

The characterization of ground states

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Abstract

We consider limits of equilibrium distributions as temperature approaches zero, for systems of infinitely many particles, and characterize the support of the limiting distributions. Such results are known for particles with positions on a fixed lattice; we extend these results to systems of particles on \mathbb{R}^n , with restrictions on the interaction.

1 Introduction

Consider a physical system consisting of a large number of interacting molecules in thermal equilibrium. Equilibrium statistical mechanics accurately models

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such systems. The fundamental qualitative feature of having fluid and solid phases, the latter appearing at low temperature and/or high pressure, can even be usefully modelled with *classical* statistical mechanics. Yet although this phase structure has been amply supported by computer simulations [FS] there is as yet not a single model, of particles moving in space and interacting through reasonable short range forces, in which such fundamental features can be proven [Ra1]. It is not difficult to model a solid if one uses less physical interactions, as in the Einstein or Debye models, but this has not yet been achieved with a satisfactory short range model, which could also describe a fluid phase. (See however [Ru1, LM, Ra2].) This is one of the main unsolved problems in condensed matter physics [Br, Uh].

One of the difficulties is that to unambiguously characterize or distinguish a phase one must use the thermodynamic limit, or, equivalently, uniformly control the behavior of the system as the system size grows indefinitely. Now consider the grand canonical ensemble for a system of finite size, for which the unnormalized probability density of particle configuration ω is $\exp -\beta[E(\omega) - \lambda|\omega|]$, where $E(\omega)$ is the energy of ω , $|\omega|$ is its particle number, λ is the chemical potential and β is the inverse temperature. If one takes the limit $\beta \rightarrow \infty$, for fixed λ , one easily sees that the probability tends to concentrate on configurations ω which minimize $E(\omega) - \lambda|\omega|$ and which are called ground state configurations. This can be useful, as one can then understand the state at large β as a perturbation of the energy ground state, and try to understand the solid phase from this. But, as we just noted, one must be careful with the order of limits; one needs to see the approximation of positive temperature states by zero temperature states *uniformly in the size of the system*, and not only is this not obvious, it can actually fail, as we show below. (For a failure of a different sort see [ER, CH].)

In other words, a major difficulty in solving this old problem, of successfully modelling the origin of the solid state in terms of short range forces, is to control the approximation of low temperature states by those at zero temperature (energy ground states) as the system size grows. One way to systematize this is to make sense of infinite volume limit “Gibbs states” $\mu_{\beta,\lambda}$ for finite β , introduce the “ground states” $\mu_{\infty,\lambda}$ as the limit points $\lim_{\beta \rightarrow \infty} \mu_{\beta,\lambda}$, and characterize the “ground state configurations” ω in the support of $\mu_{\infty,\lambda}$, the smallest closed set of configurations of probability 1. This is the path we will take as it makes the control of the limit as $\beta \rightarrow \infty$ a bit easier, having already taken the limit in the size of the system. So $\mu_{\beta,\lambda}$ and $\mu_{\infty,\lambda}$ will be probability distributions on configurations ω of particles in unbounded phys-

ical space. From the above analysis in finite volume we expect $\mu_{\infty,\lambda}$ to be supported by configurations ω which in some sense minimize $E(\omega) - \lambda|\omega|$. Of course for an infinite system $E(\omega) - \lambda|\omega|$ is typically going to be infinite, so one must adjust appropriately both the defining characteristic of the equilibrium distribution $\mu_{\beta,\lambda}$ and the optimization approached as $\beta \rightarrow \infty$. For $\mu_{\beta,\lambda}$ this was solved rather generally many years ago, and we use the result below. But for $\mu_{\infty,\lambda}$ this was only solved in the simpler situation of models with particles living in a discrete space, typically a lattice [Ru2, Sc]. Restricting oneself to lattice models is a weakness however if one is trying to model the fluid/solid transition, or more specifically to model a solid. Removing this obstacle is the main motivation for this work. We show that under certain reasonable conditions the optimization characterization of the support of $\mu_{\infty,\lambda}$ is the same for models of particles in space as for models of particles on a lattice. The proof is somewhat harder, and for good reason: it is known that without extra assumptions on the interaction the particle density can be unbounded at any positive temperature, a phenomenon not possible in typical lattice models.

