

Continuum percolation for Gibbsian point processes with attractive interactions*

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Abstract

We study the problem of continuum percolation in infinite volume Gibbs measures for particles with an attractive pair potential, with a focus on low temperatures (large β). The main results are bounds on percolation thresholds $\rho_{\pm}(\beta)$ in terms of the density rather than the chemical potential or activity. In addition, we prove a variational formula for a large deviations rate function for cluster size distributions. This formula establishes a link with the Gibbs variational principle and a form of equivalence of ensembles, and allows us to combine knowledge on finite volume, canonical Gibbs measures with infinite volume, grand-canonical Gibbs measures

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1 Introduction

The present article is concerned with percolation properties for Gibbsian point processes. We are interested in infinite volume Gibbs measures (in the sense of the Dobrushin-Lanford-Ruelle conditions) for particles in \mathbb{R}^d interacting via an attractive, finite range pair potential. The dimension is two or higher, $d \geq 2$. Around each particle x of a random configuration ω , draw a ball of radius R , for some fixed $R > 0$. *Percolation* occurs if the region in \mathbb{R}^d covered by the union of such balls, $\cup_{x \in \omega} B(x, R)$, has an unbounded connected component, with positive probability. In the notation of Meester and Roy [15], our problem is a Boolean percolation model (X, ρ) driven by a Gibbsian point process X and with deterministic radius $\rho = R$.

This problem has been studied before [17, 24, 18, 2], for both repulsive pair potentials and potentials with an attractive part. Mürmann [17] investigated finite-range potentials

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and gave a sufficient condition for the absence of percolation; a different proof, with an extension to tempered boundary conditions for attractive potentials, was given by Zessin [24]. His proof builds on integration by parts for Gibbsian measures. Pechersky and Yambartsev [18] proved a criterion for absence of percolation with the help of a coupled branching process; their result does not require that the potential has compact support. In addition, Pechersky and Yambartsev gave a sufficient condition for the presence of percolation, valid in dimension 2, for attractive potentials with possibly unbounded support. An analogous result for hard spheres in dimension 2 was shown by Aristoff [2]. Stucki [22] gave results in arbitrary dimension for pair and many-body potentials.

The cited works all formulate criteria in terms of the activity z – i.e., the intensity parameter of some a priori Poisson point process – rather than the density ρ , which for interacting particles is a non-trivial function of z . As a consequence, for attractive potentials, the cited results cannot distinguish between two very different physical pictures. First, percolation can be a high-density effect, as expected for hard spheres; second, it can be an energetic effect – at low temperature, it may happen that the interaction favors the formation of large connected components, which because of entropy may coexist with large almost empty regions of space containing a few small components. In such a situation the density threshold for percolation may be very small, as suggested by results on large deviations for cluster size distributions in the canonical ensemble [14].

The aim of the present article is, therefore, to give bounds on percolation and non-percolation thresholds in terms of the density rather than the activity. Our main result is Theorem 3.6 below, valid for finite-range, attractive potentials. Quickly summarized, Theorem 3.6 states that there are curves $\rho_{\pm}(\beta)$ such that if $P_{\beta,\rho}$ is a shift-invariant Gibbs measure at density ρ and inverse temperature β , the following holds.

- If $\rho < \rho_{-}(\beta)$, there are only bounded connected components, $P_{\beta,\rho}$ -almost surely; we have $\rho_{-}(\beta) = \exp(-\beta\nu^{*}(1 + o(1)))$ for suitable $\nu^{*} > 0$.
- If $\rho > \rho_{+}(\beta)$, there is an unbounded connected component, $P_{\beta,\rho}$ -almost surely; as $\beta \rightarrow \infty$, $\rho_{+}(\beta) \rightarrow \rho_0 > 0$ for suitable $\rho_0 > 0$.

We expect that for very large β and $\rho_{-}(\beta) < \rho < \rho_{+}(\beta)$, there are non-ergodic Gibbs measures with percolation probability strictly between 0 and 1. We have no proof of this conjecture; see, however, Proposition 3.7 for some preliminary evidence, and Appendix A for relevant lattice gas results. The reader may wish to compare the exponential decay $\exp(-\beta\nu^{*})$ of the critical density with the Clausius-Clapeyron equation of thermodynamics. The Clausius-Clapeyron equation approximates the saturation pressure – i.e., the pressure at which the gas condenses – by $\exp(-\beta L)$ where L is the latent heat.

We also provide bounds for percolation thresholds in terms of the chemical potential $\frac{1}{\beta} \log z$ (Section 3.2). The existence of such thresholds is not new; our contribution is a careful analysis of the way the pair potentials enters into relevant estimates. This allows to compare the proven thresholds with a conjecture on the low-temperature behavior of the percolation threshold (in activity / chemical potential space) that we formulate in Eq. (3.5).

The key technical tool for the proof of Proposition 3.7 is a variational formula for a large deviations rate for cluster size distributions in the canonical ensemble (Theorem 3.2); the large deviations principle was investigated in [14]. The variational formula establishes a relation with the Gibbs variational principle and allows us to apply a form of equivalence of ensemble [10]. This in turn enables us to combine the knowledge for grand-canonical, infinite volume Gibbs measures in [17, 18] with results on the canonical ensemble [14].

We conclude the introduction with a word of caution on the physical interpretation of percolation. We should stress that a percolation transition need not be a phase transition – for the ideal gas at activity z (Poisson point process with intensity z), the pressure is an analytic function no matter the value of z , even though there is a percolation transition at high enough z [15]. Nevertheless, for attractive pair potentials and at low temperature, the percolation transition might coincide with a phase transition. In fact, for nearest neighbor attractive lattice gases (or Ising model), and temperatures below some threshold T_+ , the percolation transition and the phase transition coincide (see the review by Georgii, Häggström and Maes [11]). In dimension two, T_+ equals the Curie temperature T_C , but in higher dimensions $T_+ < T_C$ [1], illustrating again that percolation and phase transition in general do not coincide. For the reader's convenience, we summarize some relevant results in Appendix A.

The remainder of the article is organized as follows. In Sections 2 and 3 we formulate the setting and our results. Section 4 defines the topology of local convergence and summarizes continuity properties of important functions such as the relative entropy rate. Sections 5 to 7 are devoted to the proofs.

2 Setting

2.1 Pair potential

The pair potential is a function $v : [0, \infty) \rightarrow \mathbb{R} \cup \{\infty\}$ that serves to define the total energy of an N -particle configuration

$$U_N(x_1, \dots, x_N) := \sum_{1 \leq i < j \leq N} v(|x_i - x_j|), \quad x_1, \dots, x_N \in \mathbb{R}^d.$$

By a slight abuse of notation, we shall drop the subscript and write $U(\mathbf{x})$ instead of $U_N(\mathbf{x})$.

Assumption 2.1. *The pair potential satisfies the following basic assumptions:*

- *Either v is everywhere finite or there is a $r_{\text{hc}} > 0$ such that $v(r) = \infty$ for $r < r_{\text{hc}}$ and $v(r) < \infty$ for $r > r_{\text{hc}}$. (We impose no condition on $v(r_{\text{hc}})$.)*
- *v has compact support: $r_1 := \sup \text{supp } v < \infty$.*
- *v is bounded from below: $\inf v > -\infty$.*
- *v has an attractive tail: there exist $r_1, r_0 > 0$ such that $r_1 > r_0 > 0$ and for all $r \in (r_0, r_1)$, $v(r) < 0$.*

If $r_{\text{hc}} > 0$, we say that v has a *hard core*. If v has compact support, we shall also say that v has *finite range*.

For $\mathbf{k} \in \mathbb{Z}^d$, let $C(\mathbf{k})$ be the unit cube $[k_1 + 1, k_1 + 2) \times \dots \times [k_d + 1, k_d + 2)$ and

$$N_{C(\mathbf{k})}(x_1, \dots, x_N) := |\{j \in \{1, \dots, N\} \mid x_j \in C(\mathbf{k})\}|$$

the number of particles in $C(\mathbf{k})$.

Assumption 2.2. *The pair potential v is superstable: there are constants $a > 0$, $b < \infty$ such that for all $N \in \mathbb{N}$ and all $\mathbf{x} = (x_1, \dots, x_N) \in (\mathbb{R}^d)^N$,*

$$U(\mathbf{x}) \geq \sum_{\mathbf{k} \in \mathbb{Z}^d} \left(a N_{C(\mathbf{k})}(\mathbf{x})^2 - b N_{C(\mathbf{k})}(\mathbf{x}) \right). \quad (2.1)$$

Every superstable interaction is *stable*, i.e., there exists $B > 0$ such that $U(\mathbf{x}) \geq -Bn$ for all $n \in \mathbb{N}$ and $\mathbf{x} \in \mathbb{R}^n$: by Eq. (2.1) we may choose $B = b$. If v satisfies Assumption 2.1 and is non-integrably divergent at the origin, then v is superstable; see [21, 20] for a proof and other sufficient conditions.

Assumption 2.3. *The potential is integrable in $\{v < \infty\}$: $\int_{|x|>r_{hc}} |v(|x|)|dx < \infty$.*

Assumption 2.4. *There is an $r_{\min} > 0$ such that for every $N \in \mathbb{N}$, U has a global minimizer $(x_1, \dots, x_N) \in (\mathbb{R}^d)^N$ with interparticle distance bounded from below by r_{\min} :*

$$1 \leq i < j \leq N \Rightarrow |x_i - x_j| \geq r_{\min}.$$

In addition, v is Hölder-continuous in $[r_{\min}, \infty)$.

A sufficient condition for the lower bound on interparticle distances is that $v(r)/r^d \rightarrow \infty$ as $r \rightarrow 0$, as can be shown along [23, Lemma 2.2].

Assumption 2.5. *There is a $C > 0$ such that for every $N \in \mathbb{N}$, U has a global minimizer $(x_1, \dots, x_N) \in (\mathbb{R}^d)^N$ with diameter bounded by $CN^{1/d}$:*

$$\max\{|x_i - x_j| \mid 1 \leq i < j \leq N\} \leq CN^{1/d}.$$

Under Assumption 2.1, this condition is trivially fulfilled in dimension 1. In dimension 2, sufficient conditions are given, for example, in [23], where much more is proven on the ground states. To the best of our knowledge, there is no result in dimension 3 or higher; in fact, providing upper bounds on interparticle distances for Lennard-Jones type interactions seems to be a non-trivial problem in non-linear optimization, see the article by Blanc [3] and the references therein.

Let us briefly comment on our conditions on the pair potential. Assumption 2.1 simply defines the class of pair potentials we are interested in. Superstability as in Assumption 2.2 is a standard condition that ensures the existence of infinite volume Gibbs measures, see the next subsection. The integrability assumption 2.3 will allow us to use a bound on Mayer expansions going back to Brydges and Federbush [4].¹ Assumptions 2.4 and 2.5 are needed for precise statements about Gibbs measures at low temperature β^{-1} and densities above some threshold of the form $\exp(-\beta v^*)$.

2.2 Infinite volume Gibbs measures

Let Ω be the set of locally finite point configurations,

$$\Omega := \{\omega \subset \mathbb{R}^d \mid \forall r > 0 : |\omega \cap B(0, r)| < \infty\},$$

with $B(0, r)$ the open ball of radius r centered at the origin. We equip Ω with the σ -algebra \mathcal{F} generated by the counting variables $N_B(\omega) := |\omega \cap B|$, $B \subset \mathbb{R}^d$ Borel-measurable, and denote the probability measures on (Ω, \mathcal{F}) with the letter \mathcal{P} . The following subsets of \mathcal{P} will be relevant for us: shift-invariant measures \mathcal{P}_θ , tempered measures, and infinite-volume Gibbs measures $\mathcal{G}(\beta, \mu)$; we proceed with their definition.

