then* $I(c) = \{1\}$,
- *if* $c = c_n$ *for some* $1 \le n < \eta + 1$ *then* $I(c) = I^{(n)}$.

Proof. It is easy to see that

$$\min_{\kappa\in\mathbb{N}\cup\{\infty\}} \Big(\theta_\kappa - \frac{c}{\kappa}\Big) = \min_{x\in[0,1]} (g(x) - cx).$$

Since g is strictly convex and piecewise linear, the minimum on the right hand side can be found by comparing the derivative of g with c.

- If $c = c_n$ for some $1 \le n < \eta + 1$ then the minimum is attained on $[1/\kappa_{n+1}, 1/\kappa_n]$ and is equal to $\theta_{\kappa_n} - \frac{c}{\kappa_n}$.
- If $c_1 < c$ then the minimum is attained at $x = 1$ and is equal to $-c$.
- If $c_n < c < c_{n-1}$ for some $2 \le n < \eta + 1$ then the minimum is attained at $1/\kappa_n$ and is equal to $\theta_{\kappa_n} - \frac{c}{\kappa_n}$.
- If $c < c_\eta$ then the minimum is attained at 0 and is equal to $\tilde{\varphi}$.
- In the case $\eta = \infty$, $c_\infty > 0$ we additionally have to consider $c = c_\infty$. In that case the minimum is also attained at 0 and is equal to $\tilde{\varphi}$.

This proves (5.2) and the remaining statements follow easily. ☐

Theorem 1.5 follows now directly from (5.1) in combination with Lemmas 5.1 and 5.2.

6. A potential with more than one phase transition

By Theorem 1.5, we always have at least two phases: a high temperature phase where particles do not interact, and a low temperature phase where the connected components of interacting particles are unbounded. We now give an example of a potential where at least one further, intermediate, phase exists.

To explain the idea, consider the potential v such that $v = \infty$ on $[0, \nu_0) \cup (\nu_0, R)$, $v = 0$ on $[R, \infty)$ and $v(\nu_0) = -M$ for some $M > 0$ and $R > 2\nu_0$. Obviously it does not satisfy Assumption (V), but it provides the correct intuitive picture on which we build our example below. For this potential, configurations have finite energy only if any two of its points are either precisely at distance ν_0 or do not interact. The largest configurations in $\mathbb{R}^d$ such that all distances are equal to ν_0 are regular simplices of $d+1$ points. Hence, optimal configurations of n particles are organised in $\lfloor n/(d+1) \rfloor$ such simplices at distances $> R$ to each other and one subset of such a simplex with $i_n = n-(d+1)\lfloor n/(d+1) \rfloor$ points.

In particular, $\varphi(n) = -2M\binom{d+1}{2}\lfloor n/(d+1)\rfloor - 2M\binom{i_n}{2}$ for any $n \in \mathbb{N}$, and $\tilde\varphi = -M$. Hence, at zero temperature, we see a phase in which only the simplices are present. In our modification below, this phase is shifted to positive temperature. In the simplest case, where $d = 1$, we have $\varphi(n) = -2M\lfloor \frac{n}{2}\rfloor$, and the diagram of the points $(1/\kappa, \varphi(\kappa)/\kappa)$ with $\kappa \in \mathbb{N} \cup \{\infty\}$ is depicted in Figure 3.