Our arguments are necessarily technical since we are forced to deal carefully with limits, but this is justified by the direct relevance of our results to matters of importance to physical theory. We note that ground states are also used significantly in optimization schemes outside physics; see for instance [HR].

2 Convergence to Ground State Configurations

First some notation and assumptions. We assume a two-body interaction potential $U(s, t)$ dependent only on the separation of the point particles at positions s, t in \mathbb{R}^n , including a hard core at separation 1 and diverging as the separation decreases to 1:

$$U(s, t) \begin{cases} = \infty & \text{for } |s - t| \leq 1, \\ \rightarrow \infty & \text{for } |s - t| \searrow 1. \end{cases}$$

We assume U has finite range $R > 1$, and that $U \geq -m$, for some $m > 0$. Denote the chemical potential by λ .

We denote by Ω the set of all finite or countably infinite configurations $\omega \subset \mathbb{R}^n$ of particles which are separated by a distance at least 1. By ω_j we

denote the positions of the particles in ω , and by $b_1(\omega)$ the set of balls $b_1(\omega_j)$ of diameter 1 centered at positions ω_j . For $A \subset \mathbb{R}^n$ we denote by Ω_A the set of configurations $\omega = \omega_A \equiv \omega \cap A$, which have all their particles in A . The number of particles in ω_A will be denoted by $|\omega_A|$. With the usual topology Ω is compact.

Now we will introduce the notion of the Gibbs state. We first introduce for every bounded A and $\omega \in \Omega_A$ the energy:

$$H(\omega) = \sum_{i < j} U(\omega_i, \omega_j) + \lambda |\omega|. \quad (1)$$

For two collections of particles, $\omega' \in \Omega_A$, $\omega'' \in \Omega$, we define the interaction between them as

$$H(\omega', \omega'') = \sum_{i,j} U(\omega'_i, \omega''_j). \quad (2)$$

and the sum

$$H(\omega' | \omega'') = H(\omega') + H(\omega', \omega''). \quad (3)$$

We say that the probability measure $\mu_{\beta, \lambda}$ on Ω is a Gibbs measure, corresponding to the interaction U , inverse temperature β and chemical potential λ , if for any finite A and any function f on Ω_A we have

$$\begin{aligned} & \int f(\omega_A) d\mu_{\beta, \lambda}(\omega) \\ &= \int \left[\int f(\omega_A) \exp \{-\beta H(\omega_A | \omega_{A^c})\} d\pi_A(\omega_A) \right] Z_{\beta, \lambda}^{-1}(A, \omega_{A^c}) d\mu_{\beta, \lambda}(\omega). \end{aligned} \quad (4)$$

Here

- $A^c = \mathbb{R}^n \setminus A$,
- π_A is the Poisson measure on Ω_A , which on the k -particle subset of Ω_A is just the Lebesgue measure, normalized by the factor $e^{-|A|} \frac{|A|^k}{k!}$,
- the *partition function*

$$Z_{\beta, \lambda}(A, \omega_{A^c}) = \int \exp \{-\beta H(\omega_A | \omega_{A^c})\} d\pi_A(\omega_A).$$

It is easy to see that any such measure gives probability 1 to the set of configurations in which no two particles are at distance 1.

The probability distribution $q_{A,\omega_{A^c}} \equiv q_{\beta,\lambda,A,\omega_{A^c}}$ on Ω_A , given by the density $Z_{\beta,\lambda}^{-1}(A,\omega_{A^c}) \exp\{-\beta H(\omega_A|\omega_{A^c})\}$ with respect to the measure π_A , is called the *conditional Gibbs distribution*, corresponding to the boundary condition ω_{A^c} . The equation (4) is called the Dobrushin-Lanford-Ruelle (DLR) conditions; see [D1, D2, D3, LR]. (The conditions are a way to replace, for systems of infinite size, the usual formula which one uses for finite systems.) Any measure obtainable from such a Gibbs state by the limit $\beta \rightarrow \infty$ will be called a *ground state*.