For $x \in \mathbb{R}^d$, the shift $\theta_x : \Omega \rightarrow \Omega$ is defined by $\theta_x \omega := \{y - x \mid y \in \omega\}$. A measure $P \in \mathcal{P}$ is *shift-invariant* if $P(\theta_x(A)) = P(A)$ for all measurable $A \subset \Omega$ and all $x \in \mathbb{R}^d$. The collection of shift-invariant measures is denoted \mathcal{P}_θ . We say that $P \in \mathcal{P}$ is *tempered* if for P -almost all ω ,

$$\exists t(\omega) > 0 \forall \ell \in \mathbb{N} : \sum_{\mathbf{k} \in \mathbb{Z}^d \cap [-\ell, \ell]^d} \left(N_{C(\mathbf{k})}(\omega) \right)^2 \leq t(\omega) \ell^d, \tag{2.2}$$

where $C(\mathbf{k})$ is the unit cube $[k_1, k_1 + 1) \times \dots \times [k_d, k_d + 1)$. Fix $\beta > 0$ and $\mu \in \mathbb{R}$. Let $\Lambda \subset \mathbb{R}^d$ be a bounded Borel set and $\zeta \in \Omega$ a configuration satisfying the temperedness condition (2.2). For $n \in \mathbb{N}$, define the measure Q_n on Λ^n as the measure with Lebesgue density

$$\frac{1}{n!} \exp\left(-\beta \sum_{1 \leq i < j \leq n} v(|x_i - x_j|) - \beta \sum_{i=1}^n \sum_{y \in \zeta \cap \Lambda^c} v(|x_i - y|)\right).$$

¹After completion of this article there has been some improvement on convergence criteria [6, 16]; in some cases the improved convergence criteria should allow for a weakening of Assumption 2.3.

The image of Q_n under $(x_1, \dots, x_n) \mapsto \{x_1, \dots, x_n\}$ is a measure on Ω which we denote again by Q_n . Let Q_0 be the probability measure on Ω which gives probability 1 to the event that $\omega = \emptyset$. Define $P_{\beta, \mu, \Lambda|\zeta}$ by

$$P_{\beta, \mu, \Lambda|\zeta} := \frac{1}{\Xi_{\Lambda|\zeta}(\beta, \mu)} \sum_{n=0}^{\infty} z^n Q_n, \quad z = \exp(\beta\mu).$$

The normalization $\Xi_{\Lambda|\zeta}(\beta, \mu)$ is defined by the requirement that $P_{\beta, \mu, \Lambda|\zeta}$ is a probability measure on Ω .

We say that $P \in \mathcal{P}$ is a (β, μ) -Gibbs measure if and only if P is tempered and for every Λ and every measurable $f : \Omega \rightarrow [0, \infty)$,

$$\int_{\Omega} P(d\omega) f(\omega) = \int_{\Omega} P(d\zeta) \int_{\Omega} P_{\beta, \mu, \Lambda|\zeta}(d\omega) f(\omega \cup (\zeta \cap \Lambda^c)). \tag{2.3}$$

We denote the set of (β, μ) -Gibbs measures as $\mathcal{G}(\beta, \mu)$; the sets $\mathcal{G}(\beta, \mu)$, $(\beta, \mu) \in \mathbb{R}_+ \times \mathbb{R}$, are pairwise disjoint [10, Remark 3.7]. The existence of Gibbs measures for lower regular, superstable potentials – this class includes our potentials satisfying Assumptions 2.1 and 2.2 – is shown in [21, 8]: for all $\beta > 0$, $\mu \in \mathbb{R}$, $\mathcal{G}(\beta, \mu)$ and $\mathcal{G}(\beta, \mu) \cap \mathcal{P}_{\theta}$ are non-empty, convex sets. With suitable topologies, they are Choquet simplices and, in particular, compact [21, Theorems 5.6 and 5.8].

2.3 Palm measure; energy and entropy densities

For each $P \in \mathcal{P}_{\theta}$, there is a unique finite measure P° on (Ω, \mathcal{F}) such that for all measurable, non-negative functions $f : \mathbb{R}^d \times \Omega \rightarrow [0, \infty)$,

$$\int_{\Omega} \sum_{x \in \omega} f(x, \theta_x \omega) P(d\omega) = \int_{\Omega} \int_{\mathbb{R}^d} f(x, \omega) dx P^{\circ}(d\omega). \tag{2.4}$$

P° is the *Palm measure* of P [5, Chapter 13]. It is known that $P^{\circ}(0 \notin \omega) = 0$ and $P^{\circ}(\Omega) = \rho(P)$, where $\rho(P)$ is the expected number of particles in $[0, 1]^d$, called *density*. The defining equation (2.4), specialized to $f(x, \omega) = \mathbf{1}_C(x)g(\omega)$ with $C \subset \mathbb{R}^d$ Borel-measurable, yields the useful identity

$$\int_{\Omega} g(\omega) P^{\circ}(d\omega) = \frac{1}{|C|} \int_{\Omega} \sum_{x \in \omega \cap C} g(\theta_x \omega) P(d\omega). \tag{2.5}$$

$|C|$ is the Lebesgue volume of C .

Remark 2.6. The Palm measure is the continuum analogue of a simple lattice object: if $\Omega = \{\omega \mid \omega \subset \mathbb{Z}^d\} \equiv \{0, 1\}^{\mathbb{Z}^d}$ and P is a shift-invariant measure on Ω , the Palm measure becomes $P^{\circ}(A) = P(A \cap \{0 \in \omega\})$.

For a shift-invariant, tempered measure P , we define the expected energy per unit volume, or *energy density*, as

$$U(P) := \frac{1}{2} \int_{\Omega} \left(\sum_{y \in \omega} v(|y|) \right) P^{\circ}(d\omega) = \frac{1}{2} \int_{\Omega} \left(\sum_{x \in \omega \cap [0, 1]^d} \sum_{y \in \omega} v(|y - x|) \right) P(d\omega).$$

$U(P)$ takes values in $\mathbb{R} \cup \{\infty\}$. For superstable potentials as in Eq. (2.1), the energy is bounded from below: $U(P) \geq -b^2/4a$.

The entropy per unit volume, or *entropy density* is defined as a relative entropy rate. Let $Q \in \mathcal{P}_{\theta}$ be the Poisson point process with intensity 1 and $P \in \mathcal{P}_{\theta}$. For

$\Lambda = [-L, L]^d \subset \mathbb{R}^d$, let P_Λ be the image of P under the projection map $\omega \mapsto \omega \cap \Lambda$. Define Q_Λ in a similar way. The relative entropy is

$$I(P_\Lambda; Q_\Lambda) := \int_\Omega f(\omega) \log f(\omega) Q_\Lambda(d\omega) = \int_\Omega \log f(\omega) P_\Lambda(d\omega)$$

if P_Λ has Radon-Nikodym derivative $dP_\Lambda/dQ_\Lambda = f$, and $I(P_\Lambda; Q_\Lambda) := \infty$ if P_Λ is not absolutely continuous with respect to Q_Λ . The limit

$$S(P) := 1 - \lim_{|\Lambda| \rightarrow \infty} \frac{1}{|\Lambda|} I(P_\Lambda; Q_\Lambda) \in \mathbb{R} \cup \{-\infty\} \tag{2.6}$$

exists for all $P \in \mathcal{P}_\theta$, see [12]. Continuity properties of $U(P)$ and $S(P)$ with respect to a suitable topology on \mathcal{P} are recalled in Section 4 below.

Remark 2.7. The additive constant 1 is included in Eq. 2.6 for aesthetic reasons; if we did not include it, we would need an additive constant in Eq. (3.1).

Example 2.8. Let P be a Poisson point process with intensity parameter z . Then

$$\begin{aligned} I(P_\Lambda; Q_\Lambda) &= \sum_{n=0}^{\infty} \left(\log \frac{(z|\Lambda|)^n \exp(-z|\Lambda|)}{|\Lambda|^n \exp(-|\Lambda|)} \right) \frac{(z|\Lambda|)^n}{n!} e^{-z|\Lambda|} \\ &= (1 - z)|\Lambda| + z|\Lambda| \log z \end{aligned}$$

thus $S(P) = -z(\log z - 1)$.

2.4 Cluster densities

Let $r_1 > 0$ be the range of the potential as in Assumption 2.1. Fix $R \geq r_1$. For $\omega \in \Omega$, let G_ω be the graph with vertex set ω and edge set $\{\{x, y\} \mid x, y \in \omega, 0 < |x - y| \leq R\}$. When $x \in \omega$, let $\mathcal{C}_\omega(x) \subset \omega$ be the connected component of x in G_ω . When $x \in \mathbb{R}^d \setminus \omega$, we set $\mathcal{C}_\omega(x) := \emptyset$ and $|\mathcal{C}_\omega(x)| := 0$. For $P \in \mathcal{P}_\theta$ and $k \in \mathbb{N}$, the *expected number of k -clusters per unit volume* or *k -cluster density* is

$$\rho_k(P) := k^{-1} P^\circ(|\mathcal{C}_\omega(0)| = k) = \frac{1}{k|C|} \int_\Omega \sum_{x \in \omega \cap C} \mathbf{1}(|\mathcal{C}_\omega(x)| = k) P(d\omega). \tag{2.7}$$

The last identity holds for every Borel set C , compare Eq. (2.5). Note that for every $P \in \mathcal{P}_\theta$, $\sum_{k=1}^{\infty} k \rho_k(P) \leq \rho(P)$. For later purpose we also define finite volume empirical densities as

$$\rho_{k,\Lambda}(\omega) := \frac{1}{k|\Lambda|} \sum_{x \in \omega} \mathbf{1}(|\mathcal{C}_{\omega \cap \Lambda}(x)| = k).$$

Thus $\rho_{k,\Lambda}(\omega)$ is the number of k -clusters in $\omega \cap \Lambda$, divided by the volume $|\Lambda|$. We have, for all $\omega \in \Omega$, $\sum_{k=1}^{N_\Lambda(\omega)} k \rho_{k,\Lambda}(\omega) = N_\Lambda(\omega)/|\Lambda|$. Cluster densities are relevant for percolation because there is percolation if and only if $\sum_{k=1}^{\infty} k \rho_k(P) < \rho(P)$, see Proposition 3.3 below.

2.5 Large deviations for cluster size distributions

Finally we recall a large deviation principle shown in [14]. Fix $R > r_1$. For $\Lambda = [0, L]^d$ and $N \in \mathbb{N}$, let

$$Z_\Lambda(\beta, N) := \frac{1}{N!} \int_{\Lambda^N} e^{-\beta U(x_1, \dots, x_N)} dx_1 \cdots dx_N.$$

be the canonical partition function and $\mathbb{P}_{\beta, N, \Lambda}$ the probability measure on Λ^N with density $[N! Z_\Lambda(\beta, N)]^{-1} \exp(-\beta U(x_1, \dots, x_N))$. The image of $\mathbb{P}_{\beta, N, \Lambda}$ under the mapping

$\mathbb{R}^N \rightarrow \Omega, (x_1, \dots, x_N) \mapsto \{x_1, \dots, x_N\}$ is a measure on (Ω, \mathcal{F}) , for which by a slight abuse of notation we use the same letter $\mathbb{P}_{\beta, \Lambda, N}$.

Equip $\mathbb{R}_+^{\mathbb{N}}$ with the product topology and the associated Borel σ -algebra, and let $\rho_\Lambda : (\Omega, \mathcal{F}, \mathbb{P}_{\beta, N, \Lambda}) \rightarrow \mathbb{R}_+^{\mathbb{N}}$ be the random variable $\rho_\Lambda(\omega) := (\rho_{k, \Lambda}(\omega))_{k \in \mathbb{N}}$. We are interested in the behavior of ρ_Λ in the *thermodynamic limit*

$$N \rightarrow \infty, \quad L \rightarrow \infty, \quad \frac{N}{|\Lambda|} \rightarrow \rho \tag{2.8}$$

for $\rho > 0$. First we recall the definition of the free energy $f(\beta, \rho)$ and the close-packing density ρ_{cp} . Consider the limit

$$f(\beta, \rho) := - \lim \frac{1}{\beta|\Lambda|} \log Z_\Lambda(\beta, N)$$

along (2.8). It is well-known [20] that the limit exists and is finite when the density ρ is strictly smaller than the *close-packing density* $\rho_{cp} > 0$, and is infinite when $\rho > \rho_{cp}$. When the potential has no hard core ($r_{hc} = 0$), we have $\rho_{cp} = \infty$ and the limit $f(\beta, \rho)$ is finite for all $\rho > 0$.

