Large deviations and the equivalence of ensembles for Gibbsian particle systems with superstable interaction

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Summary. For Gibbsian systems of particles in $\mathbf{R}^d$, we investigate large deviations of the stationary empirical fields in increasing boxes. The particle interaction is given by a superstable, regular pair potential. The large deviation principle is established for systems with free or periodic boundary conditions and, under a stronger stability hypothesis on the potential, for systems with tempered boundary conditions, and for tempered (infinite-volume) Gibbs measures. As a by-product we obtain the Gibbs variational formula for the pressure. We also prove the asymptotic equivalence of microcanonical and grand canonical Gibbs distributions and establish a variational expression for the thermodynamic entropy density.

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1 Introduction

One of the classical themes of Equilibrium Statistical Mechanics is the study of the fluctuations of extensive quantities, such as the particle numbers and the energies of particle configurations in finite boxes, in the infinite-volume limit. This includes the problems of existence and variational characterization of the pressure, and of the asymptotic equivalence of the Gibbs ensembles (on the level of measures). Whereas these questions are fairly well understood in the case of lattice systems (see [2] and the references therein), the situation is less satisfactory in the case of continuous systems of particles in Euclidean space. In this paper we develop a large deviation theory for such particle systems, with the aim of contributing to a systematic study of the questions above.

The general setting is as follows. We consider the Euclidean space $\mathbf{R}^d$ of any dimension $d \geq 1$. A configuration of particles (without multiple occupancies) is described by a locally finite subset ω of $\mathbf{R}^d$, i.e., a set $\omega \subset \mathbf{R}^d$ having finite intersection with every bounded set. We write Ω for the set of all such configurations ω. Ω is equipped with the σ-algebra $\mathcal{F}$ generated by the counting variables $N_B : \omega \to \mathrm{card}(\omega \cap B)$ for Borel subsets B of $\mathbf{R}^d$. It is well-known [4, 5] that $\mathcal{F}$ is the Borel σ-algebra for a natural Polish toplogy on Ω. The translation group $\Theta = (\vartheta_x)_{x \in \mathbf{R}^d}$ acting on $(\Omega, \mathcal{F})$ is defined by $\vartheta_x \omega = \{y - x : y \in \omega\}$, $\omega \in \Omega$, $x \in \mathbf{R}^d$. The mapping $(x, \omega) \to \vartheta_x \omega$ is known to be measurable [5]. We let $\mathcal{P}$ denote the set of all probability measures P on $(\Omega, \mathcal{F})$ with finite expected particle numbers $P(N_\Delta) \equiv \int N_\Delta dP$ in bounded Borel sets $\Delta \subset \mathbf{R}^d$, and we write $\mathcal{P}_\Theta$ for the set of all Θ-invariant $P \in \mathcal{P}$. For each $P \in \mathcal{P}_\Theta$ there exists a number $\rho(P) < \infty$, the *intensity* of P, such that $P(N_\Delta) = \rho(P)\,|\Delta|$ for all Borel sets Δ. Here $|\Delta|$ is the Lebesgue measure of Δ.

We introduce a topology $\tau_\mathcal{L}$ on $\mathcal{P}$ as follows. Let $\mathcal{L}$ denote the class of all measurable functions $f : \Omega \to \mathbf{R}$ which are *local*, in that $f(\omega) = f(\omega \cap \Delta)$ for some bounded Borel set Δ and all $\omega \in \Omega$, and *tame*, in that $|f| \le c(1 + N_\Delta)$ for (without loss the same) Δ and some constant $c < \infty$. The *topology* $\tau_\mathcal{L}$ *of local convergence* is then defined as the weak* topology on $\mathcal{P}$ relative to $\mathcal{L}$, i.e., as the smallest topology on $\mathcal{P}$ making the mappings $P \to P(f) \equiv \int f\,dP$ continuous. In particular, the mappings $P \to P(N_\Delta)$ for bounded Borel sets Δ are continuous relative to $\tau_\mathcal{L}$. This shows that $\tau_\mathcal{L}$ is much finer than the usual weak topology on $\mathcal{P}$ which is based on the above-mentioned Polish toplogy on Ω.

For each $n \ge 0$, we consider the half-open cube $\Lambda_n = [-n - \frac{1}{2}, n + \frac{1}{2}[^d$ of volume $v_n = (2n+1)^d$ and the associated *invariant empirical field*

$$R_{n,\omega} = v_n^{-1} \int_{\Lambda_n} \delta_{\vartheta_x \omega^{(n)}}\, dx \tag{1.1}$$

of any configuration $\omega \in \Omega$. In (1.1), we replaced ω by the Λ_n-periodic continuation

$$\omega^{(n)} = \{x + (2n+1)i : x \in \omega \cap \Lambda_n,\ i \in \mathbf{Z}^d\}$$

of its restriction to Λ_n. This has the advantage of making $R_{n,\omega}$ translation invariant. Thus $R_{n,\omega} \in \mathcal{P}_\Theta$ for all n and ω. If $\mathcal{P}_\Theta$ is equipped with the evaluation σ-algebra generated by the maps $P \to P(A)$, $A \in \mathcal{F}$, the random measure $R_n : \omega \to R_{n,\omega}$ becomes a measurable mapping from Ω to $\mathcal{P}_\Theta$. The asymptotic behavior of the empirical fields can be described as follows: For each $P \in \mathcal{P}_\Theta$,

$$\tau_\mathcal{L}\text{ - }\lim_{n\to\infty} R_n = P_\mathcal{I}^{\cdot} \qquad \text{in } P\text{-probability}, \tag{1.2}$$

where $\omega \to P_\mathcal{I}^\omega$ is a regular conditional probability of P relative to the σ-algebra $\mathcal{I}$ of Θ-invariant sets in $\mathcal{F}$. This follows immediately from Wiener's multidimensional mean ergodic theorem, cf. [4].

In this paper we study large deviations from the ergodic theorem (1.2) when P is Gibbsian relative to a suitable pair interaction φ. More precisely, we establish a large deviation principle for R_n when the particles are distributed according to a Gibbs distribution in Λ_n with free or periodic boundary condition and the underlying potential φ is superstable and satisfies a decay condition called regularity (see Theorem 2). Under the stronger hypothesis that φ diverges at the origin sufficiently fast, we obtain a uniform large deviation principle relative to Gibbs distributions with boundary configurations $\zeta \in \Omega$ satisfying a uniform condition of temperedness (Theorem 3(a)). By virtue of the well-known superstability estimates of Ruelle [9], this leads to a large deviation principle for tempered Gibbs measures on $(\Omega, \mathcal{F})$ (Theorem 3(b)). The rate function is, of course, given by the excess of the free energy density over its equilibrium value; the latter is given by the pressure. A basic ingredient of all this is the existence and lower semicontinuity of the (internal) energy density (Theorem 1). Finally, we prove a limit theorem for conditional Poisson distributions of microcanonical type, implying the equivalence of Gibbs ensembles on the level of measures (Theorem 4). This is an instance of the maximum entropy principle and is closely related to a (microcanonical) Gibbs variational formula for the thermodynamic entropy density.

In the Poissonian case of no interaction, the analoguous results were obtained earlier in [4]. Our results here rely heavily on this paper. A weak version of a large deviation principle for particles with superstable interaction of finite range is also contained in [6]. The case of particles with hard core (which is contained in the present work) was already treated in [3].

2 Statement of results

We begin describing the particle interactions which we will consider. We assume, for simplicity, that the interaction is only pairwise and thus given by an even measurable function $\varphi : \mathbf{R}^d \to \mathbf{R} \cup \{\infty\}$. Such a φ is called a *potential*. For each $n \geq 0$,

$$H_n(\omega) \equiv H_{n,\mathrm{free}}(\omega) = \tfrac{1}{2} \sum_{x,y \in \omega \cap \Lambda_n, x \neq y} \varphi(y-x)\,, \qquad \omega \in \Omega, \tag{2.1}$$

is called the associated *Hamiltonian* in Λ_n with *free boundary condition.* A potential φ is said to be *stable* if there exists a constant $b = b(\varphi) < \infty$ such that

$$H_n \geq -bN_n \qquad \text{for all } n \geq 0. \tag{2.2}$$

Here $N_n = N_{\Lambda_n}$. In particular, (2.2) implies that $\varphi \geq -2b$. Sufficient conditions for φ to be stable can be found in [8] . Let us say that φ is *purely repulsive* if φ is nonnegative and bounded away from zero near the origin, i.e., if there exists some $\delta = \delta(\varphi) > 0$ such that

$$\varphi \geq \delta\, 1_{\{|\cdot| \leq \delta\}}. \tag{2.3}$$

Here and below, $|\cdot|$ stands for the maximum norm on $\mathbf{R}^d$. A potential φ is called *superstable* if

$$\varphi = \varphi^s + \varphi^r \tag{2.4}$$

for a stable φ^s and a purely repulsive φ^r. The use of this concept was revealed by the pioneering work of Ruelle [7, 9].

Besides the hypothesis of superstability which assures that large particle numbers in a bounded region require a large amount of energy we shall also need a condition on the decay of φ. A potential φ is called *lower regular* if there exists a decreasing function $\psi : [0,\infty[\to [0,\infty[$ such that

$$\varphi(x) \geq -\psi(|x|) \qquad \text{for all } x \in \mathbf{R}^d \tag{2.5}$$

and

$$\int_0^\infty \psi(s) s^{d-1} ds < \infty. \tag{2.6}$$

φ will be called *regular* if φ is lower regular and, in addition, there exists some $r(\varphi) < \infty$ such that

$$\varphi(x) \leq \psi(|x|) \qquad \text{whenever } |x| \geq r(\varphi). \tag{2.7}$$

Our first result is the existence of the energy density of any $P \in \mathcal{P}_\Theta$. To state it we need to recall that the *Palm measure* of $P \in \mathcal{P}_\Theta$ is defined as the unique finite measure P° on $(\Omega, \mathcal{F})$ satisfying

$$\int P(d\omega) \sum_{x \in \omega} f(x, \vartheta_x \omega) = \int dx \int P^\circ(d\omega)\, f(x, \omega) \tag{2.8}$$

for all measurable functions $f : \mathbf{R}^d \times \Omega \to [0, \infty[$. We have $P^\circ(\Omega) = P^\circ(\{\omega \in \Omega : \omega \ni 0\}) = \rho(P)$, and the normalized Palm measure $\rho(P)^{-1} P^\circ$ can be viewed as the natural version of the conditional probability $P(\,\cdot\,|\{\omega \in \Omega : \omega \ni 0\})$; see [5] for more details. Let us introduce the set

$$\mathcal{P}_\Theta^{(2)} = \{P \in \mathcal{P}_\Theta : P(N_\Delta^2) < \infty \text{ for all bounded Borel sets } \Delta\} \tag{2.9}$$

of all second-order elements of $\mathcal{P}_\Theta$. For each $n \geq 0$ and $P \in \mathcal{P}_\Theta$ we let

$$\Phi_n(P) = v_n^{-1}\, P(H_n), \tag{2.10}$$

be the expected φ-energy per volume in Λ_n. In view of (2.2), Φ_n is well-defined (possibly equal to $+\infty$), and $\Phi_n \geq -b\rho$. In Section 3 we shall prove the following.