Let the set G of *ground state configurations* be defined as:

$$G = \{\omega \in \Omega : \text{for every bounded } \Lambda \subset \mathbb{R}^n \text{ and every } \omega' = (\omega'_\Lambda, \omega_{\Lambda^c}), \\ H(\omega'_\Lambda|\omega_{\Lambda^c}) - H(\omega_\Lambda|\omega_{\Lambda^c}) \geq 0\}.$$

This set is nonempty, see [Ra2].

Our main result is the following

Theorem 1 *Let μ_∞ be any limit point of the family of Gibbs states μ_β as $\beta \rightarrow \infty$, i.e. a ground state. Then $\mu_\infty(G) = 1$.*

Theorem 1 holds in more a general situation, when the interaction has no hard core, but possess instead the superstability property. (We discuss superstability in the last section.) The proof is more complicated, and we will not present it here.

Theorem 1 is equivalent to

Theorem 2 *Assume that $\omega \in G^c$. Then there exists an open neighborhood W of ω such that $\int_W d\mu_\beta(\sigma) \rightarrow 0$ as $\beta \rightarrow \infty$.*

Proof of Theorem 2. Before giving the formal proof we present its plan. If $\omega \in G^c$ then the following holds: there exists a finite volume B , inside which the configuration $\omega \equiv (\omega_B, \omega_{B^c})$ can be modified into $\bar{\omega} \equiv (\bar{\omega}_B, \omega_{B^c})$ in such a way that

$$\Delta(\omega) \equiv H(\omega_B|\omega_{B^c}) - H(\bar{\omega}_B|\omega_{B^c}) > 0. \quad (5)$$

We will be done if we can find open neighborhoods W, \bar{W} of the configurations ω and $\bar{\omega}$, such that

$$\frac{\mu_\beta(W)}{\mu_\beta(\bar{W})} \rightarrow 0 \quad (6)$$

as $\beta \rightarrow \infty$. So we need to find an upper bound for $\mu_\beta(W)$ and a lower bound for $\mu_\beta(\bar{W})$. To do this we will use the following simple

Lemma 3 *For every value of the chemical potential λ there exists a distance $\rho(\lambda) > 1$ such that the following holds for all ρ in the interval $(1, \rho(\lambda))$:*

Let $M \subset \mathbb{R}^n$ be any bounded volume and $\xi \in \Omega_{M^c}$ – any “boundary condition”. Denote by $\Omega_{M,\rho}(\xi) \subset \Omega_M$ the subset

$$\left\{ \begin{array}{l} \sigma \in \Omega_M : \text{two particles of } \sigma \text{ are separated by } < \rho, \text{ or a particle of } \sigma \\ \text{is at distance } < \rho \text{ from a particle of } \xi \end{array} \right\}. \quad (7)$$

Then the conditional Gibbs probability $q_{\beta,M,\xi}(\Omega_{M,\rho}(\xi))$ goes to 0 as $\beta \rightarrow \infty$. This convergence, of course, is not uniform in M , but for every M it is uniform in ξ . In other words,

$$q_{\beta,M,\xi}(\Omega_M \setminus \Omega_{M,\rho}(\xi)) = 1 - \gamma(\beta, M, \xi, \rho), \quad (8)$$

where for every M, ρ the function $\gamma(\beta, M, \xi, \rho) \rightarrow 0$ as $\beta \rightarrow \infty$, uniformly in ξ .

The same statement holds for the subset

$$\Omega_{M,\rho} = \{\sigma \in \Omega_M : \text{two particles of } \sigma \text{ are at distance } < \rho\}, \quad (9)$$

since for every ξ we have $\Omega_{M,\rho} \subset \Omega_{M,\rho}(\xi)$.