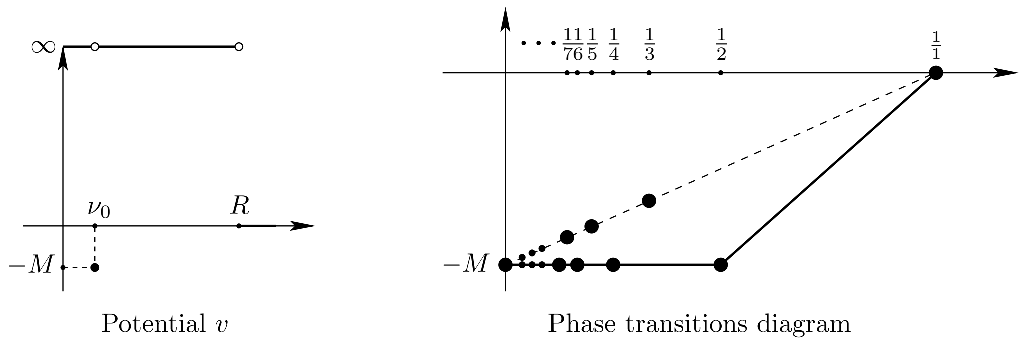


FIGURE 3

The potential v violates Assumption (V)(4), as it is not negative just to the left of R. This is the reason why the slope of the largest convex minorant is equal to zero close to 0, and this is why the phase of simplices is present only at zero temperature. Introducing a (small) negative part in v to the left of R will shift this phase to positive temperature.

Now we consider a potential of similar shape, but modified in such a way that it fulfills Assumption (V). We will see that the diagram in Figure 3 is a degeneration of the phase transitions diagram of this example.

Fix $T > 6$ and $M > \varepsilon > 0$. Consider a continuous potential v (shown in Figure 4) with support equal to $[0, 2T + 6]$, satisfying

(i) $v(x) = +\infty$ for $x \in [0, T]$ and finite otherwise;
(ii) $v(x) \geq 3M$ for $x \in [T + 1, 2T + 3]$;
(iii) $\min v = -M = v(T + 1/2)$;
(iv) $v(x) < 0$ for $x \in [2T + 4, 2T + 6)$;
(v) $\min\{v(x) \colon x > 2T + 3\} = -\varepsilon = v(2T + 5)$.

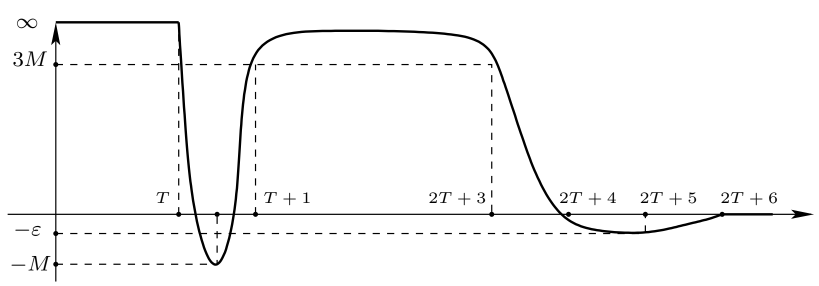


FIGURE 4

The potential v satisfies Assumption (V) with $\nu_0 = T$ and $R = 2T + 6$. For simplicity we will consider its action on one-dimensional point configurations, i.e., we put $d = 1$. Our goal is to prove that $\eta = 2$.

For each n, denote by $x_1 < \cdots < x_n$ a minimiser of V_n, which exists by Lemma 3.1. Obviously, $x_{i+1} - x_i > T$ for all i. In the following lemma we prove that only neighbouring points in this configuration interact, and that the points are split into pairs with strong interaction $-M$ between the points in each pair and weak interaction $-\varepsilon$ between the pairs.

Lemma 6.1.

(i) *Precisely* $n-1-\lfloor\frac{n-1}{2}\rfloor$ *of the nearest-neighbour distances* $x_{i+1}-x_i$ *are equal to* $T+\frac{1}{2}$*, the others are equal to* $2T+5$*. No two successive distances are equal to* $T+\frac{1}{2}$*. In particular, if* n *is even then*

$$x_{i+1}-x_i=\begin{cases} T+\frac{1}{2} & \text{for odd } i,\\ 2T+5 & \text{for even } i.\end{cases}$$

(ii) *For each* $n\in\mathbb{N}$*,*

$$\varphi(n)=-2M\Big(n-1-\Big\lfloor\frac{n-1}{2}\Big\rfloor\Big)-2\varepsilon\Big\lfloor\frac{n-1}{2}\Big\rfloor.$$

(iii) $\tilde\varphi=-M-\varepsilon$.

Proof. Since $x_{i+1}-x_i>T$ for all i, we have $x_{i+3}-x_i>3T>2T+6$, and so each point interacts with at most two points on its left and at most two points at its right.