Theorem 1 *Suppose φ is superstable and lower regular. Then, for each $P \in \mathcal{P}_\Theta$, the limit $\Phi(P) = \lim_{n\to\infty} \Phi_n(P)$ exists and satisfies*

$$\Phi(P) = \begin{cases} P^\circ(f_\varphi) & \text{if } P \in \mathcal{P}_\Theta^{(2)} \\ \infty & \text{otherwise,} \end{cases} \tag{2.11}$$

where

$$f_\varphi(\omega) = \tfrac{1}{2} \sum_{0 \neq y \in \omega} \varphi(y)\,, \qquad \omega \in \Omega. \tag{2.12}$$

Moreover, the function $\Phi : \mathcal{P}_\Theta \to \mathbf{R} \cup \{\infty\}$ is lower semicontinuous (relative to $\tau_\mathcal{L}$).

$\Phi(P)$ is called the *energy density* of P. It is clear that Φ is affine. To state our large deviation results we next need to introduce the entropy density. We let $Q \in \mathcal{P}_\Theta$ denote the Poisson point random field on $\mathbf{R}^d$ with intensity $\rho(Q) = 1$. For each $P \in \mathcal{P}_\Theta$ and $n \geq 0$ we write

$$P_n = P(\{\omega \in \Omega : \omega \cap \Lambda_n \in \cdot\,\})$$

for the restriction of P to Λ_n. We think of P_n as an element of $\mathcal{P}$ which is supported on $\Omega_n = \{\omega \in \Omega : \omega \subset \Lambda_n\}$. The negative *entropy density* of P is then defined as the (existing) limit

$$I(P) = \lim_{n\to\infty} v_n^{-1}\, I(P_n; Q_n), \tag{2.13}$$

where $I(\,\cdot\,;\,\cdot\,)$ stands for the relative entropy; see [4] for more details. I is an affine function with $\tau_\mathcal{L}$-compact level sets [4].

Suppose now we are given an inverse temperature $\beta > 0$ and an activity $z > 0$. (Later on, we shall assume without loss that the units are chosen so that $\beta = z = 1$.) The *excess free energy density* of $P \in \mathcal{P}_\Theta$ is then given by

$$I_{z,\beta}(P) = I(P) + \beta\Phi(P) - \rho(P)\,\log z + p(z,\beta), \tag{2.14}$$

where

$$p(z,\beta) = -\min[I + \beta\Phi - \rho \log z]. \tag{2.15}$$

Theorem 2 below asserts that $p(z,\beta)$ is nothing other than (β times) the pressure, and $I_{z,\beta}$ is the rate function in a large deviation principle for the distribution of the empirical fields R_n under the Gibbs distributions with free or periodic boundary conditions. (Configurational boundary conditions will be considered later in Theorem 3.)

For $n \geq 0$, the *Hamiltonian* in Λ_n with *periodic boundary condition* is defined by

$$\begin{aligned} H_{n,\mathrm{per}}(\omega) &= v_n \Phi(R_{n,\omega}) \\ &= \tfrac{1}{2} \sum_{x\in\omega\cap\Lambda_n, y\in\omega^{(n)}, y\neq x} \varphi(y-x). \end{aligned} \tag{2.16}$$

The last equation follows from (2.11) and the easily verified fact that the Palm measure of $R_{n,\omega}$ is given by

$$R^\circ_{n,\omega} = v_n^{-1} \sum_{x\in\omega\cap\Lambda_n} \delta_{\vartheta_x \omega^{(n)}}, \tag{2.17}$$

cf. [4]. For a given boundary condition bc $\in$ {per, free}, the associated *Gibbs distribution* in Λ_n with parameters $z,\beta > 0$ is defined by

$$P_{n,z,\beta,\mathrm{bc}}(d\omega) = Z^{-1}_{n,z,\beta,\mathrm{bc}}\, z^{N_n(\omega)} \exp\left[-\beta H_{n,\mathrm{bc}}(\omega)\right] \, Q_n(d\omega), \tag{2.18}$$

where

$$Z_{n,z,\beta,\mathrm{bc}} = Q_n(z^{N_n} \exp[-\beta H_{n,\mathrm{bc}}]) \tag{2.19}$$

is the so-called partition function. It follows from (2.2) resp. Theorem 1 and (3.3) below that $Z_{n,z,\beta,\mathrm{bc}}$ is finite. Thus $P_{n,z,\beta,\mathrm{bc}}$ is well-defined. Again, we think of it as an element of $\mathcal{P}$ with support Ω_n.

Theorem 2 *Let φ be superstable and regular, $z,\beta > 0$, and $F : \mathcal{P}_\Theta \to \mathbf{R} \cup \{\infty\}$ a measurable functional satisfying $F \geq -c(1+\rho)$ for some $c < \infty$. Then, for* bc = per *or* free,

$$\limsup_{n\to\infty} v_n^{-1} \log P_{n,z,\beta,\mathrm{bc}}(e^{-v_n F(R_n)}) \leq -\inf[I_{z,\beta} + F_{\mathrm{lsc}}] \tag{2.20}$$

and

$$\liminf_{n\to\infty} v_n^{-1} \log P_{n,z,\beta,\mathrm{bc}}(e^{-v_n F(R_n)}) \geq -\inf[I_{z,\beta} + F^{\mathrm{usc}}], \tag{2.21}$$

where F_{lsc} is the largest lower semicontinuous minorant and F^{usc} the lowest upper semicontinuous majorant of F relative to $\tau_{\mathcal{L}}$. In addition, $I_{z,\beta}$ has $\tau_{\mathcal{L}}$-compact level sets, and

$$p(z,\beta) = \lim_{n\to\infty} v_n^{-1} \log Z_{n,z,\beta,\mathrm{bc}}. \tag{2.22}$$

Note that (2.20) and (2.21) take the familiar form of a large deviation principle when F is chosen to be zero on some measurable set $A \subset \mathcal{P}_\Theta$ and equal to $+\infty$ outside A. The existence of the limit in (2.22) is the classical result on the existence of the pressure, cf. [7, 8, 9]. Its coincidence with (2.15) is called the Gibbs variational formula. The upper bound (2.20) will be proved in Section 4 and the lower bound (2.21) in Section 5.

We now turn to large deviations for Gibbs distributions with configurational boundary conditions, and for infinite-volume Gibbs measures. We need some notations. Let $C = [-\frac{1}{2}, \frac{1}{2}[^d = \Lambda_0$ be the centered half-open unit cube and $L = \mathbf{Z}^d$. The sets $C+i, i \in L$, form a partition of $\mathbf{R}^d$. For $n \geq 0$ we set $L_n = L \cap \Lambda_n = \{i \in L : |i| \leq n\}$ and

$$T_n = \sum_{i \in L_n} N_{C+i}^2 \quad . \tag{2.23}$$

For $t > 0$ we define

$$\Omega(t) = \{T_n \leq t v_n \text{ for all } n \geq 0\}. \tag{2.24}$$

The configurations in $\Omega^\star = \bigcup_{t>0} \Omega(t)$ are called *tempered*. The multidimensional ergodic theorem shows that $P(\Omega^\star) = 1$ for all $P \in \mathcal{P}_\Theta^{(2)}$.

For each $\zeta \in \Omega^\star$ and $n \geq 0$ we let

$$H_{n,\zeta}(\omega) = H_n(\omega) + \sum_{x \in \omega \cap \Lambda_n, y \in \zeta \setminus \Lambda_n} \varphi(y - x) \tag{2.25}$$

denote the Hamiltonian in Λ_n with *boundary condition* ζ. The associated Gibbs distributions $P_{n,z,\beta,\zeta}$ are defined by (2.18) with bc $= \zeta$. By Lemma 4.2, the last sum in (2.25) exists when φ is regular. Under the hypothesis (2.26) below, Lemma 6.1 and the estimates in the proof of Lemma 6.3 even imply that $Z_{n,z,\beta,\zeta} < \infty$, so that $P_{n,z,\beta,\zeta}$ is well-defined.

A measure $P \in \mathcal{P}$ is called a *tempered Gibbs measure* for $z, \beta > 0$ if $P(\Omega^\star) = 1$ and, for all $n \geq 0$ and measurable functions $f \geq 0$ on Ω,

$$P(f) = \int P(d\zeta) \int P_{n,z,\beta,\zeta}(d\omega) f(\omega \cup (\zeta \setminus \Lambda_n)).$$

Note that the identity above is equivalent to the equilibrium equations in [9]. The following theorem provides a uniform large deviation principle for Gibbs distributions with (uniformly) tempered boundary conditions, and a large deviation principle for tempered Gibbs measures. Its proof will be given in Section 6.

Theorem 3 *Suppose φ is regular and strongly repulsive in the sense that*

$$\varphi(x)|x|^d \to \infty \qquad \text{as } |x| \to 0. \tag{2.26}$$

Also, let F be as in Theorem 2 and $z, \beta > 0$.

(a) *For each $t > 0$, we have*

$$\limsup_{n\to\infty} v_n^{-1} \log \sup_{\zeta \in \Omega(t)} P_{n,z,\beta,\zeta}(e^{-v_n F(R_n)}) \leq -\inf[I_{z,\beta} + F_{\rm lsc}] \tag{2.27}$$

and

$$\liminf_{n\to\infty} v_n^{-1} \log \inf_{\zeta \in \Omega(t)} P_{n,z,\beta,\zeta}(e^{-v_n F(R_n)}) \geq -\inf[I_{z,\beta} + F^{\rm usc}]. \tag{2.28}$$

Moreover, (2.22) holds with bc $= \zeta$ *uniformly for all $\zeta \in \Omega(t)$.*

(b) *Each tempered Gibbs measure P with parameters z, β satisfies a large deviation principle for R_n with rate function $I_{z,\beta}$, in that inequalities (2.20) and (2.21) hold with P instead of $P_{n,z,\beta,\rm bc}$.*

We note that hypothesis (2.26), together with the lower regularity of φ, implies that φ is superstable; see Proposition 3.2.8 of [8]. (2.26) holds in particular when φ has a hard core. We also note that an application of the contraction principle to Theorems 2 and 3 leads to analoguous large deviation principles for the individual empirical fields R_n° in (2.17); see [4] for more details.

Our last result is a version of the equivalence of ensembles. For any non-degenerate interval $D \subset [0,\infty[$ and real ε we consider the *microcanonical Gibbs distribution*

$$\begin{aligned} Q_{n|D,\varepsilon,\mathrm{per}} &\equiv Q_n\left(\,\cdot\,|N_n \in v_n D, H_{n,\mathrm{per}} \le v_n\varepsilon\right) \\ &= Q_n\left(\,\cdot\,|\rho(R_n)\in D, \Phi(R_n)\le\varepsilon\right) \end{aligned} \tag{2.29}$$

in Λ_n with periodic boundary condition. As we will see, the conditioning event has positive probability for all sufficiciently large n whenever $\varepsilon > \inf\phi(D)$. Here $\phi : [0,\infty[\to \mathbf{R}\cup\{\infty\}$ is defined by

$$\phi(\nu) = \inf\{\Phi(P) : P \in \mathcal{P}_\Theta,\, \rho(P)=\nu,\, I(P)<\infty\}. \tag{2.30}$$

Since Φ, ρ and I are affine, ϕ is convex. ϕ is finite on an interval $[0,\nu(\varphi)[$, where $\nu(\varphi)=\infty$ except when φ has a hard core, see Lemma 7.1. Intuitively, $\nu(\varphi)$ is the close-packing density of $\{\varphi=\infty\}$-balls.