Without the hard core condition Lemma 3 does not hold, and has to be replaced by a weaker statement. Our proof of Lemma 3 uses the divergence of the repulsion near the hard core.

The proof of Theorem 2 proceeds now as follows. Let \bar{B} be the open R -neighborhood of B in \mathbb{R}^n . Due to the Lemma it is enough to consider the case of ω such that $\omega_{\bar{B}} \notin \Omega_{\bar{B},\rho(\lambda)}$.

By an r -perturbation of a finite configuration $\varpi \in \Omega$ we will mean any finite configuration \varkappa with the same number of particles, such that for every particle $\varpi_j \in \varpi$ the intersection $\varkappa \cap b_1(\varpi_j)$ consists of precisely one particle $\varkappa_j \in \varkappa$, and $\text{dist}(\varpi_j, \varkappa_j) < r$.

Now we define the open neighborhood W of ω by putting

$$W = \{(\varkappa, \xi) : \varkappa \in \Omega_r(\omega, \bar{B}), \xi \in \Omega_{\bar{B}^c}\}, \quad (10)$$

where $\Omega_r(\omega, \bar{B})$ is the set of all those r -perturbations \varkappa of $\omega_{\bar{B}}$ which also belong to $\Omega_{\bar{B}}$. It is immediate to see that if $r \leq \rho(\lambda)/2$ then for every $(\varkappa, \xi) \in W$

$$\begin{aligned} |H(\varkappa_B) - H(\omega_B)| &< Cr, \\ |H(\varkappa_B, \varkappa_{\bar{B} \setminus B}) - H(\omega_B, \omega_{\bar{B} \setminus B})| &< Cr, \end{aligned}$$

for some $C = C(B)$. Let r be so small that $Cr < \frac{\Delta(\omega)}{10}$. Then, by DLR,

$$\begin{aligned} &\int_W d\mu_\beta(\varkappa, \xi) \\ &= \int_{\Omega_r(\omega, \bar{B})} \frac{\left[\int_{\Omega_r(\omega, \varkappa_{\bar{B} \setminus B})} \exp\{-\beta H(\varkappa_B | \varkappa_{\bar{B} \setminus B})\} d\pi_B(\varkappa_B) \right]}{Z_B(\varkappa_{\bar{B} \setminus B})} d\mu_\beta(\varkappa, \xi) \\ &\leq \exp\left\{-\beta \left[H(\omega_B | \omega_{B^c}) - \frac{\Delta(\omega)}{10} \right]\right\} \int_{\Omega_r(\omega, \bar{B})} \frac{1}{Z_B(\varkappa_{\bar{B} \setminus B})} d\mu_\beta(\varkappa, \xi), \end{aligned}$$

where

$$\Omega_r(\omega, \varkappa_{\bar{B} \setminus B}) = \{\tilde{\varkappa} \in \Omega_r(\omega, \bar{B}) : \tilde{\varkappa}_{\bar{B} \setminus B} = \varkappa_{\bar{B} \setminus B}\}, \quad (11)$$

and $Z_B(\varkappa_{\bar{B} \setminus B})$'s are the partition functions.

In the same way, and recalling the meaning of $\bar{\omega}$, we put

$$\bar{W} = \{(\varkappa, \xi) : \varkappa \in \Omega_r(\bar{\omega}, \bar{B}), \xi \in \Omega_{\bar{B}^c}\}. \quad (12)$$

Without loss of generality we can assume that for the same C and every $(\varkappa, \xi) \in \bar{W}$

$$\begin{aligned} |H(\varkappa_B) - H(\bar{\omega}_B)| &< Cr, \\ |H(\varkappa_B, \varkappa_{\bar{B} \setminus B}) - H(\bar{\omega}_B, \omega_{\bar{B} \setminus B})| &< Cr. \end{aligned}$$