The following holds [14]: for all $\beta > 0$ and $\rho \in (0, \rho_{cp})$, in the limit (2.8), the random variable $\rho_\Lambda(\omega)$ satisfies a large deviation principle with speed $\beta|\Lambda|$. The rate function is of the form $f(\beta, \rho, (\rho_k)_{k \in \mathbb{N}}) - f(\beta, \rho)$ for a function $f(\beta, \rho, \cdot) : [0, \infty)^{\mathbb{N}} \rightarrow \mathbb{R} \cup \{\infty\}$ that is convex and lower semi-continuous with compact sublevel sets. Moreover,

$$f(\beta, \rho) = \min \left\{ f(\beta, \rho, (\rho_k)_{k \in \mathbb{N}}) \mid (\rho_k)_{k \in \mathbb{N}} \in [0, \infty)^{\mathbb{N}}, \sum_{k=1}^{\infty} k \rho_k \leq \rho \right\},$$

Note that the rate function $f(\beta, \rho, \cdot)$ (but not the free energy $f(\beta, \rho)$!) depends on the connectivity radius $R \geq r_1$; to lighten notation, however, we leave the R -dependence implicit.

3 Results

Here we formulate our main results. Section 3.1 provides a variational characterization of percolation. Sections 3.2 and 3.3 formulate bounds on percolation thresholds in terms of the chemical potential $\mu = \beta^{-1} \log z$ and the density ρ . Section 3.1 on the one hand and Sections 3.2 and 3.3 on the other hand are logically independent, except for Proposition 3.7.

Throughout the remainder of the article we shall assume without further mention that the pair potential satisfies Assumptions 2.1 and 2.2, and the connectivity radius R is larger or equal to the potential range r_1 .

3.1 Variational characterization of percolation

Our first result expresses the rate function $f(\beta, \rho, (\rho_k))$ of [14] in terms of a variational problem.

Theorem 3.1. *For every $\rho \in (0, \rho_{cp})$, $\beta > 0$ and $(\rho_k)_{k \in \mathbb{N}} \in \mathbb{R}_+^{\mathbb{N}}$,*

$$f(\beta, \rho, (\rho_k)_{k \in \mathbb{N}}) = \min \{ U(P) - \beta^{-1} S(P) \mid P \in \mathcal{P}_\theta, \rho(P) = \rho, \forall k \in \mathbb{N} : \rho_k(P) = \rho_k \} \tag{3.1}$$

with the convention $\min \emptyset = \infty$.

The theorem says in particular that the minimum in Eq. (3.1) is attained, see Lemma 4.2 below.

We recall Theorem 3.4 from [10]. Fix $\beta > 0$ and $\mu \in \mathbb{R}$. Then $P \in \mathcal{P}_\theta$ is a (β, μ) -Gibbs measure if and only if it minimizes $U(P) - \beta^{-1}S(P) - \mu\rho(P)$; the minimum $-p(\beta, \mu)$ is minus the pressure. This is the *Gibbs variational principle*. Together with Theorem 3.1, it allows us to establish the following relation between minimizers of $f(\beta, \rho, \cdot)$ and infinite volume Gibbs measures.²

Theorem 3.2. Fix $\rho \in (0, \rho_{cp})$ and $\beta > 0$. Then, for every $(\rho_k)_{k \in \mathbb{N}} \in \mathbb{R}_+^{\mathbb{N}}$, the following two statements are equivalent:

1. $(\rho_k)_{k \in \mathbb{N}}$ is a minimizer of $f(\beta, \rho, \cdot)$.
2. There is a chemical potential $\mu \in \mathbb{R}$ and a shift-invariant Gibbs measure $P \in \mathcal{P}_\theta \cap \mathcal{G}(\beta, \mu)$ such that $\rho(P) = \rho$ and for all $k \in \mathbb{N}$, $\rho_k(P) = \rho_k$.

The next elementary proposition establishes a relation between cluster densities and percolation, valid for general shift-invariant point processes.

Proposition 3.3. Let $P \in \mathcal{P}_\theta$. The following statements are equivalent:

1. $\sum_{k=1}^\infty k\rho_k(P) < \rho(P)$.
2. $P(\text{there is a cluster with infinitely many particles}) > 0$.
3. $P(\text{there is a cluster with infinite diameter}) > 0$.

A quantitative relation is given in Eq. (6.1) below. We shall refer to both (2) and (3) as $P(\text{there is an infinite cluster}) > 0$, or more briefly as percolation. An immediate consequence of Theorem 3.2 and Prop. 3.3 is the following characterization of percolation in shift-invariant Gibbs measures. Set

$$\mathcal{G}_\theta(\beta, \rho) := \left\{ P \in \bigcup_{\mu \in \mathbb{R}} \mathcal{G}(\beta, \mu) \mid P \in \mathcal{P}_\theta, \rho(P) = \rho \right\}.$$

The Gibbs variational principle implies that $\mathcal{G}_\theta(\beta, \rho)$ consists of the minimizers of $U(P) - \beta^{-1}S(P)$ under the constraint $\rho(P) = \rho$; compare with the proof of Theorem 3.2 below.

Corollary 3.4. Let $\beta > 0$ and $\rho \in (0, \rho_{cp})$. Consider the following statements:

1. There is a $P \in \mathcal{G}_\theta(\beta, \rho)$ such that $P(\text{there is an infinite cluster}) > 0$.
2. $f(\beta, \rho, \cdot)$ has a minimizer (ρ_k) such that $\sum_{k=1}^\infty k\rho_k < \rho$.
3. For every $P \in \mathcal{G}_\theta(\beta, \rho)$, $P(\text{there is an infinite cluster}) = 1$.
4. Every minimizer (ρ_k) of $f(\beta, \rho, \cdot)$ satisfies $\sum_{k=1}^\infty k\rho_k < \rho$.

We have (1) \Leftrightarrow (2) and (3) \Leftrightarrow (4).

A similar characterization holds for non-percolation. We note that Corollary 3.4 establishes a relation between percolation for infinite volume Gibbs measures and cluster size distributions in finite volume canonical ensembles as examined in [14].

3.2 Percolation thresholds: grand-canonical ensemble

Set $E_1 := 0$ and

$$E_k := \inf_{(\mathbb{R}^d)^k} U(x_1, \dots, x_k) \quad (k \in \mathbb{N}), \quad e_\infty := \inf_{k \in \mathbb{N}} \frac{E_k}{k} > -\infty.$$

Let $r_0 < r_1$ as in Assumption 2.1 and suppose that v is continuous in (r_0, r_1) . Set

²Georgii states his result under the additional assumption that the potential is non-integrably divergent at the origin. A close inspection of the proof shows, however, that we can dispense with this condition because our potentials have finite range; see the comment in [10] before Lemma 7.3.

$-M := \inf_{r>r_0} v(r) < 0$. For $m < M$, choose $\tilde{r}_m \in (r_0, r_1)$ such that $v(\tilde{r}_m) \leq -m$, see Figure 2 in [18]. Note $e_\infty \leq -dm$. Consider the conditions

$$\forall \mu > \mu_+ \forall P \in \mathcal{G}(\beta, \mu) P(\text{there is an infinite } R\text{-cluster}) = 1 \tag{3.2}$$

$$\forall \mu < \mu_- \forall P \in \mathcal{G}(\beta, \mu) P(\text{there is an infinite } R\text{-cluster}) = 0. \tag{3.3}$$

Set

$$\begin{aligned} \mu_+(\beta; R) &:= \inf\{\mu_+ \in \mathbb{R} \mid \mu_+ \text{ satisfies (3.2)}\}, \\ \mu_-(\beta; R) &:= \sup\{\mu_- \in \mathbb{R} \mid \mu_- \text{ satisfies (3.3)}\}. \end{aligned}$$

Clearly $\mu_-(\beta; R) \leq \mu_+(\beta; R)$.

Theorem 3.5. *Let $R \geq r_1$, $m \in (0, M)$ and $R_m > \sqrt{d+3} \tilde{r}_m \geq \sqrt{d+3} r_0$.*

1. *Suppose that v satisfies Assumption 2.3. Then*

$$e_\infty \leq \liminf_{\beta \rightarrow \infty} \mu_-(\beta; R).$$

In addition, for every $\mu < e_\infty$ and sufficiently large β , there is a unique (β, μ) -Gibbs measure P ; it is shift-invariant, has no infinite cluster (P -almost surely), and satisfies

$$P^\circ(|\mathcal{C}_\omega(0)| = k) = k\rho_k(P) \leq ke^k |B(0, R)|^{k-1} \exp(-\beta k(e_\infty - \mu)). \tag{3.4}$$

2. *Suppose that v is continuous in (r_0, r_1) . Then*

$$\limsup_{\beta \rightarrow \infty} \mu_+(\beta; R_m) \leq -m.$$

We conjecture that for every fixed $R \geq r_1$, under suitable conditions on v , we have $\mu_-(\beta; R) = \mu_+(\beta; R)$ for sufficiently large β and

$$\lim_{\beta \rightarrow \infty} \mu_-(\beta; R) = \lim_{\beta \rightarrow \infty} \mu_+(\beta; R) = e_\infty. \tag{3.5}$$

See Appendix A for the corresponding lattice gas result.

3.3 Percolation thresholds: canonical ensemble

Let $\nu^* := \inf_{k \in \mathbb{N}} (E_k - ke_\infty)$. It is known that for potentials with an attractive tail, $\nu^* > 0$ [14]. Consider the conditions

$$\forall \rho > \rho_+ \forall P \in \mathcal{G}_\theta(\beta, \rho) P(\text{there is an infinite } R\text{-cluster}) = 1, \tag{3.6}$$

$$\forall \rho < \rho_- \forall P \in \mathcal{G}_\theta(\beta, \rho) P(\text{there is an infinite } R\text{-cluster}) = 0. \tag{3.7}$$

Set

$$\begin{aligned} \rho_+(\beta; R) &:= \inf\{\rho_+ \in (0, \rho_{cp}) \mid \rho_+ \text{ satisfies (3.6)}\}, \\ \rho_-(\beta; R) &:= \sup\{\rho_- \in (0, \rho_{cp}) \mid \rho_- \text{ satisfies (3.7)}\}. \end{aligned}$$

Clearly $\rho_-(\beta; R) \leq \rho_+(\beta; R)$. For $\mu \in \mathbb{R}$, we define $\rho(\beta, \mu)$ as the smallest density ρ of Gibbs measures $P \in \mathcal{P}_\theta \cap \mathcal{G}(\beta, \mu)$; equivalently, as the left derivative, with respect to μ , of the pressure $p(\beta, \mu) = \sup_\rho (\rho\mu - f(\beta, \rho))$. Set

$$\rho_m := \liminf_{\beta \rightarrow \infty} \rho(\beta, -m).$$

Theorem 3.6. *Let $R \geq r_1$, $m \in (0, M)$ and $R_m > \sqrt{d+3} \tilde{r}_m \geq \sqrt{d+3} r_0$.*

1. *Suppose that v satisfies Assumption 2.3. Then*

$$-\nu^* \leq \liminf_{\beta \rightarrow \infty} \beta^{-1} \log \rho_-(\beta; R).$$

In addition, for every fixed $\nu > \nu^$, sufficiently large β , $\rho = \exp(-\beta\nu)$, there is a unique measure P in $\mathcal{G}_\theta(\beta, \rho)$. It has no infinite cluster, P -almost surely, and satisfies*

$$P^\circ(|\mathcal{C}_\omega(0)| = k) = k\rho_k(P) \leq C\rho \exp(-\beta ck) \tag{3.8}$$

for suitable $C, c > 0$ and all $k \in \mathbb{N}$.