We write $\mathrm{acc}_{n\to\infty}P^{(n)}$ for the set of all accumulation points (relative to $\tau_{\mathcal{L}}$) of a sequence $P^{(n)}$ in $\mathcal{P}$.

Theorem 4 *Suppose φ is superstable and regular, let $D\subset[0,\infty[$ be a non-degenerate interval with $\inf D < \nu(\varphi)$, and $\varepsilon > \inf\phi(D)$. Then there exists some $\beta\ge 0$ and $z>0$ such that*

$$\emptyset \ne \operatorname*{acc}_{n\to\infty} Q_{n|D,\varepsilon,\mathrm{per}} \subset \{\, I_{z,\beta}=0\} \supset \operatorname*{acc}_{n\to\infty} P_{n,z,\beta,\mathrm{per}} \ne \emptyset. \tag{2.31}$$

In particular, if $\{I_{z,\beta}=0\}$ consists of a unique element $P_{z,\beta}$ then

$$\lim_{n\to\infty} Q_{n|D,\varepsilon,\mathrm{per}} = \lim_{n\to\infty} P_{n,z,\beta,\mathrm{per}} = P_{z,\beta}.$$

Moreover,

$$\begin{aligned} \lim_{n\to\infty}\quad & v_n^{-1}\log Q_n(N_n\in v_nD, H_{n,\mathrm{per}}\le v_n\varepsilon) \\ &= -\inf\{I(P) : P\in\mathcal{P}_\Theta, \rho(P)\in D, \Phi(P)\le\varepsilon\}. \end{aligned} \tag{2.32}$$

If $\varepsilon<\inf\phi(D)$ or $\inf D>\nu(\varphi)$ the limit in (2.32) equals $-\infty$.

(2.31) expresses the asymptotic equivalence of microcanonical and grandcanonical Gibbs distributions. (2.32) is an analogue of the classical existence result for the thermodynomic entropy density, cf. [8]. The difference here is that the particle number is not fixed but ranges in a whole interval, and that we use periodic boundary conditions. In addition, (2.32) provides a microcanonical Gibbs variational formula. The proof of Theorem 4 will be given in Section 7 which also contains some additional information on the involved functions. With the same techniques, one can derive the asymptotic equivalence of small canonical and grand canonical ensembles. In addition, an obvious extension of Lemma 7.2 in the spirit of Sections 4 and 5 leads to a large deviation principle for the empirical fields R_n under the microcanonical distributions $Q_{n|D,\varepsilon,\mathrm{per}}$. We leave this to the reader.

3 The energy density

In this section we prove Theorem 1. We begin with some basic estimates. For $P \in \mathcal{P}_\Theta$ we set $\rho^{(2)}(P) = P(N_C^2)$, where again $C = \Lambda_0$ is the centered half-open unit cube. Since

$$N_\Delta^2 \leq m \sum_{j=1}^m N_{\Delta_j}^2 \qquad \text{when} \quad \Delta \subset \bigcup_{j=1}^m \Delta_j, \tag{3.1}$$

$\rho^{(2)}(P) < \infty$ if and only if $P \in \mathcal{P}_\Theta^{(2)}$, cf. (2.9).

Suppose now we are given a superstable lower regular potential φ. The presence of the purely repulsive part φ^r of φ implies that, for fixed n, H_n tends to infinity quadratically as $N_n \to \infty$. This is asserted in our first lemma. Recall the definitions (2.23) and (2.10) of T_n and Φ_n.

Lemma 3.1 *There exist constants $a > 0$, $b < \infty$ such that for each $n \geq 0$*

$$H_n \geq a\,T_n - b\,N_n \tag{3.2}$$

and

$$\Phi_n \geq a\,\rho^{(2)} - b\,\rho. \tag{3.3}$$

Proof. (3.2) follows from (2.4), (2.2) and (2.3) by partitioning Λ_n into $k^d\,v_n$ half-open cubes Δ_j of size $1/k$ (where k is the smallest integer exceeding $1/\delta$ for the number δ in (2.3)), and applying (3.1) with $\Delta = C{+}i, i \in L_n$, and $m = k^d$. (One can take $a = \delta/2k^d$. b exceeds the constant in (2.2) by $\delta/2$.) (3.3) follows from (3.2) by integration. $\square$

As a consequence of (3.3), if $P \notin \mathcal{P}_\Theta^{(2)}$ then $\Phi_n(P) = \infty$ for all $n \geq 0$ and thus $\lim_{n\to\infty} \Phi_n(P) = \infty$. To prove Theorem 1 we can therefore assume that $P \in \mathcal{P}_\Theta^{(2)}$. In this case, $\Phi_n(P)$ admits a convenient description in terms of the Palm measure P° of P.

Lemma 3.2 *For all $P \in \mathcal{P}_\Theta^{(2)}$ and $n \geq 0$ we have $\Phi_n(P) = P^\circ(f_{\varphi,n})$, where*

$$f_{\varphi,n}(\omega) = \tfrac{1}{2} \sum_{0 \neq y \in \omega} \varphi(y)\,|\Lambda_n \cap (\Lambda_n - y)|/v_n, \qquad \omega \in \Omega.$$

Proof. Consider the (measurable) function

$$f_n(x,\omega) = \tfrac{1}{2} \sum_{0 \neq y \in \omega} \varphi(y) 1_{\Lambda_n \cap (\Lambda_n - y)}(x),$$

$x \in \mathbf{R}^d, \omega \in \Omega$. Since $\varphi \geq -2b$, $f_n(x,\omega) \geq -b 1_{\Lambda_n}(x) N_n(\vartheta_{-x}\omega)$. Also,

$$\int P^\circ(d\omega) \int dx\; 1_{\Lambda_n}(x) N_n(\vartheta_{-x}\omega) = P(N_n^2) < \infty$$

for all $P \in \mathcal{P}_\Theta^{(2)}$, by (2.8). Equation (2.8) therefore also holds for $f = f_n$. But for $f = f_n$, the left-hand side of (2.8) coincides with $\Phi_n(P)$ and the right-hand side with $P^\circ(f_{\varphi,n})$. $\square$

Since $|\Lambda_n \cap (\Lambda_n - y)|/v_n \to 1$ as $n \to \infty$, it is natural to expect that $P^\circ(f_{\varphi,n}) \to P^\circ(f_\varphi)$, which will give us the first assertion of Theorem 1. To make this rigorous we need the lower regularity of φ. Let again $L = \mathbf{Z}^d$ and, for each $i \in L$,

$$\psi_i = \psi(\, d(C, C+i)\,), \tag{3.4}$$

where $d(C, C+i) = (|i|-1)_+$ is the distance of C and $C+i$. Hypothesis (2.6) implies that $\sum_{i \in L} \psi_i < \infty$. Moreover,

$$f_\varphi \geq -\tfrac{1}{2} \sum_{i \in L} \psi_i \, N_{C+i}\,, \tag{3.5}$$

and the function on the right-hand side is P°-integrable for all $P \in \mathcal{P}_\Theta^{(2)}$ because for all $i \in L$

$$\begin{aligned} P^\circ(N_{C+i}) &= \int P(d\omega) \sum_{x \in \omega \cap C} N_{C+i}(\vartheta_x \omega) \\ &\leq P(N_C N_{\Lambda_1 + i}) \leq P(N_C^2)^{1/2}\, P(N_{\Lambda_1}^2)^{1/2} \\ &\leq 3^d \, \rho^{(2)}(P). \end{aligned} \tag{3.6}$$

In the last step we used (3.1). It follows that $\Phi(P) \equiv P^\circ(f_\varphi)$ is well-defined for all $P \in \mathcal{P}_\Theta^{(2)}$. We now compare $\Phi(P)$ with $\Phi_n(P)$.

Lemma 3.3 *There exists a sequence $\epsilon_n \to 0$ such that for all $P \in \mathcal{P}_\Theta^{(2)}$ and $n \geq 0$,*

$$\Phi(P) \geq \Phi_n(P) - \epsilon_n \, \rho^{(2)}(P).$$

Proof. Let $P \in \mathcal{P}_\Theta^{(2)}$ and $n \geq 0$ be given. Since $|\Lambda_n \cap (\Lambda_n - y)|/v_n \leq 1$, (2.5) and Lemma 3.2 imply that $\Phi(P) \geq \Phi_n(P) - \epsilon_n(P)$, where

$$\epsilon_n(P) = \tfrac{1}{2} \int P^\circ(d\omega) \sum_{0 \neq y \in \omega} \psi(y)\, |\Lambda_n \setminus (\Lambda_n - y)|/v_n.$$

Distinguishing the cubes $C + i$ containing y, we conclude from (3.4) and (3.6) that $\epsilon_n(P) \leq \epsilon_n \, \rho^{(2)}(P)$, where

$$\epsilon_n = \tfrac{1}{2}\, 3^d \sum_{i \in L} \psi_i \max_{y \in C+i} |\Lambda_n \setminus (\Lambda_n - y)|/v_n.$$

But the dominated convergence theorem shows that $\epsilon_n \to 0$ as $n \to \infty$. □

Proof of Theorem 1. We first show that, for all $P \in \mathcal{P}_\Theta$, $\lim_{n\to\infty} \Phi_n(P)$ exists and has the claimed value. The case $P \notin \mathcal{P}_\Theta^{(2)}$ was already discussed after Lemma 3.1. For $P \in \mathcal{P}_\Theta^{(2)}$, Lemma 3.2 and Fatou's lemma imply that

$$\Phi(P) = P(\liminf_{n\to\infty} f_{\varphi,n}) \leq \liminf_{n\to\infty} \Phi_n(P)$$

because the functions $f_{\varphi,n}$ are not less than the right-hand side of (3.5). Together with Lemma 3.3, this shows that $\Phi(P) = \lim_{n\to\infty} \Phi_n(P)$.