Then

$$\begin{aligned}
& \int_{\bar{W}} d\mu_\beta(\boldsymbol{\varkappa}, \xi) \\
&= \int_{\Omega_r(\omega, \bar{B})} \frac{\left[\int_{\Omega_r(\bar{\omega}, \boldsymbol{\varkappa}_{\bar{B} \setminus B})} \exp\{-\beta H(\boldsymbol{\varkappa}_B | \boldsymbol{\varkappa}_{\bar{B} \setminus B})\} d\pi_B(\boldsymbol{\varkappa}_B) \right]}{Z_V(\boldsymbol{\varkappa}_{\bar{B} \setminus B})} d\mu_\beta(\boldsymbol{\varkappa}, \xi) \\
&\geq \exp\left\{-\beta \left[H(\bar{\omega}_B | \omega_{B^c}) + \frac{\Delta(\omega)}{10} \right]\right\} \int_{\Omega_r(\omega, \bar{B})} \frac{\left[\int_{\Omega_r(\bar{\omega}, \boldsymbol{\varkappa}_{\bar{B} \setminus B})} d\pi_B(\boldsymbol{\varkappa}_B) \right]}{Z_V(\boldsymbol{\varkappa}_{\bar{B} \setminus B})} d\mu_\beta(\boldsymbol{\varkappa}, \xi),
\end{aligned}$$

But the integral $\int_{\Omega_r(\bar{\omega}, \boldsymbol{\varkappa}_{\bar{B} \setminus B})} d\pi_B(\boldsymbol{\varkappa}_B)$ is just the Poisson measure of the set $\Omega_r(\bar{\omega})$, so it is a positive number (not depending on β). The comparison of the last two estimates proves our theorem. \square

Proof of Lemma 3. Using the above ideas it is straightforward. Let $i(n)$ be the maximal number of particles with which any given particle can interact. Suppose a particle ϖ_1 is ρ -close to ϖ_2 . Due to the divergence of the repulsion near the hard core, the energy of the interaction of particles ϖ_1 and ϖ_2 diverges as $\rho \searrow 1$, so we can assume that $U(\varpi_1, \varpi_2) > \lambda + i(n)m + 1$ once $\rho - 1$ is small enough. But then if we erase the particle ϖ_1 , we gain at least one unit of energy. The rest of the argument follows the same line as above. \square

3 Counterexamples

In this section we will explain that some results which one might expect to obtain in this area in fact do not hold.

Let U be some pair potential, which is translation and rotation invariant, i.e. $U(s, t) = U(|s - t|)$. We suppose U to be superstable. Superstability is a property which means that the repulsion part of the interaction dominates the attraction part, see [Ru3] for more details. The Lennard-Jones potential is an example of such an interaction. Let λ be some chemical potential.

Our initial modest goal was to prove that for all reasonable interactions U the following holds:

Statement. *Let $\beta_n \rightarrow \infty$ be a sequence of inverse temperatures, going to infinity, and let μ_n be a weakly converging sequence of Gibbs states, corresponding to the interaction U , chemical potential λ and inverse temperatures*

β_n , i.e. $\mu_n \in \mathcal{G}(U, \lambda, \beta_n)$. Then the limiting state μ_∞ is supported by the set G of ground state configurations.

For every U, λ there exist a pair of constants $\underline{R} < \overline{R}$, such that for every $\omega = \{\omega_k\} \in G$

$$\inf_{i < j} |\omega_i - \omega_j| > \underline{R}, \quad (13)$$

and every ball $B_r \subset \mathbb{R}^n$ of radius $r > \overline{R}$ contains at least one particle $\omega_i \in \omega$.

If true, these properties would be a zero-level approximation to the ordered structure which is expected (in some sense) to be formed by solids. (For the use of these Delone properties in modelling the ground states of quasicrystals see [BHZ, BL, Ke, La, Ra2, RW, VGW].)

We have to say that we do not expect the above picture to hold without extra assumptions, though these assumptions are expected to be mild and physically natural. The following results point to difficulties that must be overcome.