2. *Suppose that v is continuous in (r_0, r_1) . Then*

$$\limsup_{\beta \rightarrow \infty} \rho_+(\beta; R_m) \leq \rho_m.$$

The constants C and c in Eq. (3.8) can be chosen uniform in regions of the form $\beta \geq \beta_\epsilon, \rho \leq \exp(-\beta(\nu^* + \epsilon))$.

If in addition v satisfies Assumptions 2.4 and 2.5, then ρ_m is larger than the preferred ground state density³ ρ_* , and in particular, bounded away from zero; this follows from Theorem 3.2 in [13]. Moreover, we expect that for every $R \geq r_1$, as $\beta \rightarrow \infty$,

$$\lim_{\beta \rightarrow \infty} \beta^{-1} \log \rho_-(\beta; R) = -\nu^*, \quad \lim_{\beta \rightarrow \infty} \rho_+(\beta; R) = \rho_*$$

and for $\rho_-(\beta; R) < \rho < \rho_+(\beta; R)$ and very large β , there should be non-ergodic Gibbs measures with percolation probability strictly between 0 and 1. This is what happens for lattice gases (see Appendix A). For continuum systems, we have no proof of this conjecture; we have, however, the following bound:

Proposition 3.7. *Suppose that v satisfies Assumptions 2.4 and 2.5. Let $R \geq r_1$. There are $\beta_0, \rho_0, C > 0$ such that for all $\beta \geq \beta_0$, all $\rho \leq \rho_0$ and all $P \in \mathcal{G}_\theta(\beta, \rho)$, the following holds: if $\rho = \exp(-\beta\nu) > \exp(-\beta\nu^*)$, then*

$$\forall K \in \mathbb{N} : \sum_{k=1}^K k\rho_k(P) \leq \frac{C\rho\beta^{-1} \log \beta}{\nu^* - \nu}.$$

In view of Proposition 3.3 we would like to say that for $\rho \gg \exp(-\beta\nu^*)$, we have $\sum_{k=1}^\infty k\rho_k(P) < \rho$. Set $q_k = k\rho_k(P)/\rho$, $q_\infty = 1 - \sum_{k \in \mathbb{N}} q_k$, and interpret (q_k) as a probability measure on $\mathbb{N} \cup \{\infty\}$. Thus we would like to say that $q_\infty > 0$. Instead Proposition 3.7 tells us that as $\beta \rightarrow \infty$ and $\rho \geq \exp(-\beta\nu^*)$, q gives more and more mass to large cluster sizes, even though we may have $q_\infty = 0$ all the way through.

4 Topology on \mathcal{P} and continuity properties

In this section we specify the topology on \mathcal{P} that we use, recall some continuity properties of the functionals to be studied, and explain why the variational problems considered in this article have minimizers. We follow [12, 9].

Let $\mathcal{M}(\Omega)$ be the set of finite measures on (Ω, \mathcal{F}) . The topology $\tau_{\mathcal{L}}$ of local convergence on $\mathcal{M}(\Omega)$ is defined as follows. Let \mathcal{L} be the class of measurable functions $f : \Omega \rightarrow \mathbb{R}$ that are local and tame, i.e., $f \in \mathcal{L}$ if and only if there is a Borel subset $B \subset \mathbb{R}^d$ and a constant $c > 0$ such that f is a function of $\omega_B := \omega \cap B$ alone and for all $\omega \in \Omega$,

³Let $e(\rho) = \lim_{\beta \rightarrow \infty} f(\beta, \rho)$, then ρ_* is the minimizer of $\rho \mapsto e(\rho)/\rho$.

$|f(\omega)| \leq c(1 + N_B(\omega))$. Then $\tau_{\mathcal{L}}$ is the smallest topology with respect to which all maps of the form $P \mapsto \int_{\Omega} f(\omega)P(d\omega)$, $f \in \mathcal{L}$, are continuous.

The topology of local convergence is a convenient alternative, in the Gibbsian world, to the topology of weak convergence of probability measures on the space Ω , which equipped with the vague topology is a Polish space. Weak convergence is more commonly used in point process theory. Indeed various maps listed below are lower semi-continuous in the local topology but not necessarily in the weak topology. Moreover there is an elegant compactness criterion in terms of the relative entropy [12, 9]. The inclusion of tame local functions rather than bounded local functions in the definition of the topology reflects the lower bound of the energy by minus a constant times the number of particles.

The following holds [12, 9]:

- \mathcal{P} and \mathcal{P}_{θ} are closed subsets of $\mathcal{M}(\Omega)$. We endow them with the traces of the topology $\tau_{\mathcal{L}}$.
- The Palm measure $\mathcal{P}_{\theta} \rightarrow \mathcal{M}(\Omega)$, $P \mapsto P^{\circ}$ is continuous.
- The particle density $\mathcal{P}_{\theta} \rightarrow \mathbb{R}$, $P \mapsto \rho(P)$ is continuous.
- The entropy density $\mathcal{P}_{\theta} \rightarrow \mathbb{R} \cup \{-\infty\}$, $P \mapsto S(P)$ is affine, upper semi-continuous, and has superlevel sets $\{S \geq -c\}$ that are compact and sequentially compact.
- The energy density $\mathcal{P}_{\theta} \rightarrow \mathbb{R} \cup \{\infty\}$, $P \mapsto U(P)$ is lower semi-continuous.

Furthermore, the cluster densities are continuous:

Lemma 4.1. *For every $k \in \mathbb{N}$, the map $\mathcal{P}_{\theta} \rightarrow \mathbb{R}$, $P \mapsto \rho_k(P)$, is continuous.*

Proof. Let $g_k(\omega) := \mathbf{1}(|\mathcal{C}_{\omega}(0)| = k)$. The function g_k is local and bounded, thus in particular, tame. Therefore, by definition of $\tau_{\mathcal{L}}$, $P \mapsto \int_{\Omega} g_k dP$ is continuous. Since $P \mapsto \rho_k(P)$ is the composition of the latter map with the continuous map $P \mapsto P^{\circ}$, it follows that $P \mapsto \rho_k(P)$ is continuous. \square

Now we can easily check that the variational problem in Theorem 3.1 admits a minimizer.

Lemma 4.2. *Fix $\beta, \rho > 0$ and $(\rho_k)_{k \in \mathbb{N}} \in [0, \infty)^{\mathbb{N}}$. Let $\mathcal{A} \subset \mathcal{P}_{\theta}$ be the set of measures satisfying $\rho(P) = \rho$ and $\rho_k(P) = \rho_k$, for every $k \in \mathbb{N}$. If $\mathcal{A} \neq \emptyset$, the function $\mathcal{A} \ni P \mapsto U(P) - \beta^{-1}S(P)$ has a minimizer.*

Proof. If $U(P) - \beta^{-1}S(P) = \infty$ for every $P \in \mathcal{A}$, there is nothing to show. If $U(P) - \beta^{-1}S(P) < \infty$ for some $P \in \mathcal{A}$, let (P_n) be a minimizing sequence. The sequence $(U(P_n) - \beta^{-1}S(P_n))_{n \in \mathbb{N}}$ is bounded from above and, because $U(P)$ is bounded from below, $S(P_n)$ is bounded from below too. Since the superlevel sets $\{S \geq -c\}$ are $\tau_{\mathcal{L}}$ -sequentially compact, there is a subsequence P_{n_j} converging to some $P \in \mathcal{P}_{\theta}$. The continuity of the maps $\rho(\cdot)$ and $\rho_k(\cdot)$ ensures that $P \in \mathcal{A}$, and the lower semi-continuity of U and $-S$ shows that P is a minimizer. \square

5 Proof of Theorem 3.1

The main idea for the proof of Theorem 3.1 is to apply a large deviations principle for the stationary empirical field proven in [9, 12] and the contraction principle [7, Section 4.2.1]. Two complications stand in our way. First, the large deviations principle in [9, 12] was shown in the grand-canonical rather than the canonical ensemble. Second, the cluster size densities can only be expressed as functions of the stationary empirical field if we modify their definition and, loosely speaking, define them with periodic boundary conditions; this yields a modified variable $\rho_{\Lambda}^{\text{per}}$. In order to circumvent these difficulties, we proceed as follows:

- We show first that the large deviations principle in the canonical ensemble for ρ_Λ implies a large deviations principle in the grand-canonical ensemble (Lemma 5.1).
- We apply the contraction principle and show that $\rho_\Lambda^{\text{per}}$ satisfies a large deviations principle with convex rate function (Lemma 5.3).
- Next we show that (truncations of) ρ_Λ and $\rho_\Lambda^{\text{per}}$, in the grand-canonical ensemble, are *exponentially equivalent* [7, Section 4.2.2]; this follows from Ruelle’s super-stability bounds [21]. As a consequence, the grand-canonical rate functions for ρ_Λ and $\rho_\Lambda^{\text{per}}$ must be equal (Lemma 5.4).
- Taking Legendre transforms, we deduce the desired identity for the canonical rate function (Lemma 5.5).

For the purpose of this section it is most convenient to work with measures that are not normalized and to suppress the β -dependence in the notation. Let

$$Q_{N,\Lambda}^{\text{can}}(A) := \frac{1}{N!} \int_A \exp(-\beta U(x_1, \dots, x_N)) dx_1 \cdots dx_N$$

be a measure on Λ^N with total mass $Z_\Lambda(\beta, N)$. The image of $Q_{N,\Lambda}^{\text{can}}$ under the map $\Lambda^N \rightarrow \Omega, (x_1, \dots, x_N) \mapsto \{x_1, \dots, x_N\}$ is a measure on (Ω, \mathcal{F}) , for which we use the same letter $Q_{N,\Lambda}^{\text{can}}$. Furthermore define

$$Q_{\mu,\Lambda} = \delta_\emptyset + \sum_{N=1}^\infty z^N Q_{N,\Lambda}^{\text{can}}, \quad z = \exp(\beta\mu).$$

We use the same letter for the measure on Ω and the measure on disjoint unions $\dot{\cup}_{N \geq 0} \Lambda^N$. Λ^0 is a dummy space corresponding to $\omega = \{\emptyset\}$: the event that there is no point at all has $Q_{\mu,\Lambda}$ -measure 1. Remember that $\mathbb{R}_+^{\mathbb{N}}$ is equipped with the product topology and the corresponding Borel σ -algebra.

Lemma 5.1. *Under $Q_{\mu,\Lambda}$ as $|\Lambda| \rightarrow \infty, N \rightarrow \infty$ at fixed $\beta > 0$ and $\mu \in \mathbb{R}$, the cluster size distribution $\rho_\Lambda := (\rho_{k,\Lambda})_{k \in \mathbb{N}}$ satisfies a large deviations principle with speed $\beta|\Lambda|$ and rate function*

$$J_{\beta,\mu}((\rho_k)_k) = \inf_{\rho > 0} \left(f(\beta, \rho, (\rho_k)_k) - \mu\rho \right). \tag{5.1}$$

We recall that $f(\beta, \cdot, \cdot) : \mathbb{R}_+ \times \mathbb{R}_+^{\mathbb{N}} \rightarrow \mathbb{R}$ is a lower semi-continuous, convex function, defined in all of $\rho > 0$ and not only $\rho \in (0, \rho_{\text{cp}})$. When $\rho > \rho_{\text{cp}}$ or $\sum_{k+1}^\infty k\rho_k > \rho$, it takes the value ∞ [14].

Proof of Lemma 5.1. We consider Eq. (5.1) as the definition of a function $J_{\beta,\mu}$ and show that $J_{\beta,\mu}$ is a rate function for $(\rho_{k,\Lambda})$. Set $z := \exp(\beta\mu)$.