To prove the lower semicontinuity of Φ we note first that each Φ_n is lower semicontinuous. This is because H_n satisfies (2.2) and is thus the supremum of functions in $\mathcal{L}$. Now let $c \in \mathbf{R}$ and $(P_\alpha)_{\alpha\in D}$ be a net in $\{\Phi \le c\}$ which converges (in $\tau_{\mathcal{L}}$) to some $P \in \mathcal{P}_\Theta$. Then $\rho(P_\alpha) \to \rho(P) < \infty$. We thus can assume without loss that $s \equiv \sup_\alpha \rho(P_\alpha) < \infty$. In view of (3.3) and the first part of this proof, we have for all $\alpha \in D$

$$c \ge \Phi(P_\alpha) \ge a\,\rho^{(2)}(P_\alpha) - b\,\rho(P_\alpha)$$

and thus $\rho^{(2)}(P_\alpha) \le (c + bs)/a \equiv c'$. Together with Lemma 3.3 this implies that

$$\begin{aligned} \Phi_n(P) - \epsilon_n c' &\le \liminf_{\alpha\in D} \Phi_n(P_\alpha) - \epsilon_n c' \\ &\le \liminf_{\alpha\in D} \Phi(P_\alpha) \le c \end{aligned}$$

for all $n \ge 0$. Letting $n \to \infty$ we see that $P \in \{\Phi \le c\}$. $\square$

We conclude this section proving the compactness of the level sets of the functionals $I_{z,\beta}$ defined in (2.14).

Lemma 3.4 *For any two numbers c_1, c_2, the set $\{I + \Phi \le c_1 + c_2\,\rho\}$ is $\tau_{\mathcal{L}}$-compact.*

Proof. The set above is closed because ρ is continuous and I and Φ are lower semicontinuous. In fact, I even has compact level sets, see Proposition 2.6 of [4]. The same is true for I^z, the relative entropy density with reference measure Q^z, the Poisson point random field with intensity $\rho(Q^z) = z > 0$. It is easy to see that $I^z = I_{z,0} = I - \rho \log z + z - 1$. By (2.2), $\Phi \ge -b\rho$. The set under consideration is therefore contained in the compact set $\{I^z \le c_1 + z - 1\}$, where $z = \exp(b + c_2)$. $\square$

4 The upper estimate

Let φ be superstable and regular and $F : \mathcal{P}_\Theta \to \mathbf{R} \cup \{\infty\}$ a measurable function such that $F \ge -c(1+\rho)$ for some $c < \infty$. In this section we shall prove the following result.

Proposition 4.1 *For* bc = per *or* free,

$$\limsup_{n\to\infty} v_n^{-1} \log\, Q_n(\,\exp[-v_n F(R_n) - H_{n,\mathrm{bc}}]) \le -\inf[I + \Phi + F_{\mathrm{lsc}}].$$

In the case bc = per, the above proposition follows directly from the results of [4] combined with those of Section 3. Namely, let $G = F + \Phi$. The integrand under consideration then equals $\exp[-v_n\, G(R_n)]$. By Theorem 1 and (3.3), $G \ge -c'(1+\rho)$ with $c' = c + b$, and G is clearly measurable because so is Φ. Theorem 3.1 of [4] thus implies that the lim sup in Proposition 4.1 is not larger than $-\inf[I + G_{\mathrm{lsc}}]$. But $G_{\mathrm{lsc}} \ge F_{\mathrm{lsc}} + \Phi$ because Φ is lower semicontinuous.

The proof of Proposition 4.1 for bc = free is based on a comparison with the case of periodic boundary conditions. We need several lemmas. First, we use the regularity of φ to estimate the interaction of suitably separated configurations.

For each integer $k \geq 0$ we define

$$\delta_k = \tfrac{1}{2} \sum_{\ell \geq k} \partial\psi(\ell)\, v_\ell\,, \tag{4.1}$$

where $\partial\psi(\ell) = \psi(\ell-1) - \psi(\ell) \geq 0$ for $\ell \geq 1$, $\partial\psi(0) = 0$, and ψ is as in (2.5) and (2.7). By (3.4),

$$\psi_i = \sum_{\ell \geq |i|} \partial\psi(\ell) \tag{4.2}$$

for all $i \in L$. Hence

$$\sum_{\ell \geq 0} \partial\psi(\ell)\, v_\ell = \sum_{i \in L} \psi_i < \infty$$

and thus $\delta_k \to 0$ as $k \to \infty$. For all $n \geq 0$, $\omega \in \Omega_n$ and $\zeta \in \Omega$ we have

$$\sum_{x \in \omega, y \in \zeta} \psi(y-x) \leq \sum_{i \in L_n, j \in L} \psi_{i-j}\, N_{C+i}(\omega)\, N_{C+j}(\zeta). \tag{4.3}$$

We estimate the long-distance contribution to the right-hand side of (4.3) in two cases. (The second case will be used later in Section 6.)

Lemma 4.2 *For all $n \geq 0$, $\omega \in \Omega_n$ and $k \geq 0$,*

$$\begin{aligned} &\sum_{i \in L_n, j \in L : |i-j| \geq k} \psi_{i-j} \quad N_{C+i}(\omega)\, N_{C+j}(\zeta) \\ &\qquad \leq \quad \begin{cases} \delta_k (1 + 2^d)\, T_n(\omega) & \text{if } \zeta = \omega^{(m)} \text{ for some } m \geq n, \\ \delta_k \left[T_n(\omega) + v_n\, t\, 2^d \right] & \text{if } \zeta \in \Omega(t) \text{ for some } t > 0. \end{cases} \end{aligned}$$

Proof. In view of (4.2), the sum above is not larger than

$$\sum_{\ell \geq k} \partial\psi(\ell) \sum_{i \in L_n, j \in L_\ell + i} N_{C+i}(\omega) N_{C+j}(\zeta).$$

Using the inequality $uv \leq (u^2 + v^2)/2$ we obtain the upper bound

$$\tfrac{1}{2} \sum_{\ell \geq k} \partial\psi(\ell)\, [v_\ell\, T_n(\omega) + S_{n,\ell}(\zeta)]$$

with

$$S_{n,\ell}(\zeta) = \sum_{j \in L} N_{C+j}(\zeta)^2 \ \text{ card } (L_n \cap (L_\ell + j)).$$

For $\zeta = \omega^{(m)}$ with $m \geq n$ we have

$$\begin{aligned} S_{n,\ell}(\omega^{(m)}) &= \sum_{j' \in L_n} N_{C+j'}(\omega)^2 \sum_{i \in L_n} \text{card}\{j \in L_\ell + i : j \equiv j' \ \bmod\ 2m+1\} \\ &\leq v_n\, (2^d v_\ell / v_m)\, T_n(\omega) \leq 2^d\, v_\ell\, T_n(\omega). \end{aligned}$$

On the other hand, if $\zeta \in \Omega(t)$ then

$$
\begin{aligned}
S_{n,\ell}(\zeta) &\leq (v_n \wedge v_\ell)\, T_{n+\ell}(\zeta) \\
&\leq v_{n\wedge\ell}\; t\; v_{2(n\vee\ell)} \leq t\, 2^d\, v_n\, v_\ell
\end{aligned}
$$

which implies the lemma in the second case. □

Recall the notation $r(\varphi)$ in (2.7).

Lemma 4.3 *For all* $n \geq 0$ *and* $k \geq r(\varphi)$, $|H_n - H_{n+k,\mathrm{per}}| \leq 2^d \delta_k T_n$ *on* Ω_n.

Proof. After a comparison of (2.1) and (2.16), the lemma follows immediately from (2.5) and (2.7) together with (4.3) and Lemma 4.2. □

Next we need to compare R_n with R_{n+k}. For $n \geq 0, s > 0$ we define

$$
\Omega(s,n) = \{\omega \in \Omega : T_n(\omega) \leq s\, v_n\}\,. \tag{4.4}
$$

Lemma 4.4 *For all* $k \geq 1$, $s > 0$ *and* $f \in \mathcal{L}$,

$$
\lim_{n\to\infty} \sup_{\omega\in\Omega(s,n+k)} |R_{n+k,\omega}(f) - R_{n,\omega}(f)| = 0.
$$

Proof. The case of bounded f is trivial. We thus assume for simplicity that $|f| \leq N_\Delta$ for some centered cube $\Delta \supset C$ with $f = f(\cdot \cap \Delta)$. For each n we can write, setting $m = n + k$,

$$
\begin{aligned}
|R_{m,\omega}(f) - R_{n,\omega}(f)| &\leq (v_n^{-1} - v_m^{-1}) \int_{\Lambda_m} N_{\Delta+x}(\omega^{(m)} dx \\
&\quad + v_n^{-1} \int_{\Lambda_m\setminus\Lambda_n} N_{\Delta+x}(\omega^{(m)}) dx \\
&\quad + v_n^{-1} \int_{\partial\Lambda_n} \Big(N_{\Delta+x}(\omega^{(m)}) + N_{\Delta+x}(\omega^{(n)}) \Big)\, dx,
\end{aligned}
$$

where $\partial\Lambda_n = \{x \in \Lambda_n : x + \Delta \not\subset \Lambda_n\}$. On the other hand, for each m with $\Lambda_m \supset \Delta + C$ and all $V \subset \Lambda_m$ we have

$$
\begin{aligned}
\int_V N_{\Delta+x}(\omega^{(m)}) dx &\leq \sum_{i\in L} N_{C+i}(\omega^{(m)})\, |\{x \in V : (\Delta + x) \cap (C + i) \neq \emptyset\}| \\
&\leq 2^d\, |\Delta| \sum_{i\in L\cap(V+\Delta+C)} N_{C+i}(\omega^{(m)}) \\
&\leq 4^d\, |\Delta| \sum_{j\in L_m(V)} N_{C+j}(\omega) \\
&\leq 4^d\, |\Delta|\, \mathrm{card} L_m(V)^{1/2}\, T_m(\omega)^{1/2}
\end{aligned}
$$

with $L_m(V) = \{j \in L_m : j \equiv i \mod 2m+1 \text{ for some } i \in V + \Delta + C\}$. In the cases $V = \Lambda_m, V = \Lambda_m \setminus \Lambda_n$, and $V = \partial\Lambda_n$ we have $\mathrm{card} L_m(V) \leq c_\Delta |V|$ for some constant

$c_\Delta < \infty$. Combining all estimates above one can now easily complete the proof. $\square$

Lemma 4.5 *For any three constants $c_1, c_2, c_3 > 0$ there exists some $s = s(c_1, c_2, c_3) < \infty$ such that*

$$Q_n(e^{c_1 N_n - c_2 T_n}; \Omega(s,n)^c) \leq e^{-c_3 v_n}$$

for all $n \geq 0$.

Proof. Let s be so large that $sc_2 \geq c_3 + e^{c_1} - 1$. The result then follows from the inequality

$$1_{\Omega(s,n)^c} \leq \exp[c_2(T_n - s v_n)]$$

and the fact that $Q_n(e^{c_1 N_n}) = \exp[(e^{c_1} - 1)v_n]$. $\square$

Before completing the proof of Proposition 4.1 we need one further notation. We let $\mathcal{U}$ denote the system of all sets of the form

$$U = \left\{(P_1, P_2) \in \mathcal{P}_\Theta \times \mathcal{P}_\Theta : \max_{1 \leq i \leq k} |P_1(f_i) - P_2(f_i)| \leq \epsilon\right\}$$

with $k \geq 1, \epsilon > 0$, and $f_1, \ldots, f_k \in \mathcal{L}$. By definition, $\mathcal{U}$ is a uniformity base for $\tau_{\mathcal{L}}$.