Let $\mu \in \mathcal{G}(U, \lambda, \beta)$ be a Gibbs field with inverse temperature β , and the superstable interaction has attractive part. Denote by $\rho_\mu(x)$ the expected number of particles of the field μ in the unit ball centered at the point $x \in \mathbb{R}^n$.

Proposition 4 *For every λ, β and U without hard core there exists a state $\bar{\mu} \in \mathcal{G}(U, \lambda, \beta)$, such that the function $\rho_{\bar{\mu}}(\cdot)$ is unbounded on \mathbb{R}^n .*

That statement means that the relation (13) cannot hold in general.

Proposition 5 *Suppose that the state $\tilde{\mu} \in \mathcal{G}(U, \lambda, \beta)$ has the density function $\rho_{\tilde{\mu}}(\cdot)$, which is polynomially bounded, i.e. there exists a polynomial $P(\cdot)$, such that $\rho_{\tilde{\mu}}(x) \leq P(x)$, $x \in \mathbb{R}^n$. Then there exists a constant $C = C(U, \lambda)$, such that $\rho_{\tilde{\mu}}(x) \leq C$.*

The proof of Proposition 5 can be obtained by the application of the technique of compact functions, developed by R. Dobrushin in [D4], see also [DP]. Being proven, Proposition 5 can be used to deduce the existence of the constants $\underline{R}, \overline{R}$ above, under condition that the random fields we are dealing with have their density functions polynomially bounded (and hence, uniformly bounded).

Proposition 4 can be derived from Proposition 5 and the following construction. We will consider the 1D case; the generalization to higher dimensions is obvious. Let us suppose that $U(r) \geq 0$ for $r < r_1$, $U(r) < 0$ for

$r_1 < r < r_2$, and $r_1 < 1/3$, $r_2 > 2$. Let I_n be the unit segment centered at the integer point $n \in \mathbb{R}^1$. Let ϖ^{-1}, ϖ^1 be two configurations in the segments I_{-1}, I_1 , and consider the conditional Gibbs distribution $q(\omega^0 | \varpi^{-1}, \varpi^1)$ in I_0 , given configuration $\varpi^{-1} \cup \varpi^1$ outside. Let $K > 0$ be fixed. Clearly, there exists a number $N(1)$, such that if $|\varpi^{-1}| > N(1)$, $|\varpi^1| > N(1)$, then $2K > \mathbb{E}(|\omega^0|) > K$. Indeed, there will be a part of the segment I_0 , where the potential defined by the particles $\varpi^{-1} \cup \varpi^1$ will be attractive (\equiv negative), and the more particles we will have in $\varpi^{-1} \cup \varpi^1$, the deeper this well will be. Let now ϖ^{-2}, ϖ^2 be two configurations in the segments I_{-2}, I_2 , and consider the conditional Gibbs distribution $q(\omega | \varpi^{-2}, \varpi^2)$ in $I_{-1} \cup I_0 \cup I_1$, given configuration $\varpi^{-2} \cup \varpi^2$ outside. Clearly, there exists a number $N(2)$, such that if $|\varpi^{-2}| > N(2)$, $|\varpi^2| > N(2)$, then $\mathbb{E}(|\omega^1|) > N(1)$, $\mathbb{E}(|\omega^{-1}|) > N(1)$, and so again $\mathbb{E}(|\omega^0|) > K$. Here we denote by ω^k the restriction of ω on the segment I_k . If the number $N(2)$ is not too big, then we have in addition that $\mathbb{E}(|\omega^0|) < 2K$. We can repeat this construction inductively in n . As a result, by taking a limit point we get an infinite volume Gibbs state on \mathbb{R}^1 , such that $\mathbb{E}(|\omega^0|) > K$. If K is chosen large enough: $K > C(U, \lambda)$, then the so constructed state has the function $\rho(\cdot)$ unbounded, due to Proposition 5.

In the previous section we presented a proof of our Statement, restricted to the case of interactions with hard core. This assumption plays a technical role, and with an extra effort it can be removed.

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