Let us show that there are no points with interacting distance between $T+1$ and $2T+3$, where the potential is large. Suppose this is not true and $x_j-x_i\in[T+1,2T+3]$ for some $j>i$ (recall that j can only be $i+1$ or $i+2$). Consider a new configuration $y_1<\cdots<y_n$ given by $y_k=x_k$ for $k\le i$ and $y_k=x_k+2T+6$ for $k\ge i+1$, i.e., we separate the first i points of the configuration x from the others. This removes all the three interactions that involve x_i and x_{i+1}:

$$V_n(y_1,\dots,y_n)=V_n(x_1,\dots,x_n)-2\big(v(x_{i+1}-x_{i-1})+v(x_{i+1}-x_i)+v(x_{i+2}-x_i)\big)$$

Since either $v(x_{i+1}-x_i)$ or $v(x_{i+2}-x_i)$ is greater or equal than $3M$ and the other two are greater or equal than $-M$ we obtain $V_n(y_1,\dots,y_n)<V_n(x_1,\dots,x_n)$, which contradicts x being a minimiser.

Now we conclude that each point in the configuration x interacts only with its neighbours. Indeed, for any i, we have $x_{i+2}-x_i=(x_{i+2}-x_{i+1})+(x_{i+1}-x_i)>2T>T+1$. The above implies that $x_{i+2}-x_i>2T+3$. This implies that either $x_{i+1}-x_i$ or $x_{i+2}-x_{i+1}$ is greater than $T+1$ and hence is greater than $2T+3$, by the above. This in turn implies that $x_{i+2}-x_i>3T+3>2T+6$, i.e., x_{i+2} and x_i do not interact.

Therefore, since v assumes its minimum on $[T,T+1]$ at $T+\frac{1}{2}$ with value $-M$ and its minimum outside $[T,T+1]$ at $2T+5$ with value $-\varepsilon$, all nearest-neighbour distances are either equal to $T+\frac{1}{2}$ or $2T+5$. For each i, at most one of the distances $x_{i+2}-x_{i+1}$ and $x_{i+1}-x_i$ belongs to the interval $[T,T+1]$. Hence, no two successive distances are equal to the optimal distance, $T+\frac{1}{2}$. Because $M>\varepsilon$, the distance $T+\frac{1}{2}$ is more favourable than the distance $2T+5$, hence the number of distances equal to $T+\frac{1}{2}$ is maximal, i.e., equal to $n-1-\lfloor\frac{n-1}{2}\rfloor$, and the other $\lfloor\frac{n-1}{2}\rfloor$ distances are equal to $2T+5$. From this, it is easy to conclude the proof. ☐

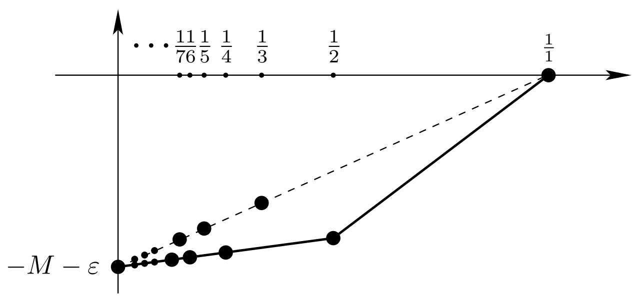


FIGURE 5. Phase transitions diagram

Now we argue that there are exactly two phase transitions. Indeed, for any $n \in \mathbb{N}$, we have

$$\varphi(n) = \begin{cases} n\tilde{\varphi} - \tilde{\varphi} & \text{if } n \text{ is odd,} \\ n\tilde{\varphi} + 2\varepsilon & \text{if } n \text{ is even.} \end{cases}$$

Hence all points $(1/n, \varphi(n)/n)$ with n odd lie on the straight line passing through $(0, \tilde{\varphi})$ and $(1, 0)$, whereas the others lie on the straight line passing through $(0, \tilde{\varphi})$ and $(-\frac{\tilde{\varphi}}{2\varepsilon}, 0) = (\frac{1}{2} + \frac{M}{2\varepsilon}, 0)$, which lies below the first line because $M > \varepsilon$. Hence we obtain the phase transitions diagram of Figure 5.

We obtain two phase transitions: one at $c_1 = -\varphi(2) = 2M$ from singletons to particle clouds with even cardinality, and then at $c_2 = 2\varepsilon$ to infinite clouds.

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