Proof of Proposition 4.1 in the case bc = free. For given $s > 0$ and arbitrary n we can write

$$Q_n(\exp[-v_n F(R_n) - H_n]) = p_n(s) + q_n(s),$$

where $p_n(s)$ is defined by restricting the integral on the left-hand side to the set $\Omega(s,n)$ and $q_n(s)$ is the remaining contribution corresponding to $\Omega(s,n)^c$. Let $\tau > 0$ be any given number, and let $s = s(c + b, a, \tau + c)$ be chosen according to Lemma 4.5. Here c is the constant appearing in the hypothesis $F \geq -c(1+\rho)$, and a, b are as in (3.2). It then follows that $q_n(s) \leq \exp[-\tau v_n]$ for all n.

To estimate the main term $p_n(s)$ we choose an arbitrary integer $k \geq r(\varphi)$. Then for each $n \geq 0$ we can write, setting again $m = n + k$ and using Lemma 4.3 and (2.16),

$$\begin{aligned} p_n(s) &= e^{v_m - v_n} Q_m\Big(\exp[-v_n F(R_n) - H_n]; \Omega(s,n) \cap \{N_{\Lambda_m \setminus \Lambda_n} = 0\}\Big) \\ &\leq \exp[v_m - v_n + 2^d \delta_k\, s\, v_n]\, Q_m(\exp[-G_m]), \end{aligned}$$

where $G_m = v_n F(R_n) + v_m \Phi(R_m) + \infty \cdot 1_{\Omega(s,m)^c}$. Next we choose any $U \in \mathcal{U}$ and $\ell > 0$ and define $F^\ell = F \wedge \ell$,

$$F_U^\ell(P) = \inf\{F^\ell(P') : (P, P') \in U\},$$

and $G_U^\ell = F_U^\ell + \Phi$. Lemma 4.4 asserts that $(R_m, R_n) \in U$ on $\Omega(s,m)$ for sufficiently large m. Since $v_n F \geq v_m F^\ell - (v_m - v_n)\ell$, we conclude that for these m

$$v_m^{-1} G_m \geq G_U^\ell(R_m) - (1 - v_n/v_m)\ell.$$

But this is all what is needed for the large deviation upper bound (3.2) of [4], cf. the proof of Lemma 5.6 there. (Measurability of G_U^ℓ is not required.) Hence

$$\limsup_{n\to\infty} v_m^{-1} \log Q_m(\exp[-G_m]) \leq -\inf[I + (G_U^\ell)_{\mathrm{lsc}}].$$

In view of the lower semicontinuity of Φ, $(G_U^\ell)_{\rm lsc} \geq (F_U^\ell)_{\rm lsc} + \Phi$. Also, Lemma 3.4 shows that the argument of Remark 1.4 of [2] can be applied, yielding

$$\sup_{\ell>0, U\in\mathcal{U}} \inf[I + \Phi + (F_U^\ell)_{\rm lsc}] = \inf[I + \Phi + F_{\rm lsc}] \equiv \gamma.$$

Hence

$$\limsup_{n\to\infty} v_n^{-1} \log p_n(s) \leq 2^d \delta_k s - \gamma.$$

Since k is arbitrary, we finally get

$$\limsup_{n\to\infty} v_n^{-1} \log [p_n(s) + q_n(s)] \leq -\gamma \wedge \tau,$$

and letting $\tau \to \infty$ we obtain the result. □

5 The lower estimate

We still assume that φ is superstable and regular. Our proof of the lower bound (2.21) follows the standard device of changing the measure so that untypical events become typical, and controlling the Radon-Nikodym density by means of McMillan's theorem. But some refinements are necessary. The basic observation is that the familiar approximation of invariant by ergodic probability measures can be sharpened as follows. For $q > 0$ we define

$$\Gamma_q = \Big\{\omega \in \Omega : \varphi(x-y) \leq q \text{ and } |x-y| \geq 1/q \text{ for any two distinct } x, y \in \omega\Big\}. \quad (5.1)$$

It is easy to check that Γ_q is measurable.

Lemma 5.1 *Let $P \in \mathcal{P}_\Theta$ be such that $I(P) + \Phi(P) < \infty$. For each open neighbourhood U of P and any $\epsilon > 0$ there exists some Θ-ergodic $P' \in U$ such that $I(P') < I(P) + \epsilon$, $\Phi(P') < \Phi(P) + \epsilon$, and $P'(\Gamma_q) = 1$ for some $0 < q < \infty$.*

Proof. 1) Let $n \geq 0$ be given. Since $\Phi(P) < \infty$, we have $\rho^{(2)}(P) < \infty$ and thus, by Lemma 3.3, $\Phi_n(P) < \infty$. Hence $P_n(\Gamma_q) \uparrow 1$ as $q \uparrow \infty$. Therefore we can choose a number $0 < q(n) < \infty$ such that $p_n \equiv P_n(\Gamma_{q(n)}) \to 1$ as $n \to \infty$. We also fix an integer $k \geq 1$ such that $2k \geq r(\varphi)$, where $r(\varphi)$ is as in (2.7). We can assume without loss that $q(n) \geq \psi(k)$ for all n. In the following we use again the abbreviation $m = n + k$.

2) Let $\hat{P}^{(n)} \in \mathcal{P}$ be the probability measure relative to which the particle configurations in the disjoint blocks $\Lambda_m + (2m+1)i$, $i \in L$, are independent with identical distribution $P'_n \equiv P_n(\,\cdot\,|\Gamma_{q(n)})$. This means in particular that the corridors $(\Lambda_m \setminus \Lambda_n) + (2m+1)i$, $i \in L$, contain no particles. We also set

$$P^{(n)} = v_m^{-1} \int_{\Lambda_m} \hat{P}^{(n)} \circ \vartheta_x^{-1}\, dx.$$

It is then obvious that $P^{(n)} \in \mathcal{P}_\Theta$, and a standard argument shows that $P^{(n)}$ is ergodic; see, for example, Theorem 14.12 of [1]. Since $\Gamma_{q(n)}$ is Θ-invariant and $\hat{P}^{(n)}(\Gamma_{q(n)}) = 1$, it also follows that $P^{(n)}(\Gamma_{q(n)}) = 1$.

3) Next we show that $\limsup_{n\to\infty} I(P^{(n)}) \le I(P)$. By an analogue of Lemma 5.5 of [4],

$$\begin{aligned} I(P^{(n)}) &\le I(P_n'; Q_m)/v_m \\ &= [I(\,P_n(\,\cdot\,|\Gamma_{q(n)})\,;\,Q_n\,) + v_m - v_n]/v_m. \end{aligned}$$

On the other hand, since $I(P) < \infty$ we have $P_n \ll Q_n$ with a density f_n, and thus

$$\begin{aligned} I(\,P_n(\,\cdot\,|\Gamma_{q(n)})\,;\,Q_n\,) &= P_n(\log f_n/p_n; \Gamma_{q(n)})/p_n \\ &\le (I(P_n; Q_n) + 1)/p_n - \log p_n \end{aligned}$$

because $x \log x \ge -1$ for all $x \ge 0$ and thus

$$P_n(\log f_n; \Gamma_{q(n)}^c) = Q_n(f_n \log f_n; \Gamma_{q(n)}^c) \ge -1.$$

Since $(v_m - v_n)/v_m \to 0$ and $p_n \to 1$ as $n \to \infty$, the desired result follows.

4) The regularity of φ implies that $\limsup_{n\to\infty} \Phi(P^{(n)}) \le \Phi(P)$. Indeed, since obviously $P^{(n)} \in \mathcal{P}_\Theta^{(2)}$, (2.11) and (2.8) yield

$$\begin{aligned} \Phi(P^{(n)}) &= \int P^{(n)}(d\omega) \sum_{x\in\omega\cap C} f_\varphi(\vartheta_x\omega) \\ &= v_m^{-1} \int_{\Lambda_m} du \int \hat{P}^{(n)}(d\omega)\ \tfrac{1}{2} \sum_{x,y\in\omega, y\neq x} 1_{C+u}(x)\varphi(y-x) \\ &= v_m^{-1} \int \hat{P}^{(n)}(d\omega)\ \tfrac{1}{2} \sum_{x,y\in\omega, y\neq x} \varphi(y-x)|\Lambda_m \cap (x-C)| \\ &= a_n + b_n. \end{aligned}$$

Here $a_n = v_m^{-1}\,\hat{P}^{(n)}(H_n)$ and

$$b_n = v_m^{-1} \int \hat{P}^{(n)}(d\omega)\ \tfrac{1}{2} \sum_{x\in\omega\cap\Lambda_n, y\in\omega\setminus\Lambda_m} \varphi(y-x),$$

and we have used that for $\hat{P}^{(n)}$-almost all ω and all $x \in \omega$ either $x \in \Lambda_n$, and thus $x - C \subset \Lambda_m$, or $\Lambda_m \cap (x - C) = \emptyset$. Now,

$$\begin{aligned} a_n &= P_n(H_n; \Gamma_{q(n)})/p_n v_m \\ &\le \Phi_n(P)\, v_n/p_n v_m + b\, P(N_n; \Gamma_{q(n)}^c)/p_n v_m \\ &\le \Phi_n(P)\,(1 + o(1)) + b\, P(N_n^2)^{1/2}(1-p_n)^{1/2}/p_n v_m \\ &= \Phi_n(P)\,(1 + o(1)) + o(1) \end{aligned}$$

because of (2.2) and (3.1), and $b_n = o(1)$ because of (2.7), (4.3), the inequality

$$\hat{P}^{(n)}(N_{C+i}N_{C+j}) = \hat{P}^{(n)}(N_{C+i})\hat{P}^{(n)}(N_{C+j}) \le \rho(P)^2/p_n^2$$

for $i \in L_n, j \notin L_m$, and the summability of $i \to \psi_i$.

5) We finally show that $P^{(n)}(f) \to P(f)$ as $n \to \infty$ for all $f \in \mathcal{L}$. Since this is quite obvious when f is bounded, we assume for simplicity that $|f| \leq N_\Delta$, where Δ is any cube with $f = f(\cdot \cap \Delta)$. Then we can write

$$|P^{(n)}(f) - P(f)| \leq (s_n + t_n)/v_m$$

with

$$s_n = \int_{\{x+\Delta \subset \Lambda_m\}} dx \, \Big| P_n(f \circ \vartheta_x | \Gamma_{q(n)}) - P(f \circ \vartheta_x) \Big|$$

and

$$t_n = \int_{\partial \Lambda_m} dx \, \Big[\hat{P}^{(n)}(N_{\Delta+x}) + P(N_{\Delta+x}) \Big] ,$$

where $\partial \Lambda_m$ is as in the proof of Lemma 4.4. Now $P(N_{\Delta+x}) = |\Delta| \rho(P)$,

$$\hat{P}^{(n)}(N_{\Delta+x \bmod 2m+1} | \Gamma_{q(n)}) \leq |\Delta| \rho(P)/p_n ,$$

and therefore $t_n = o(v_m)$. On the other hand, the integrand defining s_n is at most

$$\begin{aligned} |1 - p_n^{-1}| \, P_n(N_{\Delta+x}; \Gamma_{q(n)}) \quad &+ \quad P_n(N_{\Delta+x}; \Gamma_{q(n)}^c) \\ &\leq \quad |\Delta| \rho(P) |1 - p_n^{-1}| + P(N_\Delta^2)^{1/2} (1 - p_n)^{1/2} , \end{aligned}$$

whence $s_n = o(v_m)$. This completes the last step of the proof. □

The main advantage of the classes

$$\mathcal{P}_{\Theta,q} = \{ P \in \mathcal{P}_\Theta : P(\Gamma_q) = 1 \} \tag{5.2}$$

is the following continuity property of Φ.