Lower bound. Let $\mathcal{O} \subset \mathbb{R}_+^{\mathbb{N}}$ be an open set. For every N and Λ ,

$$Q_{\mu,\Lambda}((\rho_{k,\Lambda})_k \in \mathcal{O}) \geq z^N Q_{N,\Lambda}^{\text{can}}((\rho_k)_k \in \mathcal{O}).$$

Fix $\rho > 0$ and apply the previous inequality to N, Λ with $N \rightarrow \infty, |\Lambda| \rightarrow \infty$ such that $N/|\Lambda| \rightarrow \rho$. We get

$$\liminf \frac{1}{\beta|\Lambda|} \log Q_{\mu,\Lambda}((\rho_{k,\Lambda})_k \in \mathcal{O}) \geq \mu\rho - \inf_{(\rho_k) \in \mathcal{O}} f(\beta, \rho, (\rho_k)).$$

Since the inequality holds for every $\rho > 0$, we can take the supremum over $\rho > 0$ on the right-hand side, and to conclude note

$$\begin{aligned} \sup_{\rho > 0} \left(\mu\rho - \inf_{(\rho_k) \in \mathcal{O}} f(\beta, \rho, (\rho_k)) \right) &= \sup_{\rho > 0} \sup_{(\rho_k) \in \mathcal{O}} \left(\mu\rho - f(\beta, \rho, (\rho_k)) \right) \\ &= \sup_{(\rho_k) \in \mathcal{O}} \sup_{\rho > 0} \left(\mu\rho - f(\beta, \rho, (\rho_k)) \right) \\ &= - \inf_{(\rho_k) \in \mathcal{O}} J_{\beta,\mu}((\rho_k)). \end{aligned}$$

Upper bound. We use ideas explained in [20, Section 3.4.5]. Let $\mathcal{A} \subset \mathbb{R}_+^{\mathbb{N}}$ be a closed set. For every $\rho > 0$ as $|\Lambda| \rightarrow \infty$ and $N/|\Lambda| \rightarrow \rho$,

$$\limsup \frac{1}{\beta|\Lambda|} \ln Q_{N,\Lambda}^{\text{can}}((\rho_k, \Lambda)_k \in \mathcal{A}) \leq - \inf_{(\rho_k) \in \mathcal{A}} f(\beta, \rho, (\rho_k)). \tag{5.2}$$

Let $b < \infty$ be the stability constant from Eq. 2.1. When $N/|\Lambda| \rightarrow 0$, note that

$$Q_{N,\Lambda}^{\text{can}}((\rho_k, \Lambda) \in \mathcal{A}) \leq Z_\Lambda(\beta, N) \leq \exp(\beta Nb) \frac{|\Lambda|^N}{N!}$$

from which we get

$$\limsup_{|\Lambda| \rightarrow \infty} \frac{1}{|\Lambda|} \log Q_{N,\Lambda}^{\text{can}}((\rho_k) \in \mathcal{A}) \leq \limsup_{|\Lambda| \rightarrow \infty} \frac{1}{|\Lambda|} \left(\beta Nb - N \log \frac{N}{|\Lambda|e} \right) = 0.$$

Thus Eq. (5.2) holds for all $\rho \geq 0$, provided we read the right-hand side as 0 when $\rho = 0$. Fix $\rho_0 > 0$. We claim that Eq. (5.2) holds uniformly in $\rho \in [0, \rho_0]$. More precisely, for every $\epsilon > 0$, there is a $\delta > 0$ such that: for all $\rho \in [0, \rho_0]$ and all N, Λ satisfying $|\Lambda| \geq 1/\delta$ and $|N/|\Lambda| - \rho| \leq \delta$, we have

$$\frac{1}{\beta|\Lambda|} \log Q_{N,\Lambda}^{\text{can}}((\rho_k, \Lambda)_k \in \mathcal{A}) \leq \epsilon - \inf_{(\rho_k) \in \mathcal{A}} f(\beta, \rho, (\rho_k)). \tag{5.3}$$

Indeed, if this was not the case, we could find $\epsilon > 0$, sequences $(N_j), (\Lambda_j)$ and a $\rho \in [0, \rho_0]$ such that $|\Lambda_j| \geq j$, $|N_j/|\Lambda_j| - \rho| \leq 1/j$ and

$$\frac{1}{\beta|\Lambda_j|} \ln Q_{N_j, \Lambda_j}^{\text{can}}((\rho_k, \Lambda)_k \in \mathcal{A}) \geq \epsilon - \inf_{(\rho_k) \in \mathcal{A}} f(\beta, \rho, (\rho_k)),$$

contradicting Eq. (5.2); this proves the claim. Now because of the uniformity, for every $\epsilon > 0$ and sufficiently large $|\Lambda|$,

$$\begin{aligned} & \frac{1}{\beta|\Lambda|} \log \left(\sum_{N=1}^{\lfloor \rho_0 |\Lambda| \rfloor} z^N Q_{N,\Lambda}^{\text{can}}((\rho_k, \Lambda) \in \mathcal{A}) \right) \\ & \leq \frac{\log(2 + \rho_0 |\Lambda|)}{\beta|\Lambda|} + \epsilon + \sup_N \left(\mu \frac{N}{|\Lambda|} - \inf_{(\rho_k) \in \mathcal{A}} f(\beta, N/|\Lambda|, (\rho_k)) \right) \\ & \leq o(1) + \epsilon + \sup_{\rho > 0} \left(\mu \rho - \inf_{(\rho_k) \in \mathcal{A}} f(\beta, \rho, (\rho_k)) \right) \\ & = o(1) + \epsilon - \inf_{(\rho_k) \in \mathcal{A}} J_{\beta, \mu}((\rho_k)). \end{aligned}$$

If $(\rho_k) = \mathbf{0} \notin \mathcal{A}$, the δ_\emptyset term corresponding, formally, to $N = 0$, does not contribute to $Q_{\mu, \Lambda}^{\text{can}}((\rho_k, \Lambda) \in \mathcal{A})$. If $\mathbf{0} \in \mathcal{A}$, the δ_\emptyset -term contributes a term 1 inside the logarithm, and we want to check that $\lim |\Lambda|^{-1} \log 1 \leq - \inf_{\mathcal{A}} J_{\beta, \mu}$. To this aim note that

$$\inf_{\mathcal{A}} J_{\beta, \mu}((\rho_k)) \leq \inf_{\rho > 0} (f(\beta, \rho, \mathbf{0}) - \mu \rho) \leq \liminf_{\rho \rightarrow 0} (f(\beta, \rho, \mathbf{0}) - \mu \rho) = 0.$$

The last equality is shown by choosing a connected reference configuration (x_1^0, \dots, x_N^0) which is such that (i) for suitable $r > 0$, every $\mathbf{x} \in \cup_{\pi \in \mathcal{S}_N} \times_{k=1}^N B(x_{\pi(k)}^0, r)$ is connected, (ii) on this set the energy is upper bounded by CN for suitable $C > 0$, and (iii) the balls are disjoint. Integrating in the neighborhood of \mathbf{x}^0 given by $\times_{i=1}^N B(x_i, r)$ (and permutations of this set) yields the bound

$$-\beta f(\beta, \rho, \mathbf{0}) \geq -\beta \rho \log \left(|B(0, r)| e^{1-\beta C} \right).$$

The right-hand side goes to 0 as $\rho \rightarrow 0$. Thus we need not worry about the contribution from $N = 0$.

It remains to estimate the terms from $N \geq \rho_0|\Lambda|$. Choose ρ_0 large enough so that $z \exp(\beta b + 1)/\rho_0 < 1/2$. Remember $N! \geq (N/e)^N$. Then

$$\begin{aligned} \sum_{N \geq \rho_0|\Lambda|} z^N Q_{N,\Lambda}^{\text{can}}((\rho_{k,\Lambda}) \in \mathcal{A}) &\leq \sum_{N \geq \rho_0|\Lambda|} z^N \frac{|\Lambda|^N}{N!} e^{\beta b N} \\ &\leq \sum_{N \geq \rho_0|\Lambda|} \left(\frac{z|\Lambda| \exp(\beta b + 1)}{N} \right)^N \leq 2 \exp(-\rho_0|\Lambda| \ln 2). \end{aligned}$$

If $\inf_{\mathcal{A}} J_{\beta,\mu} < \infty$, we can choose ρ_0 large enough so that $\rho_0 \log 2 > \beta \inf_{\mathcal{A}} J_{\beta,\mu}$, and we obtain

$$\limsup \frac{1}{\beta|\Lambda|} \log Q_{\mu,\Lambda}((\rho_{k,\Lambda}) \in \mathcal{A}) \leq - \inf_{(\rho_k) \in \mathcal{A}} J_{\beta,\mu}((\rho_k)). \tag{5.4}$$

If $\inf_{\mathcal{A}} J_{\beta,\mu} = \infty$, we have $f(\beta, \rho, (\rho_k)) = \infty$ for all $\rho > 0$ and $(\rho_k) \in \mathcal{A}$. But this implies that $Q_{N,\Lambda}^{\text{can}}((\rho_{k,\Lambda})_k \in \mathcal{A}) = 0$ for all N, Λ . Indeed, suppose by contradiction that there is a $N \in \mathbb{N}$ and a box $\Lambda = [0, L]^d$ such that $Q_{N,\Lambda}^{\text{can}}((\rho_{k,\Lambda})_k \in \mathcal{A}) > 0$. For $n \in \mathbb{N}$, let $L_n := n(L + R)$, $\Lambda_n := [0, L_n]^d$ and $N_n := n^d N$. Then

$$Q_{N_n,\Lambda_n}^{\text{can}}((\rho_{k,\Lambda}) \in \mathcal{A}) \geq \left(Q_{N,\Lambda}^{\text{can}}((\rho_{k,\Lambda}) \in \mathcal{A}) \right)^{n^d}$$

and

$$-\beta \inf_{(\rho_k) \in \mathcal{A}} f(\beta, \rho, (\rho_k)) \geq -\frac{1}{(L + R)^d} \log Q_{N,\Lambda}^{\text{can}}((\rho_{k,\Lambda}) \in \mathcal{A}) > -\infty,$$

contradiction. Thus $Q_{N,\Lambda}^{\text{can}}((\rho_{k,\Lambda})_k \in \mathcal{A}) = 0$ for all N and Λ , whence $Q_{\mu,\Lambda}((\rho_{k,\Lambda}) \in \mathcal{A}) = 0$; Eq. (5.4) holds trivially. \square

Next we define the stationary empirical field and the modified cluster size distribution $\rho_{\Lambda}^{\text{per}}$. For $\omega \in \Omega$ and $\Lambda = [0, L]^d$, let $\omega_{\Lambda}^{\text{per}} := \cup_{\mathbf{k} \in \mathbb{Z}^d} \theta_{L\mathbf{k}}(\omega \cap \Lambda)$ be the periodic continuation of $\omega \cap \Lambda$. The *translation invariant empirical field* is

$$R_{\Lambda,\omega} = \frac{1}{|\Lambda|} \int_{\Lambda} \delta_{\theta_x \omega_{\Lambda}^{\text{per}}} dx.$$

The Palm measure of $R_{\Lambda,\omega}$ is

$$R_{\Lambda,\omega}^{\circ} = \frac{1}{|\Lambda|} \sum_{x \in \omega \cap \Lambda} \delta_{\theta_x \omega_{\Lambda}^{\text{per}}}.$$

Remark 5.2. The stationary empirical field associates with every configuration ω a probability measure supported on configurations with the same relative coordinates as $\omega \cap \Lambda$, but randomized center of mass. For example, in dimension $d = 1$, if ω consists of two particles $0, \epsilon$, then $R_{\Lambda,\omega}$ describes configurations $\{x, x + \epsilon\}$ with x having uniform Lebesgue density $1/L$.

We define k -cluster densities with periodic boundary conditions as

$$k\rho_{k,\Lambda}^{\text{per}}(\omega) := \int_{\Omega} \mathbf{1}(|\mathcal{C}_{\tilde{\omega}}(0)| = k) R_{\Lambda,\omega}^{\circ}(d\tilde{\omega}) = \frac{1}{|\Lambda|} \left| \left\{ x \in \omega \cap \Lambda \mid |\mathcal{C}_{\omega_{\Lambda}^{\text{per}}}(x)| = k \right\} \right|.$$

We have $\rho_{k,\Lambda}^{\text{per}}(\omega) = \rho_k(R_{\Lambda,\omega})$; compare with Eq. (2.7). Set $\rho_{\Lambda}(\omega) := ((\rho_{k,\Lambda}^{\text{per}}(\omega))_{k \in \mathbb{N}})$.