Lemma 5.2 *For each $q > 0$, Φ is continuous on $\mathcal{P}_{\Theta,q}$.*

Proof. For each $n \geq 0$, H_n is local and bounded on Γ_q. Hence Φ_n is continuous on $\mathcal{P}_{\Theta,q}$. Also, a glance at Lemma 3.3 and its proof shows that the convergence $\Phi_n \to \Phi$ is uniform on $\mathcal{P}_{\Theta,q}$. This gives the result. □

Let $r \geq r(\varphi)$ be a fixed integer. For $n \geq r$ we define the modified empirical fields

$$R_{n,\omega}^{\#} = R_{n,\omega \cap \Lambda_{n-r}} . \tag{5.3}$$

Lemma 5.3 *For each ergodic $P \in \mathcal{P}_\Theta$, $R_n^{\#} \to P$ in P-probability as $n \to \infty$.*

Proof. This follows in the same way as (1.2); cf. the proof of Remark 2.4 in [4]. □

Let F be as in Theorem 2.

Proposition 5.4 *For all $P \in \mathcal{P}_\Theta$ and* bc $\in$ {per, free},

$$\liminf_{n\to\infty} v_n^{-1} \log Q_n(\exp[-v_n F(R_n) - H_{n,\mathrm{bc}}]) \geq -[I(P) + \Phi(P) + F^{\mathrm{usc}}(P)].$$

Proof. We may assume without loss that the right-hand side of the asserted inequality, denoted by $-\gamma_P$, is finite. By Lemma 5.1, we can even assume that P is ergodic and supported on $\Gamma = \Gamma_q$ for some $q \geq \psi(r)$. For $n \geq r$ let $P_n^{\#} = P_{n-r}$. We think of $P_n^{\#}$ as a measure on Ω_n which leaves $D_n = \Lambda_n \setminus \Lambda_{n-r}$ free of particles. Since $I(P) < \infty$, $P_{n-r} \ll Q_{n-r}$ with a density f_{n-r}. Hence $P_n^{\#} \ll Q_n$ with the density $f_n^{\#} = 1_{\{N_{D_n}=0\}} f_{n-r} \exp[v_n - v_{n-r}]$. Given any $\epsilon > 0$, we define

$$A_n = \left\{ F(R_n) < F^{\mathrm{usc}}(P) + \epsilon, v_n^{-1} H_{n,\mathrm{bc}} < \Phi(P) + \epsilon, v_n^{-1} \log f_n^{\#} < I(P) + \epsilon \right\}.$$

A well-known estimate (see, e.g., [4]) then shows that the lim inf in the proposition is not less than

$$-\gamma_P - 3\epsilon + \liminf_{n\to\infty} v_n^{-1} \log P_n^{\#}(A_n).$$

It is therefore sufficient to show that $P_n^{\#}(A_n) \to 1$. But

$$P_n^{\#}(\, F(R_n) < F^{\mathrm{usc}}(P) + \epsilon\,) = P(\, F(R_n^{\#}) < F^{\mathrm{usc}}(P) + \epsilon) \to 1$$

because of Lemma 5.3, and

$$P_n^{\#}(\, v_n^{-1} \log f_n^{\#} < I(P) + \epsilon\,) = P_{n-r}(v_n^{-1} \log f_{n-r} + 1 - v_n^{-1} v_{n-r} < I(P) + \epsilon) \to 1$$

by McMillan's theorem. Moreover, for bc = per we obtain from Lemmas 5.2 and 5.3 that

$$P_n^{\#}(v_n^{-1} H_{n,\mathrm{per}} < \Phi(P) + \epsilon) = P(\Phi(R_n^{\#}) < \Phi(P) + \epsilon) \to 1$$

because $P(R_n^{\#} \in \mathcal{P}_{\Theta,q}) = 1$. Thus $P_n^{\#}(A_n) \to 1$ for bc = per, and the same result follows for bc = free because

$$\sup_{\omega\in\Gamma} |H_n(\omega \cap \Lambda_{n-r}) - H_{n,\mathrm{per}}(\omega \cap \Lambda_{n-r})| \leq \tfrac{1}{2}\nu^2 \sum_{i\in L_{n-r}, j\notin L_n} \psi_{i-j} = o(v_n),$$

where $\nu = \sup N_C(\Gamma_q)$. This proves the proposition. □

The proof of Theorem 2 is now completed as follows. First, there is no loss in assuming $\beta = 1$. Next, we apply Propositions 4.1 and 5.4 to $F_z = -\rho \log z$. Since $\rho(R_n) = N_n/v_n$, this proves (2.22). Combining (2.22) with Proposition 4.1 (applied to $F + F_z$ instead of F) we arrive at the upper bound (2.20), and the lower bound (2.21) follows in the same way from (2.22) and Proposition 5.4.

6 Uniform estimates for tempered boundary conditions

This section is devoted to the proof of Theorem 3. We thus assume that φ is regular and satisfies (2.26). By Proposition 3.2.8 of [8], the stable part φ^s of φ may be chosen bounded. So we can assume that the repulsive part φ^r satisfies (2.26). This gives us the following sharpening of the basic inequality (3.2).

Lemma 6.1 *There exists a constant $b < \infty$ and an increasing function $h : \mathbf{Z}_+ \to [0, \infty[$ such that $h(0) = 0$, $h(\ell)/\ell^2 \to \infty$ as $\ell \to \infty$, and for all $n \geq 0$*

$$H_n \geq T_n^h - b\, N_n\,, \tag{6.1}$$

where

$$T_n^h = \sum_{i \in L_n} h(N_{C+i}) \,. \tag{6.2}$$

Proof. Since the stable part of φ satisfies (2.2), and in view of the remarks above, we can assume without loss that $\varphi = \varphi^r \geq 0$. Let $\chi :]0,\infty[\to [0,\infty[$ be a decreasing function such that $\varphi(x) \geq \chi(|x|)$ for all $x \neq 0$ and $\chi(s)s^d \to \infty$ as $s \to 0$. For each integer $k \geq 1$ we divide the unit cube C into k^d similar cubes $V(i)$ of size $1/k$. For $\omega \subset C$ with card $\omega = N \geq 1$ we let $N_i = \text{card}\, \omega \cap V(i), i = 1, \ldots, k^d$. Then

$$\begin{aligned}
\tfrac{1}{2} \sum_{x,y\in\omega, x\neq y} \varphi(x-y) &\geq \sum_{i=1}^{k^d} \binom{N_i}{2} \chi(1/k) \\
&= \tfrac{1}{2}\chi(1/k) \Big(\sum_{i=1}^{k^d} N_i^2 - N \Big) \\
&\geq \tfrac{1}{2}\chi(1/k)\, k^d \left[(Nk^{-d})^2 - Nk^{-d} \right].
\end{aligned}$$

If $N \geq 2^{d+1}$ and k is chosen as the largest integer with $Nk^{-d} \geq 2$, the last expression is not less than

$$h(N) \equiv 2^{-d-1} N \,\chi(2^{1+1/d} N^{-1/d}).$$

This gives (6.1) in the case $n = 1$, provided the constant b is chosen in such a way that $h(N) - bN \leq 0$ when $1 \leq N < 2^{d+1}$. The case of arbitrary n follows by summation over the cubes $C + i$, $i \in L_n$. Finally, the properties of χ imply that h is increasing and superquadratic. □

The next lemma establishes a simple relation between superquadratic and subquadratic functions on $\mathbf{Z}_+$ by means of the Legendre-Fenchel transform. Observe that this transform preserves the parabola $\ell \to \ell^2/2$.

Lemma 6.2 *Suppose* $g : \mathbf{Z}_+ \to [0,\infty[$ *is such that* $g(0) = 0$ *and* $g(\ell)/\ell^2 \to \infty$ *as* $\ell \to \infty$. *Let* $g^* : \mathbf{Z}_+ \to [0,\infty[$ *be defined by* $g^*(m) = \sup_\ell [m\ell - g(\ell)]$. *Then* g^* *is increasing,* $g^*(0) = 0$, *and* $g^*(m)/m^2 \to 0$ *as* $m \to \infty$.

Proof. This is a straightforward computation. Note that no convexity of g is required. □

The following lemma will allow us to reduce the case of tempered boundary conditions to that of the free boundary condition.

Lemma 6.3 *Let* $\epsilon > 0$, $t > 0$ *be given. If* n *is sufficiently large,*

$$\inf_{\zeta \in \Omega(t)} H_{n,\zeta} \geq H_n - \epsilon\, T_n^h - \epsilon\, v_n,$$

where h *is as in Lemma 6.1.*

Proof. In view of (2.25), (2.5) and (4.3) we must show that

$$\sup_{\zeta \in \Omega(t)} \sum_{i \in L_n, j \notin L_n} \psi_{i-j}\, N_{C+i}\, N_{C+j}(\zeta) \leq \epsilon\, T_n^h + \epsilon\, v_n \tag{6.3}$$

for large n. Let q be such that $h(\ell) \geq \ell^2$ for all $\ell \geq q$. Then $T_n \leq q^2 v_n + T_n^h$ for all n. By Lemma 4.2, the contribution of all i, j with $|i-j| \geq k$ to the sum on the left-hand side of (6.3) is not larger than $\delta_k [T_n^h + v_n(t2^d + q^2)]$. Choosing k sufficiently large we can achieve that this is less than $\epsilon(T_n^h + v_n)/2$.

To estimate the remaining part of the sum in (6.3) we define $g(\ell) = \ell\, h(\ell)^{1/2}$, $\ell \geq 0$. g is increasing with $g(0) = 0$ and satisfies $g(\ell)/\ell^2 \to \infty$ and $g(\ell)/h(\ell) \to 0$ as $\ell \to \infty$. Let g^* be as in Lemma 6.2. Then $\ell m \leq g(\ell) + g^*(m)$ for all $\ell, m \geq 0$ and therefore

$$\begin{aligned} \sum_{i \in L_n, j \notin L_n : |i-j| < k} & \psi_{i-j}\, N_{C+i}\, N_{C+j}(\zeta) \\ & \leq \Psi \sum_{i \in L_n \setminus L_{n-k}} g(N_{C+i}) + \Psi \sum_{j \in L_{n+k} \setminus L_n} g^*(N_{C+j}(\zeta)) \qquad (6.4) \end{aligned}$$

for all $n \geq k$ and $\zeta \in \Omega$. Here $\Psi = \sum_{i \in L} \psi_i$. Since $g(\ell)/h(\ell) \to 0$ as $\ell \to \infty$, the first expression on the right-hand side of (6.4) is at most $\epsilon\, T_n^h/2 + O(v_n - v_{n-k})$. Similarly, Lemma 6.2 implies that the second term on the right-hand side of (6.4) admits a bound of the form

$$\epsilon\, T_{n+k}(\zeta)/4t + O(v_{n+k} - v_n).$$

Since $v_{n+k} - v_n = o(v_n)$, it follows that, for $\zeta \in \Omega(t)$ and sufficiently large n, the left-hand side of (6.4) is not larger than $\epsilon(T_n^h + v_n)/2$. This proves (6.3). □

Proof of Theorem 3, assertion (a). Let F and t be as in the theorem, and let $0 < \epsilon < 1/2$ be given. In view of Lemma 6.3 we have for sufficiently large n

$$\begin{aligned} \bar{p}_n(t) &\equiv \sup_{\zeta \in \Omega(t)} Q_n\Big(\exp[-v_n F(R_n) - H_{n,\zeta}]\Big) \\ &\leq e^{\epsilon v_n}\, Q_n\left(\exp[-v_n F(R_n) - H_n + \epsilon T_n^h]\right). \end{aligned}$$

By Lemma 6.1 and the hypothesis on F, the exponent in the last integral is not larger than $c\, v_n + (c+b) N_n - (1-\epsilon) T_n^h$. An analogue of Lemma 4.5 thus shows that we may restrict the integral to a set of the form $\{T_n^h \leq s\, v_n\}$ with suitable $s < \infty$, the remainder being at most $e^{-\tau\, v_n}$ for any prescribed $\tau > 0$. Together with Proposition 4.1 (for bc = free), this gives the estimate

$$\limsup_{n \to \infty} v_n^{-1} \log\, \bar{p}_n(t) \leq (\epsilon + \epsilon s - \gamma) \vee (-\tau),$$

where $\gamma = \inf[I + \Phi + F_{\rm lsc}]$. Letting first $\epsilon \to 0$ and then $\tau \to \infty$ we obtain the uniform upper bound

$$\limsup_{n \to \infty} v_n^{-1} \log\, \bar{p}_n(t) \leq -\gamma. \qquad (6.5)$$

To obtain a lower estimate of

$$\underline{p}_n(t) \equiv \inf_{\zeta \in \Omega(t)} Q_n(\exp[-v_n F(R_n) - H_{n,\zeta}])$$

we can proceed just as in the proof of Proposition 5.4, the only difference being that now we must show that

$$\inf_{\zeta \in \Omega(t)} P_{n-r}(v_n^{-1}\, H_{n,\zeta} < \Phi(P) + \epsilon) \to 1 \qquad \text{as} \quad n \to \infty$$

for any given $\epsilon > 0$, each ergodic $P \in \mathcal{P}_\Theta$ which is supported on some Γ_q, and suitable $r \geq r(\varphi)$. But (2.7), (4.3) and Lemma 4.2 imply that

$$\sup_{\zeta \in \Omega(t)} H_{n,\zeta} \leq H_n + \epsilon\, v_n/2 \qquad \text{on} \quad \Gamma_q \cap \Omega_{n-r}$$

when r is large enough, and we know from the proof of Proposition 5.4 that

$$P_{n-r}(v_n^{-1} H_n < \Phi(P) + \epsilon/2) \to 1 \qquad \text{as } n \to \infty.$$

We thus arrive at the uniform lower bound

$$\liminf_{n\to\infty} v_n^{-1} \log \underline{p}_n(t) \geq -\inf[I + \Phi + F^{\mathrm{usc}}]. \tag{6.6}$$

Assertion (a) of Theorem 3 now follows from (6.5) and (6.6) in the same way as Theorem 2 from Propositions 4.1 and 5.4. □

We now turn to the large deviation principle for tempered Gibbs measures. Our main tool are the remarkable probability estimates of Ruelle [9]. The implication (a)⇒(b) of his Corollary 5.3 gives us the following.

Proposition 6.4 *For given $z, \beta > 0$, there exist constants $\gamma, \delta > 0$ such that, for all tempered Gibbs measures P with parameters z, β and all $n \geq 0$, P_n is absolutely continuous relative to Q_n with a density f_n satisfying $f_n \leq \exp[-\gamma T_n + \delta N_n]$.*

For $t > 0$ and $n \geq 0$ we define

$$\Omega_n(t) = \{\zeta \in \Omega : \zeta \setminus \Lambda_n \in \Omega(t)\}\,. \tag{6.7}$$

Corollary 6.5 *Let $z, \beta > 0$ and $\tau, c > 0$ be any constants. Then there exists some $t > 0$ such that, for each tempered Gibbs measure P with parameters z, β and all $n \geq 0$,*

$$P(e^{cN_n}; \Omega_n(t)^c) \leq e^{-\tau v_n}\,.$$

Proof. We may assume that $\tau > \log 2$. Let γ, δ be as in Proposition 6.4 and t so large that $t\,\gamma - e^{c+\delta} + 1 \geq \tau$. Then we can write

$$\begin{aligned}
P(e^{cN_n}\,;\,\Omega_n(t)^c) &\leq \sum_{\ell > n} P(e^{cN_n}; T_\ell > t\,v_\ell) \\
&\leq \sum_{\ell > n} P(\,\exp[c\,N_\ell + \gamma\,T_\ell - \gamma\,t\,v_\ell]) \\
&\leq \sum_{\ell > n} Q(\,\exp[(c+\delta)N_\ell - \gamma\,t\,v_\ell]) \\
&\leq \sum_{\ell > n} \exp[-\tau\,v_\ell]\,.
\end{aligned}$$

This implies the corollary because $v_\ell > v_n + \ell - n$ when $\ell > n$. □

Proof of Theorem 3, assertion (b). Let $z, \beta > 0$ and P be a tempered Gibbs measure for z, β. Also, let $F : \mathcal{P}_\Theta \to \mathbf{R} \cup \{\infty\}$ be such that $F \geq -c(1+\rho)$ for some $c < \infty$, $\tau > c$ an arbitrary constant, and t as in Corollary 6.5. Then

$$P(e^{v_n F(R_n)}; \Omega_n(t)^c) \leq e^{-(\tau - c)v_n}$$

and

$$\begin{aligned} P(e^{v_n F(R_n)}; \Omega_n(t)) &= \int_{\Omega_n(t)} P(d\zeta)\, P_{n,z,\beta,\zeta}(e^{v_n F(R_n)}) \\ &\leq \sup_{\zeta \in \Omega(t)} P_{n,z,\beta,\zeta}(e^{v_n F(R_n)}) \end{aligned}$$

for all n. The uniform upper bound (2.27) thus implies

$$\limsup_{n\to\infty} v_n^{-1} \log\, P(e^{v_n F(R_n)}) \leq -\inf[I_{z,\beta} + F_{\mathrm{lsc}}] \wedge (\tau - c),$$

and letting $\tau \to \infty$ we obtain the upper large deviation bound for P. The lower bound follows from the inequality

$$P(e^{v_n F(R_n)}) \geq P(\Omega(t)) \inf_{\zeta \in \Omega(t)} P_{n,z,\beta,\zeta}(e^{v_n F(R_n)})$$

together with (2.28) and the fact that $P(\Omega(t)) > 0$ for sufficiently large t. □

7 The equivalence of ensembles

In this section we prove Theorem 4. Let φ be superstable and regular. We first look at the function ϕ defined in (2.30). Let

$$\Omega_\varphi = \Big\{\omega \in \Omega : \varphi(x-y) < \infty \text{ for all } x, y \in \omega, x \neq y\Big\}$$

and

$$\nu(\varphi) = \sup\Big\{\rho(P) : P \in \mathcal{P}_\Theta, I(P) < \infty, P(\Omega_\varphi) = 1\Big\}. \tag{7.1}$$

Clearly, $\nu(\varphi)$ depends on φ only via the set $\{\varphi = \infty\}$. If φ is finite (except possibly at the origin) then $\nu(\varphi) = \infty$. For in this case we have $\Omega_\varphi = \Omega$ so that the Poisson point random fields $P = Q^z$ of arbitrarily large intensity z appear on the right-hand side of (7.1).

Lemma 7.1 *ϕ is convex. On $[0, \nu(\varphi)[$, ϕ is finite and continuous. Also, $\phi(\nu) \geq a\,\nu^2 - b\,\nu$ for all $\nu \geq 0$ and the constants a, b in (3.3), and if $\lambda \equiv \int \varphi(x)dx$ is finite then $\phi(\nu) \leq \lambda\,\nu^2/2$ for all $\nu \geq 0$. (In particular, it follows that $\lambda \geq a$.)*

Proof. The inequalities for ϕ follow from (3.3) and the easily verified fact that $\Phi(Q^z) = \lambda\, z^2/2$ for all $z > 0$. It only remains to show that ϕ is finite on $[0, \nu(\varphi)[$. For, together with the obvious convexity of ϕ, this will imply that ϕ is continuous on $]0, \nu(\varphi)[$. The continuity of ϕ at 0 is clear because $\phi(0) = 0$ and $\phi(\nu) \geq -b\,\nu$.

To prove the finiteness of ϕ we fix any $\nu < \nu(\varphi)$. By (7.1) there exists some $P \in \mathcal{P}_\Theta$ such that $\rho(P) > \nu, I(P) < \infty$, and $P(\Omega_\varphi) = 1$. A glance at the proof of Lemma

5.1 shows that its hypothesis $\Phi(P) < \infty$ can be replaced by the condition $P(\Omega_\varphi) = 1$. Therefore we can find some $P' \in \mathcal{P}_\Theta$ such that $\rho(P') > \nu, I(P') < \infty$, and $P'(\Gamma_q) = 1$ for some $q < \infty$. Since Γ_q is Θ-invariant, the Palm measure of P' is also supported on Γ_q. This and the regularity of φ immediately imply that $\Phi(P') < \infty$. Writing $s = \nu/\rho(P')$ we thus obtain that $P'' \equiv sP' + (1-s)\delta_\emptyset$ has the properties $\rho(P'') = \nu, \Phi(P'') < \infty$, and $I(P'') < \infty$. Hence $\phi(\nu) < \infty$. □

In view of (7.3) and (7.7) below, the function $\phi(\nu)$ coincides with the function $\varepsilon_0(\rho)$ on page 50 of [8]. Note, however, that not necessarily $\phi(\nu) \to \infty$ when $\nu \to \nu(\varphi) < \infty$; indeed, if φ is a pure hard core potential (taking only the values 0 and ∞) then $\phi(\nu) = 0$ for all $\nu < \nu(\varphi)$.

Next we define

$$s(\nu, \varepsilon) = -\inf\{I(P) : P \in \mathcal{P}_\Theta,\, \rho(P) = \nu,\, \Phi(P) \le \varepsilon\}. \tag{7.2}$$

Clearly, $s(\,\cdot\,,\,\cdot\,)$ is increasing in ε and concave, and (2.30) means that

$$\phi(\nu) = \inf\{s(\nu,\,\cdot\,) > -\infty\} \qquad \text{for all } \nu \ge 0. \tag{7.3}$$

Using the lower semicontinuity of Φ and the fact that I has compact level sets [4] we also see that $s(\,\cdot\,,\,\cdot\,)$ is upper semicontinuous. $s(\,\cdot\,,\,\cdot\,)$ is the entropy density, as is shown in the next lemma which proves (2.32).