Lemma 5.3. Under $Q_{\mu,\Lambda}$, $\rho_{\Lambda}^{\text{per}}$ satisfies a large deviations principle with rate function

$$J_{\beta,\mu}^{\text{per}}((\rho_k)) = \inf \{ U(P) - \beta^{-1} S(P) - \mu \rho(P) \mid P \in \mathcal{P}_{\theta}, \forall k \in \mathbb{N} : \rho_k(P) = \rho_k \}.$$

Proof. Under $Q_{\mu,\Lambda}$, the stationary empirical field satisfies a large deviations principle with rate function $U(P) - \beta^{-1}S(P) - \mu\rho(P)$ [9], with compact sublevel sets. Since $(\rho_{k,\Lambda}^{\text{per}}(\omega))_{k \in \mathbb{N}}$ can be written as a continuous function of the stationary empirical field, we can apply the contraction principle [7, Section 4.2.1] and the result follows. \square

Lemma 5.4. *For every $\beta > 0$ and $\mu \in \mathbb{R}$, we have $J_{\beta,\mu} = J_{\beta,\mu}^{\text{per}}$.*

Proof. When $x \in \Lambda$ has distance $> kR$ to the boundary $\partial\Lambda$, we have $\mathcal{C}_{\omega_\Lambda}(x) = \mathcal{C}_{\omega_\Lambda^{\text{per}}}(x)$. Set $\partial_{kR}\Lambda := \{x \in \Lambda \mid \text{dist}(x, \partial\Lambda) \leq kR\}$. Then

$$|k\rho_{k,\Lambda}(\omega) - k\rho_{k,\Lambda}^{\text{per}}(\omega)| \leq \frac{|\omega \cap \partial_{kR}\Lambda|}{|\Lambda|}$$

and for every $\epsilon > 0$,

$$P_{\mu,\Lambda}(|\rho_{k,\Lambda}(\omega) - \rho_{k,\Lambda}^{\text{per}}(\omega)| \geq \epsilon) \leq P_{\mu,\Lambda}(N_{\partial_{kR}\Lambda} \geq k\epsilon|\Lambda|).$$

Here $P_{\mu,\Lambda} := (\Xi_\Lambda(\beta, \mu))^{-1}Q_{\mu,\Lambda}$ is the grand-canonical probability measure. Because of the superstability of v , we know [21] that for some suitable $\xi > 0$ such that all n -point correlation functions $\rho_\Lambda(x_1, \dots, x_n)$ are bounded in absolute value by ξ^n ; ξ depends on β and μ but is independent of Λ or n . Integrating, we get bounds for factorial moments as

$$E_{\mu,\Lambda}[N_{\partial_{kR}\Lambda}(N_{\partial_{kR}\Lambda} - 1) \cdots (N_{\partial_{kR}\Lambda} - m + 1)] \leq (\xi|\partial_{kR}\Lambda|)^m.$$

Let $G(z) = \sum_{n=0}^\infty P_{\mu,\Lambda}(N_{\partial_{kR}\Lambda} = n)z^n$ be the probability generating function of $N_{\partial_{kR}\Lambda}(\omega)$. A Taylor expansion around $z = 1$ yields

$$\begin{aligned} P_{\mu,\Lambda}(N_{\partial_{kR}\Lambda}(\omega) = n) &= \frac{1}{n!}G^{(n)}(0) = \frac{1}{n!} \frac{d^n}{dz^n} \sum_{k=0}^\infty \frac{G^{(k)}(1)}{k!} (z-1)^k \Big|_{z=0} \\ &= \frac{1}{n!} \sum_{k=n}^\infty \frac{G^{(k)}(1)}{(k-n)!} (-1)^{k-n} \leq \frac{1}{n!} \sum_{k=n}^\infty \frac{(\xi|\partial_{kR}\Lambda|)^k}{(k-n)!} \\ &= \frac{(\xi|\partial_{kR}\Lambda|)^n}{n!} e^{\xi|\partial_{kR}\Lambda|} \leq \left(\frac{e\xi|\partial_{kR}\Lambda|}{n}\right)^n e^{\xi|\partial_{kR}\Lambda|}. \end{aligned}$$

For $M \in \mathbb{N}$ such that $M > 2e\xi|\partial_{kR}\Lambda|$, we have

$$P_{\mu,\Lambda}(N_{\partial_{kR}\Lambda}(\omega) \geq M) \leq 2\left(\frac{e\xi|\partial_{kR}\Lambda|}{M}\right)^M e^{\xi|\partial_{kR}\Lambda|}.$$

Applying the inequality to $M = k\epsilon|\Lambda|$ we obtain, for sufficiently large $|\Lambda| = L^d$,

$$P_{\mu,\Lambda}(|\rho_{k,\Lambda}(\omega) - \rho_{k,\Lambda}^{\text{per}}(\omega)| \geq \epsilon) \leq 2\left(\frac{2de\xi R}{L}\right)^{k\epsilon L^d} e^{2d\xi kRL^{d-1}}.$$

It follows that for every fixed $K \in \mathbb{N}$ and $\epsilon > 0$,

$$\lim_{|\Lambda| \rightarrow \infty} \frac{1}{|\Lambda|^d} \log P_{\mu,\Lambda}\left(\sum_{k=1}^K |\rho_{k,\Lambda}(\omega) - \rho_{k,\Lambda}^{\text{per}}(\omega)| \geq \epsilon\right) = -\infty,$$

and the same identity holds with $P_{\mu,\Lambda}$ replaced with $Q_{\mu,\Lambda}$ (note $\Xi_\Lambda(\beta, \mu) \geq 1$). As a consequence, the random variables $(\rho_{1,\Lambda}, \dots, \rho_{K,\Lambda})$ and $(\rho_{1,\Lambda}^{\text{per}}, \dots, \rho_{K,\Lambda}^{\text{per}})$ are exponentially equivalent in the sense of [7, Section 4.2.1]. The contraction principle together with Lemma 5.3 and results from [14] tell us that they satisfy large deviations principles; because of exponential equivalence, their rate functions must be equal [7, Theorem 4.2.3]. The Dawson-Gärtner theorem [7, Theorem 4.6.1] allows us to recover the rate function of the full vectors ($k \in \mathbb{N}$) from the rate functions of the truncated vectors ($1 \leq k \leq K$) and it follows that $J_{\beta,\mu} = J_{\beta,\mu}^{\text{per}}$. \square

Lemma 5.5. For every $\beta > 0$, $\rho \in (0, \rho_{cp})$ and $(\rho_k) \in \mathbb{R}_+^{\mathbb{N}}$, we have

$$f(\beta, \rho, (\rho_k)) = \inf\{U(P) - \beta^{-1}S(P) \mid P \in \mathcal{P}_\theta, \rho(P) = \rho, \forall k \in \mathbb{N} : \rho_k(P) = \rho_k\}.$$

Proof of Lemma 5.5. Fix $\beta > 0$ and $(\rho_k)_{k \in \mathbb{N}} \in \mathbb{R}_+^{\mathbb{N}}$. For $\rho > 0$, set

$$h(\rho) := \inf\{U(P) - \beta^{-1}S(P) \mid P \in \mathcal{P}_\theta, \rho(P) = \rho, \forall k \in \mathbb{N} : \rho_k(P) = \rho_k\}$$

and $g(\rho) := f(\beta, \rho, (\rho_k))$ for $\rho \in (0, \rho_{cp})$, $g(\rho) := \infty$ for $\rho < \rho_{cp}$; the value of $g(\rho_{cp})$ can be determined in such a way that g is lower semi-continuous and convex in $(0, \infty)$. Lemma 5.4 implies that h and g have the same Legendre transforms,

$$\forall \mu \in \mathbb{R} : \sup_{\rho > 0}(\rho\mu - h(\rho)) = \sup_{\rho > 0}(\rho\mu - g(\rho)).$$

Since the functions h and g are lower semi-continuous in $(0, \infty)$ and convex [9, 14], it follows that $h(\rho) = g(\rho)$ for all $\rho \in (0, \rho_{cp})$. \square

Proof of Theorem 3.1. Theorem 3.1 is an immediate consequence of Lemmas 5.5 and 4.2. \square

6 Proof of Theorem 3.2 and Prop. 3.3

Proof of Theorem 3.2. (2) \Rightarrow (1). Suppose that there is a shift-invariant Gibbs measure P with $\rho(P) = \rho$ and $\rho_k(P) = \rho_k$, for all k . By Theorem 3.1,

$$\min f(\beta, \rho, \cdot) \leq f(\beta, \rho, (\rho_k)) \leq U(P) - \beta^{-1}S(P).$$

On the other hand, let (ρ'_k) with $\sum_{k=1}^{\infty} k\rho'_k \leq \rho$. By Theorem 3.1, we find $P' \in \mathcal{P}_\theta$ such that $\rho(P') = \rho$, $\rho_k(P') = \rho'_k$ for all k , and $f(\beta, \rho, (\rho'_k)) = U(P') - \beta^{-1}S(P')$. The Gibbs variational principle implies

$$f(\beta, \rho, (\rho'_k)) - \mu\rho = U(P') - \beta^{-1}S(P') - \mu\rho(P') \geq U(P) - \beta^{-1}S(P) - \mu\rho(P).$$

Minimization over (ρ'_k) yields (remember $\rho(P) = \rho$)

$$\min f(\beta, \rho, \cdot) \geq U(P) - \beta^{-1}S(P).$$

It follows that $\min f(\beta, \rho, \cdot) = f(\beta, \rho, (\rho_k)) = U(P) - \beta^{-1}S(P)$, and (ρ_k) is a minimizer of $f(\beta, \rho, \cdot)$.

(1) \Rightarrow (2). Conversely, let (ρ_k) be a minimizer of $f(\beta, \rho, \cdot)$. Thus $f(\beta, \rho, (\rho_k)) = f(\beta, \rho)$. By Theorem 3.1, we can find $P \in \mathcal{P}_\theta$ such that $\rho(P) = \rho$, $\rho_k(P) = \rho_k$ for all k , and $f(\beta, \rho) = f(\beta, \rho, (\rho_k)) = U(P) - \beta^{-1}S(P)$. We know that $f(\beta, \rho) = \sup_{\mu}(\rho\mu - p(\beta, \mu))$, and for every $\rho \in (0, \rho_{cp})$, the supremum is actually attained. (This is because $\mu \mapsto \rho\mu - p(\beta, \mu)$ is concave and continuous in \mathbb{R} with limits $-\infty$ as $\mu \rightarrow \pm\infty$; note $\lim_{\mu \rightarrow \infty} \partial_{\mu} p(\beta, \mu) = \rho_{cp}$.) Thus let $\mu \in \mathbb{R}$ such that $f(\beta, \rho) = \rho\mu - p(\beta, \mu)$. We get $U(P) - \beta^{-1}S(P) - \mu\rho(P) = -p(\beta, \mu)$ and as a consequence of the Gibbs variational principle, we find that $P \in \mathcal{G}(\beta, \mu)$. \square

Proof of Prop. 3.3. (2) \Rightarrow (3) By definition of our probability space Ω , for every configuration ω and every bounded set A the number of particles in A is finite. Therefore, if ω has a cluster with infinitely many particles, this cluster has infinite diameter.

(3) \Rightarrow (2) If in a configuration ω there is a cluster with infinite diameter, then this cluster must contain infinitely many particles – otherwise it would have diameter bounded by R times the cardinality of the cluster.

(1) \Leftrightarrow (2) Let

$$g(\omega) := \mathbf{1}(|\mathcal{C}_\omega(0)| = \infty) = 1 - \lim_{n \rightarrow \infty} \sum_{k=1}^n \mathbf{1}(|\mathcal{C}_\omega(0) = k).$$

The function is the limit of local, measurable functions and therefore measurable. Eq. (2.5) gives

$$\int_{\Omega} g(\omega) P^\circ(d\omega) = \int_{\Omega} \sum_{x \in \omega \cap [0,1]^d} \mathbf{1}(|\mathcal{C}_\omega(x)| = \infty) P(d\omega).$$

Thus

$$\rho(P) - \sum_{k=1}^{\infty} k \rho_k(P) = \int_{\Omega} \left| \{x \in \omega \cap [0,1]^d \mid |\mathcal{C}_\omega(x)| = \infty\} \right| P(d\omega) \tag{6.1}$$

is the expected number of particles in $[0,1]^d$ belonging to an infinite cluster. If $\rho(P) - \sum_{k=1}^{\infty} k \rho_k(P) > 0$, it follows right away that with positive probability, there is an infinite cluster. If $\rho(P) - \sum_{k=1}^{\infty} k \rho_k(P) = 0$, using shift-invariance, we see that for every unit cube $C(\mathbf{k})$, $\mathbf{k} \in \mathbb{Z}^d$ (see p. 3) the probability that the cube intercepts an infinite cluster is zero; it follows that the probability that there is an infinite cluster vanishes. \square

7 Percolation properties of Gibbs measures

In this section we prove Theorems 3.5 and 3.6 and Proposition 3.7. The proofs are a combination of results from [17, 24, 18, 14], what is known from cluster expansions [20, 21], and equivalence of ensembles as in [10].

7.1 Grand-canonical ensemble

For the proof of percolation, it is convenient to discretize space. Fix $\ell > 0$. For $\mathbf{k} \in \mathbb{Z}^d$, let $C(\mathbf{k}) := [k_1\ell, (k_1 + 1)\ell) \times \dots \times [k_N\ell, (k_N + 1)\ell)$. Let \mathcal{C} be the collection of cubes $C(\mathbf{k})$, $\mathbf{k} \in \mathbb{Z}^d$. We say that two cubes are nearest neighbors if their centers have Euclidean distance ℓ . A collection $\mathcal{R} \subset \mathcal{C}$ of cubes is *connected* if any two cubes in \mathcal{R} can be joined by a path (C_1, \dots, C_n) of cubes in \mathcal{R} such that for every j , the cubes C_j and C_{j+1} are nearest neighbors. The following lemma is a variant of well-known contour arguments [20, Section 5.3].

Lemma 7.1. *Let P be a probability measure on $\{0, 1\}^{\mathcal{C}}$. There is a constant $\alpha_d > 0$ such that the following holds: if for some $\alpha > \alpha_d$, some $A > 0$, and all connected subsets $\mathcal{R} \subset \mathcal{C}$,*

$$P(\forall C \in \mathcal{R} : \omega_C = 0) \leq A \exp(-\alpha|\mathcal{R}|),$$

then P -almost surely, there is an infinite connected set $\mathcal{W} \subset \mathcal{C}$ such that $\omega_C = 1$ for all $C \in \mathcal{W}$.

Remember the notation $\omega_C = \omega \cap C$. We refer to cubes C with $\omega_C = 0$ as *empty*, and a cube with $\omega_C = 1$ as *occupied*.

Proof of Lemma 7.1. Let \mathcal{F} be the collection of the $(d-1)$ -dimensional closed faces of the cubes in \mathcal{C} . For example, $[0, \ell]^{d-1} \times \{0\} \in \mathcal{F}$. A set $\Gamma \subset \mathcal{F}$ is a *contour* if $\mathbb{R}^d \setminus \cup_{F \in \Gamma} F$ splits into exactly two connected components, one finite (*inside*) and one infinite (*outside*). Let $\text{Int } \Gamma \subset \mathcal{C}$ be the collection of cubes that are inside Γ , and $\partial_{\text{int}} \Gamma \subset \text{Int } \Gamma$ the cubes in the interior of Γ that touch the contour (e.g. for $d = 3$, sharing a face, an edge or a corner), i.e.,

$$\partial_{\text{int}} \Gamma = \{C \in \text{Int } \Gamma \mid \bar{C} \cap \left(\bigcup_{F \in \Gamma} F \right) \neq \emptyset\}.$$

Note that $\partial_{\text{int}} \Gamma$ is connected and $|\partial_{\text{int}} \Gamma| \geq c|\Gamma|$, for a suitable Γ -independent constant c .

Fix $C_0 \in \mathcal{C}$. The number of contours Γ such that $C_0 \in \text{Int } \Gamma$ and $|\Gamma| = n$ can be bounded by $c_1 n^{d/(d-1)} \exp(c_2 n)$, for some d -dependent constants $c_1, c_2 > 0$, see [20, Section 5.3]. It follows that if α is sufficiently large,

$$\sum_{n=0}^{\infty} P\left(\exists \Gamma : |\Gamma| = n, C_0 \in \text{Int } \Gamma, |\partial_{\text{int}} \Gamma| \text{ is empty}\right) < \infty.$$

The Borel-Cantelli lemma shows that P -almost surely, C_0 is enclosed in only finitely many contours with empty boundary $\partial_{\text{int}} \Gamma$. Thus we can pick a cell adjacent from outside to the union of all such contours. This cell cannot be empty, and it cannot be surrounded by another contour with empty boundary. It follows that it must be a member of an infinite connected set of occupied cells. \square

Proof of (2) in Theorem 3.5. Pechersky and Yambartsev [18] proved a similar statement in dimension $d = 2$. We show that their proof can be adapted to $d \geq 2$. Let (r_0, r_1) be as in Assumption 2.1, $-m > \inf_{(r_0, r_1)} v =: -M$ and $\tilde{r}_m \in (r_0, r_1)$ such that $v(\tilde{r}_m) \leq -m$. Since v is continuous in (r_0, r_1) , we can find $\ell, \epsilon, \delta > 0$ such that $\tilde{r}_m = \ell - \epsilon$, $0 < 2\epsilon < \ell$, and $v(r) \leq -m + \delta$ for all $r \in [\ell - 2\epsilon, \ell + 2\epsilon]$. Because of $\tilde{r}_m \geq r_0$, we also know that $v(r) \leq 0$ for all $r \geq \ell - \epsilon$.

We partition \mathbb{R}^d into the cubes $C(\mathbf{k})$ of side-length ℓ , as described before Lemma 7.1. Let $\mathcal{R} \subset \mathcal{C}$ be a finite connected collection of cubes. Set $n := |\mathcal{R}|$. Consider the events $\Omega^0(\mathcal{R})$ that there is no particle in $\Lambda_{\mathcal{R}} := \cup_{C \in \mathcal{R}} C$ and $\Omega^1(\mathcal{R})$ that every cube $C \in \mathcal{R}$ contains exactly one particle, and this particle has distance $< \epsilon$ to the center of the cube.

Choose $L \in \ell\mathbb{N}$ large enough so that $\Lambda_{\mathcal{R}} \subset [-L, L]^d =: \Lambda$ and let $P_{\Lambda} = P_{\beta, \mu, \Lambda | \emptyset}$ be the grand-canonical (β, μ) -Gibbs measure in Λ with free boundary conditions; write $\Xi_{\Lambda} = \Xi_{\Lambda | \emptyset}(\beta, \mu)$ for the associated partition function. Fix an arbitrary numbering C_1, \dots, C_n of the cells of \mathcal{R} and write \mathbf{u}^m for the center of C_m . Note that if \mathcal{R} is connected, each cube has at least one neighbor. We have

$$P_{\Lambda}(\Omega^1(\mathcal{R})) = \frac{1}{\Xi_{\Lambda}} \sum_{k=0}^{\infty} \frac{z^{n+k}}{k!} \int_{B(\mathbf{u}^1, \epsilon)} dx_1 \cdots \int_{B(\mathbf{u}^n, \epsilon)} dx_n \times \int_{(\Lambda \setminus \Lambda_{\mathcal{R}})^k} dy_1 \cdots dy_k e^{-\beta U(x_1, \dots, x_n, y_1, \dots, y_k)}.$$

Because of our choice of ℓ and ϵ , omitting the interaction between y_k 's and x_i 's in the integrand can only decrease the Boltzmann weight. Since in addition for every $\mathbf{x} \in \times_1^n B(\mathbf{u}^i, \epsilon)$

$$U(x_1, \dots, x_n) \leq (-m + \delta)(n - 1),$$

we obtain

$$P_{\Lambda}(\Omega^1(\mathcal{R})) \geq z^n |B(0, \epsilon)|^n e^{\beta(m-\delta)(n-1)} P_{\Lambda}(\Omega^0(\mathcal{R})).$$

The same argument applies to finite volume Gibbs measures with tempered boundary conditions ζ . Eq. (2.3) then shows that the previous inequality holds for every $P \in \mathcal{G}(\beta, \mu)$. It follows that, for every $P \in \mathcal{G}(\beta, \mu)$,

$$P(\Omega^0(\mathcal{R})) \leq \exp\left[-\beta|\mathcal{R}|\left(\mu + \left(1 - \frac{1}{|\mathcal{R}|}\right)(m - \delta) - \beta^{-1} \log |B(0, \epsilon)|\right)\right].$$

Lemma 7.1 applies and shows that if

$$\mu > -m + \delta - \beta^{-1} \log |B(0, \epsilon)| + \beta^{-1} \alpha_d \tag{7.1}$$

then, P -almost surely, there is an infinite connected set of occupied cubes. Since the maximum distance between particles in two adjacent cubes is $\sqrt{d+3} \ell$, it follows

that the particle configuration ω has P -almost surely an infinite R -cluster, for every $R \geq \sqrt{d+3}\ell = \sqrt{d+3}(\tilde{r}_m + \epsilon)$.

To conclude, fix $R > \sqrt{d+3}\tilde{r}_m$. Choose δ, ϵ, ℓ as above, with the additional requirement that $R > \sqrt{d+3}\ell$. Let $\beta(\delta, \epsilon) > (\alpha_d - \log |B(0, \epsilon)|)/\delta$. Then, for every $\beta \geq \beta(\delta, \epsilon)$, every $\mu > -m + 2\delta$, and every $P \in \mathcal{G}(\beta, \mu)$, there is an infinite cluster, P -almost surely. It follows that for sufficiently large β , $\mu_+(\beta; R_m) \leq -m + 2\delta$. Since δ can be chosen arbitrarily small, the proof is complete. \square

Proof of (1) in Theorem 3.5. For $\beta > 0$ and $k \in \mathbb{N}$, define the cluster partition functions

$$Z_k^{\text{cl}}(\beta) := \frac{1}{k!} \int_{(\mathbb{R}^d)^{k-1}} e^{-\beta U(0, x_2, \dots, x_k)} \mathbf{1}(\{0, x_2, \dots, x_k\} \text{ is connected}) dx_2 \dots dx_k$$

and let $R^{\text{cl}}(\beta)$ be the radius of convergence of $\sum_{k=1}^{\infty} z^k Z_k^{\text{cl}}(\beta)$, compare [17, Prop. 3.3]. Let $P \in \mathcal{G}(\beta, \mu)$ be a Gibbs measure that can be obtained as a limit of finite volume, grand canonical Gibbs measures with empty boundary conditions. Suppose that $z < R^{\text{cl}}(\beta)$. Then $P(\text{there is an infinite cluster}) = 0$ [17, Theorem 3.1]. Mürmann’s proof moreover yields, for every cube $\Lambda \subset \mathbb{R}^d$ and all $k \in \mathbb{N}$, the bound

$$\begin{aligned} &P(\exists x \in \omega \cap \Lambda : |\mathcal{C}_\omega(x)| = k) \\ &\leq \frac{z^k}{k!} \int_{(\mathbb{R}^d)^k} e^{-\beta U(x_1, \dots, x_k)} \mathbf{1}(\exists j \in \{1, \dots, k\} : x_j \in \Lambda) dx_1 \dots dx_k \\ &\leq k|\Lambda|z^k Z_k^{\text{cl}}(\beta). \end{aligned}$$