Lemma 7.2 *Let $D \subset [0,\infty[$ be a nondegenerate interval with $\inf D < \nu(\varphi)$, and let $\varepsilon > \inf \phi(D)$. Then*

$$\lim_{n\to\infty} v_n^{-1} \log Q_n(N_n \in v_n D, H_{n,\mathrm{per}} \le v_n\varepsilon) = s(D,\varepsilon) \equiv \sup_{\nu\in D} s(\nu,\varepsilon).$$

If $\inf D > \nu(\varphi)$ or $\varepsilon < \inf \phi(D)$ then the limit above equals $-\infty$.

Proof. Let $\bar{D}$ be the closure and D^o the interior of D. By the continuity of ϕ on $[0,\nu(\varphi)[$, $\inf\phi(\bar{D}) = \inf\phi(D^o) = \inf\phi(D)$. In view of the continuity of ρ and the lower semicontinuity of Φ, the set $A = \{\rho \in \bar{D}, \Phi \le \varepsilon\}$ is closed. The upper bound (2.20) for $\beta = 0, z = 1$ thus implies that

$$\limsup_{n\to\infty} v_n^{-1} \log\, Q_n(R_n \in A) \le -\min I(A) \tag{7.4}$$

(I attains its minimum over A because I has compact level sets.) On the other hand, consider the convex set $U = \{\rho \in D^o, \Phi < \varepsilon\}$. Since $\varepsilon > \inf\phi(D^o)$, $U \cap \{I < \infty\} \ne \emptyset$. A standard convexity argument (together with the fact that I, ρ and Φ are affine) thus shows that $\inf I(U) = \inf I(A) = s(D,\varepsilon)$. But

$$\liminf_{n\to\infty} v_n^{-1} \log\, Q_n(R_n \in U) \ge -\inf I(U)$$

by the arguments of Section 5. Indeed, let $P \in U$ be such that $I(P) < \infty$. For given $\epsilon > 0$, Lemma 5.1 provides us with some ergodic $P' \in U$ such that $I(P') < I(P) + \epsilon$ and $P'(\Gamma_q) = 1$ for some $q > 0$. As in the proof of Proposition 5.4, we have the estimate

$$v_n^{-1} \log Q_n(R_n \in U) \ge -I(P') - \epsilon + v_n^{-1} \log P'(R_n^\# \in U,\, v_n^{-1} \log f_n^\# \le I(P') + \epsilon),$$

and McMillan's theorem and Lemmas 5.2 and 5.3 show that the last probability tends to 1 as $n \to \infty$. The second statement of the lemma follows from (7.3) and (7.4). $\Box$

Proposition 7.3 *Suppose $D \subset [0, \infty[$ is a nondegenerate interval with $\inf D < \nu(\varphi)$, and let $\varepsilon > \inf \phi(D)$. Then the sequence $(Q_{n|D,\varepsilon,\mathrm{per}})_{n\geq 0}$ is relatively compact (in $\tau_{\mathcal{L}}$), and every accumulation point belongs to the set $M_{D,\varepsilon}$ of all I-minimizers in $\{\rho \in \bar{D}, \Phi \leq \varepsilon\}$.*

Proof. Lemma 7.2 implies that the conditioning event in (2.29) has positive probability for sufficiently large n. Thus, for all these n, $Q_{n|D,\varepsilon,\mathrm{per}}$ is well-defined. Let $\hat{P}^{(n)} \in \mathcal{P}$ denote the measure relative to which the configurations in the disjoint blocks $\Lambda_n + (2n+1)i$, $i \in L$, are independent with identical distribution $Q_{n|D,\varepsilon,\mathrm{per}}$, and $P^{(n)} \in \mathcal{P}_\Theta$ the invariant average of $\hat{P}^{(n)} \circ \vartheta_x^{-1}$, $x \in \Lambda_n$. Since $Q_{n|D,\varepsilon,\mathrm{per}}$ is invariant under translations modulo Λ_n, $P^{(n)}(f) - Q_{n|D,\varepsilon,\mathrm{per}}(f) \to 0$ as $n \to \infty$, for all $f \in \mathcal{L}$; cf. Lemma 4.6 of [2]. Just as in Step 3) of the proof of Lemma 5.1 we obtain

$$I(P^{(n)}) \leq v_n^{-1}\, I(Q_{n|D,\varepsilon,\mathrm{per}}; Q_n) = -v_n^{-1} \log Q_n(\rho(R_n) \in D, \Phi(R_n) \leq \varepsilon).$$

Lemma 7.2 thus implies that

$$\limsup_{n\to\infty} I(P^{(n)}) \leq -s(D, \varepsilon) < \infty.$$

Since I has compact (and sequentially compact) level sets, it follows that the sequence $(P^{(n)})_{n\geq 0}$, and thus also the asymptotically equivalent sequence $(Q_{n|D,\varepsilon,\mathrm{per}})_{n\geq 0}$, are relatively compact. Moreover, each accumulation point of any of these sequences belongs to the set $\{I \leq -s(D, \varepsilon)\}$. On the other hand, Lemma 5.7 of [4] asserts that $P^{(n)}$ is asymptotically equivalent to

$$Q_{n|D,\varepsilon,\mathrm{per}} R_n \equiv \int Q_{n|D,\varepsilon,\mathrm{per}}(d\omega)\, R_{n,\omega}$$

as $n \to \infty$, and the latter measures all belong to the closed convex set $\{\rho \in \bar{D}, \Phi \leq \varepsilon\}$, as is easily seen by approximating $Q_{n|D,\varepsilon,\mathrm{per}}$ by suitable discrete measures. This proves the proposition. $\Box$

To deduce the first part of (2.31) from Proposition 7.3 we choose a tangent plane $(\nu, \varepsilon') \to p + \beta\varepsilon' - \nu \log z$ to the concave function $s(\,\cdot\,,\cdot\,)$ on the subset of $\bar{D}\times]-\infty, \varepsilon]$ on which $s(\,\cdot\,,\cdot\,)$ attains its maximum $s(D, \varepsilon)$. The monotonicity of $s(\nu, \,\cdot\,)$ implies that $\beta \geq 0$. It then follows that, for all $P \in \mathcal{P}_\Theta$ with $\Phi(P) < \infty$,

$$I(P) \geq -s(\rho(P), \Phi(P)) \geq -p - \beta\Phi(P) + \rho(P) \log z$$

with equality when $P \in M_{D,\varepsilon}$. Since $M_{D,\varepsilon} \neq \emptyset$, we may conclude that $p = p(z, \beta)$ and

$$M_{D,\varepsilon} \subset \{I_{z,\beta} = 0\}. \tag{7.5}$$

Together with Proposition 7.3, this gives the first part of (2.31). The second part is the subject of the next proposition.

Proposition 7.4 *For all $z, \beta > 0$, the sequence $(P_{n,z,\beta,\mathrm{per}})_{n\geq 0}$ is relatively compact,* *and all its accumulation points belong to* $\{I_{z,\beta} = 0\}$.

Proof. We proceed just as in the proof of the last proposition. For each $n \geq 0$ we have

$$\begin{aligned} -v_n^{-1} \log Z_{n,z,\beta,\mathrm{per}} &= v_n^{-1} I(P_{n,z,\beta,\mathrm{per}}; Q_n) \\ &\quad + \beta\, P_{n,z,\beta,\mathrm{per}}(\Phi(R_n)) - P_{n,z,\beta,\mathrm{per}}(v_n^{-1} N_n) \log z\,. \end{aligned}$$

The first term on the right-hand side is not less than $I(P^{(n)})$, where $P^{(n)}$ is the invariant Λ_n-average of the Λ_n-periodic measure $\hat{P}^{(n)}$ making the configurations in the blocks $\Lambda_n + (2n+1)i$, $i \in L$, independent with identical distribution $P_{n,z,\beta,\mathrm{per}}$. Using Lemma 3.3 and the observation that $P_{n,z,\beta,\mathrm{per}}(\rho^{(2)}(R_n)) = \rho^{(2)}(P_{n,z,\beta,\mathrm{per}}) < \infty$ we see further that the second term on the right-hand side is not less than $\beta\,\Phi(P_{n,z,\beta,\mathrm{per}} R_n)$. Combining this with (2.22) we obtain

$$\limsup_{n\to\infty} \Big[I(P^{(n)}) + \beta\,\Phi(P_{n,z,\beta,\mathrm{per}} R_n) - \rho(P^{(n)}) \log z \Big] \leq -p(z,\beta) < \infty\,.$$

The compactness of the level sets of I, the lower semicontinuity of Φ, and the asymptotic equivalence of $P^{(n)}$, $P_{n,z,\beta,\mathrm{per}} R_n$, and $P_{n,z,\beta,\mathrm{per}}$ thus give the result. □

To conclude, we mention without proof that the entropy function $s(\,\cdot\,,\,\cdot\,)$ is related to the pressure by the the classical Legendre transformation as follows. For all $z, \beta > 0$,

$$p(z,\beta) = \max_{\nu \geq 0, \varepsilon \in \mathbf{R}} [s(\nu,\varepsilon) - \beta\,\varepsilon + \nu \log z]\,. \tag{7.6}$$

Conversely,

$$s(\nu,\varepsilon) = \min_{\beta \geq 0, z > 0} [p(z,\beta) + \beta\,\varepsilon - \nu \log z] \tag{7.7}$$

whenever $\nu > 0$ and $s(\nu,\varepsilon) > -\infty$.

References

[1] Georgii, H.O.: Gibbs Measures and Phase Transitions. Berlin: de Gruyter 1988

[2] Georgii, H.O.: Large deviations and maximum entropy principle for interacting random fields on $\mathbb{Z}^d$. Ann. Probab. (1993)

[3] Georgii, H.O.: Large deviations for hard core particle systems. In: Kotecky, R. (ed.) Proceedings of the 1992 Prague Workshop on Phase Transitions. Singapore: World Scientific 1993

[4] Georgii, H.O., Zessin, H.: Large deviations and the maximum entropy principle for marked point random fields. Probab. Th. Rel. Fields (1993)

[5] Matthes,K., Kerstan, J., Mecke, J.: Infinitely Divisible Point Processes. Chichester: Wiley 1978

[6] Olla, S., Varadhan, S.R.S., Yau, H.T.: Hydrodynamic limit for a Hamiltonian system with a weak noise, preprint (1992)

[7] Ruelle, D.: Classical statistical mechanics of a system of particles. Helv. Phys. Acta 36, 183-197 (1963)

[8] Ruelle, D.: Statistical Mechanics. Rigorous results. New York: Benjamin 1969

[9] Ruelle, D.: Superstable interactions in classical statistical mechanics. Commun. Math. Phys. 18, 127-159 (1970)