Let $\xi > 0$ be as in the proof of Lemma 5.4. If P is shift-invariant, Eq. (2.5) and Ruelle’s superstability bounds [21] show that

$$\begin{aligned} |\Lambda|P^\circ(|\mathcal{C}_\omega(0)| = k) &= \int_{\Omega} \mathbf{1}(\{x \in \omega \cap \Lambda : |\mathcal{C}_\omega(x)| = k\}) P(d\omega) \\ &= P(\exists x \in \omega \cap \Lambda : |\mathcal{C}_\omega(x)| = k) + O((\xi|\Lambda|)^2) \end{aligned}$$

as $|\Lambda| \rightarrow 0$. It follows that

$$\rho_k(P) \leq z^k Z_k^{\text{cl}}(\beta). \tag{7.2}$$

In order to go from shift-invariant limits of finite volume Gibbs measures to general Gibbs measures, we use the theory of Mayer expansions. It is well-known that for every $\beta > 0$, some strictly positive $R^{\text{May}}(\beta) > 0$, and activities $z = \exp(\beta\mu) < R^{\text{May}}(\beta)$, there is a unique Gibbs measure $P_{\beta, \mu} \in \mathcal{G}(\beta, \mu)$; furthermore, the pressure and the correlation functions admit absolutely convergent expansions in powers of z (with temperature-dependent coefficients) [21, Theorem 5.7]. The measure $P_{\beta, \mu}$ is shift-invariant. Since every finite volume Gibbs measure converges to an infinite volume Gibbs measure, this limit must be $P_{\beta, \mu}$, and we can apply the previous considerations to $P_{\beta, \mu}$. Thus we see that when $z < \min(R^{\text{cl}}(\beta), R^{\text{May}}(\beta))$, there is a unique Gibbs measure. It is shift-invariant, has no infinite cluster (P -almost surely), and satisfies Eq. (7.2).

Next, recall

$$Z_k^{\text{cl}}(\beta) \leq e^{-\beta k e_\infty} e^k |B(0, R)|^{k-1}, \quad R^{\text{May}}(\beta) \geq \frac{\exp(\beta e_\infty)}{\beta |||v|||}$$

where $|||v||| := |B(0, r_{\text{hc}})| + \int_{|x| > r_{\text{hc}}} |v(|x|)| dx$, see [14, Proof of Lemma 4.1] or [17, Proof of Prop. 3.1] for the first inequality and [19, Theorem 2.1] for the second inequality. We deduce

$$\liminf_{\beta \rightarrow \infty} \beta^{-1} \log \min(R^{\text{cl}}(\beta), R^{\text{May}}(\beta)) \geq e_\infty.$$

Since every $\mu_- < \beta^{-1} \log \min(R^{\text{cl}}(\beta), R^{\text{May}}(\beta))$ satisfies condition (3.3), we obtain the desired lower bound on $\mu_-(\beta; R)$. The upper bound (3.4) of $\rho_k(P)$ follows from Eq. (7.2) and the upper bound of $Z_k^{\text{cl}}(\beta)$. \square

7.2 Canonical ensemble

Theorem 3.6 is deduced from Theorem 3.5 with the help of a good control of the density as a function of the chemical potential. Recall that the pressure $p(\beta, \mu) = \sup_{\rho} (\rho\mu - f(\beta, \rho))$ is a convex function of μ . Therefore the derivative $\rho(\beta, \mu) := \partial_{\mu} p(\beta, \mu)$ exists almost everywhere and is an increasing function of μ . Moreover, if $\rho = \rho(\beta, \mu)$, then $\mathcal{G}_{\theta}(\beta, \rho) \subset \mathcal{G}(\beta, \mu)$. If $p(\beta, \mu)$ has different left and right derivatives ρ_l and ρ_r with respect to μ , the previous inclusion holds for every $\rho \in [\rho_l, \rho_r]$.

Proof of (1) in Theorem 3.6. Remember $R^{\text{May}}(\beta)$ and $R^{\text{cl}}(\beta)$ from the proof of (1) in Theorem 3.5. For $\exp(\beta\mu) < R^{\text{May}}(\beta)$, the pressure is differentiable in μ and $\rho(\beta, \mu)$ is well-defined. Fix $\epsilon > 0$ and let $\beta_{\epsilon} > 0$ large enough so that for $\beta \geq \beta_{\epsilon}$, $\exp(\beta[e_{\infty} - \epsilon]) < \min(R^{\text{May}}(\beta), R^{\text{cl}}(\beta))$. For $\beta \geq \beta_{\epsilon}$ and $\rho < \rho(\beta, e_{\infty} - \epsilon)$, we know that $\rho = \rho(\beta, \mu)$ for a unique μ ; for this μ , $\mathcal{G}_{\theta}(\beta, \rho) = \mathcal{G}(\beta, \mu) = \{P\}$ with a unique Gibbs measure P . From the proof of Theorem 3.5, we see that P assigns probability zero to the event that there is an infinite cluster. As a consequence, $\rho_-(\beta; R) \geq \rho(\beta, e_{\infty} - \epsilon)$. Since

$$\lim_{\beta \rightarrow \infty} \beta^{-1} \log \rho(\beta, e_{\infty} - \epsilon) = - \inf_{k \in \mathbb{N}} (E_k - k(e_{\infty} - \epsilon)) \tag{7.3}$$

and $\inf_{\epsilon > 0} \inf_{k \in \mathbb{N}} [E_k - k(e_{\infty} - \epsilon)] = \nu^*$ [13], we deduce $\rho_-(\beta; R) \geq \exp(-\beta\nu^*(1 + o(1)))$.

In addition, if $\nu > \nu^*$ and β is sufficiently large, we see that $\rho = \rho(\beta, \mu)$ for a unique $\mu < \beta^{-1} \log \min(R^{\text{May}}(\beta), R^{\text{cl}}(\beta))$, and the remaining part of Theorem 3.6 follows from the corresponding statement in Theorem 3.5. The claim on the uniformity of the constants stated after Theorem 3.6 follows by combining the inequalities (3.4), (7.2), and (7.3). \square

Proof of (2) in Theorem 3.6. Fix $\epsilon > 0$. By Theorem 3.5, there is a $\beta_{\epsilon} > 0$ such that for every $\beta \geq \beta_{\epsilon}$, $\mu_+(\beta; R_m) \leq -m + \epsilon$. Let $\rho(\beta, -m + \epsilon)$ be the left derivative of $p(\beta, \mu)$ with respect to μ at $\mu = -m/2 + \epsilon$. If $\rho \geq \rho_{\epsilon}(\beta)$, then $\mathcal{G}_{\theta}(\beta, \rho) \subset \mathcal{G}(\beta, \mu)$ for some $\mu \geq -m + \epsilon$. When $\beta \geq \beta_{\epsilon}$, it follows that this μ is larger than $\mu_+(\beta; R_m)$, and Theorem 3.5 tells us that for every $P \in \mathcal{G}_{\theta}(\beta, \rho) \subset \mathcal{G}(\beta, \mu)$, there is an infinite cluster, P -almost surely. Thus $\rho_+(\beta; R_m) \leq \rho(\beta, -m + \epsilon)$ and $\liminf_{\beta \rightarrow \infty} \rho_+(\beta, \mu) \leq \rho_m$. \square

Proof of Prop. 3.7. Prop. 3.7 is a consequence of Theorem 1.8 in [14] and our Theorem 3.2: the result from [14] says that the bound of our proposition holds for every minimizer $(\rho_k)_{k \in \mathbb{N}}$ of $f(\beta, \rho, \cdot)$, and Theorem 3.2 says that for every $P \in \mathcal{G}_{\theta}(\beta, \rho)$, the vector $(\rho_k(P))_{k \in \mathbb{N}}$ is a minimizer of $f(\beta, \rho, \cdot)$. \square

A Lattice gas and Ising model

Here we explain how our results relate to known results for lattice systems. We shall be very sketchy and refer the reader to to the review [11] and the references therein for precise definitions and proofs.

Consider the nearest neighbor lattice gas in \mathbb{Z}^d ($d \geq 2$) with hard-core on-site interaction and attractive nearest-neighbor interaction. As is well-known, this model can be recast as an Ising model. Occupied lattice sites ($n_x = 1$) are mapped to spin $\sigma_x = +1$ and empty lattice sites ($n_x = 0$) to spin $\sigma_x = -1$; thus $\sigma_x = 2n_x - 1$. Formally, we have

$$-\frac{J}{2} \sum_{|x-y|=1} n_x n_y - \mu \sum_x n_x = -\frac{J}{8} \sum_{|x-y|=1} \sigma_x \sigma_y - \frac{dJ + \mu}{2} \sum_x \sigma_x + \text{const},$$

which determines the external magnetic field h of the Ising model in terms of the chemical potential μ of the lattice gas as $h = (\mu + dJ)/2$. The parameter $J > 0$ measures both the strength of attraction between particles and the strength of the ferromagnetic coupling between spins.

The relevant notion of percolation is *dependent site percolation*. *Dependent* refers to the underlying measure on $\{0, 1\}^{\mathbb{Z}^d}$, which is a Gibbs measure rather than a product of Bernoulli measures, and *site percolation* refers to the notion of connectivity – two occupied lattice sites $x, y \in \mathbb{Z}^d$ are connected if there is a path (x_1, \dots, x_n) of nearest neighbor ($|x_{j+1} - x_j| = 1$) joining $x_1 = x$ and $x_n = y$, such that each site of the path is occupied, $n_{x_j} = 1$. The Ising analogue of the problem studied in this article is *percolation of +clusters*.

Our first remark is that at low temperature, the phase transition and the percolation transition coincide; this observation, as alluded to in the introduction, is the driving motivation for the present article's investigation. Fix a temperature $T > 0$ and vary the external field h (or the chemical potential μ). At temperatures above the *Curie temperature* $T_C > 0$, there is no phase transition (the pressure stays analytic and the Gibbs measure is unique); at $T < T_C$, there is a first-order phase transition at $h = 0$. On the other hand, let $P_{T,h}^+$ be the Gibbs measure with + boundary conditions. We know that for all $T > 0$, there is a threshold $h(T) \in \mathbb{R}$ such that the $P_{T,h}^+$ -probability of having an infinite cluster is 0 at external fields $h < h(T)$, and 1 at fields $h > h(T)$. Furthermore, there is a temperature $T_+ > 0$ such that $h(T) = 0$ for $T < T_+$ and $h(T) < 0$ for $T > T_+$ [1], and it is known that $T_+ < T_C$ in high dimensions. Thus at temperatures above the Curie temperature, there is a percolation transition but no phase transition; at temperatures between T_+ and T_C , as h is increased, the percolation transition happens *before* the phase transition; and below T_+ , the percolation transition coincides with the phase transition.

The next observation is that the value at which the transition takes place is consistent with our grand-canonical Theorem 3.5: indeed, the zero external field $h = 0$ corresponds, in the lattice gas picture, to a chemical potential $\mu = -dJ$, which can be interpreted as a ground state energy per particle – if in \mathbb{Z}^d every lattice site is occupied, the energy per particle is $e_\infty = -dJ$.

Finally, this agreement of thresholds extends to the canonical ensemble. At $T < T_C$ and external field $h = 0$, there are two shift-invariant Gibbs measures $P_{T,h}^\pm$, with magnetizations $m_\pm(T)$. Low temperature contour expansions show that as $T \rightarrow 0$, $m_\pm(T) = \pm 1 + O(\exp(-J/T))$. Transforming as $\rho_\pm(T) = (m_\pm(T) + 1)/2$, we obtain that the corresponding curves for the lattice gas satisfy $\rho_-(T) = O(\exp(-J/T))$ and $\rho_+(T) = 1 + O(\exp(-J/T))$, which compares nicely with Theorem 3.6: for $T < T_+$, the magnetizations $m_\pm(T)$ of the Ising model are also percolation thresholds (this is not true for $T_+ < T < T_C$).

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