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Existence of Ground State Configurations

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Abstract. We prove the existence of ground state configurations for systems of infinitely many particles interacting, in d-dimensional Euclidean space, through many-body potentials with hard core.

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1. Introduction

We are concerned with systems of interacting particles in d-dimensional Euclidean space $\mathbb{E}^d$, $d \geq 1$, with particles of one or more species. We assume the interaction includes a hard core, which need not be spherically symmetric, so the system is perhaps better described as interacting molecules or bodies. We will assume fixed some Euclidean invariant interaction potential ϕ, which associates an energy $\phi(C)$, in $\mathbb{R} \cup +\infty$, to any finite collection $C \subset \mathbb{E}^d$ of at least two bodies, subject to the weak conditions listed in the next section.

Heuristically, we are looking for configurations x, spatially extended throughout $\mathbb{E}^d$, which minimize a global energy $H(x)$ which is a sum of contributions, one for each particle/body b in x, of amount

$$\hat{L}(x;b) = -\mu(b) + \sum_{C\subset x,\ C\ni b} \phi(C), \tag{1}$$

where $\mu(b)$ is the chemical potential of b. There is no direct meaning to $H(x)$ since in interesting cases it is infinite; instead we will use the traditional criterion for ground state configurations based on a form of local optimality for all local regions.

To give a proper definition of ground state configurations we first need some notation. For each particle species i, of which there are $M \geq 1$, we assume given some body b_i (that is, a compact, connected set with dense interior and boundary of zero volume, representing the hard core for that species) and chemical potential μ_i. We define X as the space of all possible packings of $\mathbb{E}^d$ by congruent copies of the bodies, with the usual metrizable topology in which two packings are close if, within a large ball around the origin of $\mathbb{E}^d$, the two packings are uniformly close: that is, close in the Hausdorff metric on compact sets [Ra1]. (A collection of bodies forms a packing if their interiors do not intersect.) X is compact in that topology. Assume given a cube $B \subset \mathbb{E}^d$, and two packings $x, y \in X$. Then: $N_i[B;(y,x)]$ will denote the sum of the relative volumes $\mathrm{vol}(b\cap B)/\mathrm{vol}(b)$ of all those bodies b, of species i, such that either $b \in y$, or $b \in x$ and the interior of b intersects the boundary ∂B of B; $\bar{N}[B;(y,x)] = \{N_i[B;(y,x)]\}$; $\bar{\mu} = \{\mu_i\}$; and $\bar{\mu}\cdot\bar{N}[B;(y,x)] = \sum_i \mu_i N_i[B;(y,x)]$. A related but more complicated quantity is the local potential energy defined as follows, using the notation $v[A]$ to denote the volume, and $i(A)$ the interior, of $A \subset \mathbb{E}^d$:

$$\begin{aligned} E[B;(y,x)] = &\sum_{b\in y: b\subset B} \sum_{C\ni b} \phi(C) \\ &+ \sum_{b\in x: i(b)\cap\partial B\neq\emptyset} \frac{v[b\cap B]}{v[b]} \sum_{C'\ni b} \phi(C'). \end{aligned} \tag{2}$$

We are now ready to define ground state configurations.

Definition 1. A configuration x is a ground state configuration (for given $\bar{\mu}$) if for *every* fixed cube $B \subset \mathbb{E}^d$

$$\inf_y \{E[B;(y,x)] - \bar{\mu}\cdot\bar{N}[B;(y,x)]\} = E[B;(x,x)] - \bar{\mu}\cdot\bar{N}[B;(x,x)]. \tag{3}$$

This (traditional) criterion for a configuration x to be a minimizer for the global H is simply that it be locally stable: no change in x in a finite region can lower the contribution to $H(x)$ associated with that finite region. One consequence is that a minimizing configuration has the lowest possible energy density, as computed by averaging over an expanding sequence of regions.

The *existence* of such ground state configurations x is by no means obvious, and proof of their existence is our main result. (We compare this problem with the parallel one for lattice gas models in Section 3.) The special cases of our result in which ϕ only takes the values $+\infty$ and 0 and the chemical potentials μ_i are taken to have special values (appropriate to the bodies b_i), reduces to a theorem of Bowen [B] on completely saturated packings in $\mathbb{E}^d$. One example of this type to which we will refer is the following.

Example 1. Consider configurations in the plane of only one type of body, a unit square, with energy function ϕ consisting only of the hard core, and $\mu = 1$. For this example it is easy to construct ground state configurations, for instance tilings of the plane. The example will be useful below in testing general strategies of proving the existence of ground state configurations.

2. Statement and Proof of Results

We assume our Euclidean invariant interaction potential ϕ satisfies the following general properties:

i) There is some R, larger than twice the diameter of any of the b_i, such that $\phi(C) = 0$ if there is no ball of radius R containing all the bodies of C;
ii) ϕ is finite and continuous when restricted to the manifold of (positions and orientations of) packings of any given finite number, greater than 2, of bodies of given species;
iii) For pairs of bodies, $\phi = +\infty$ if their interiors intersect, ϕ is finite and continuous when the pair does not intersect, and either:
   a) ϕ is finite and continuous on all packings of pairs; or
   b) ϕ is bounded below, has value $+\infty$ for touching pairs, and $\phi \to +\infty$ as the separation of the pair vanishes.

Our main result is the following.

Theorem 1. *For any system of interacting particles/bodies with given interaction ϕ satisfying conditions i)–iii) and given chemical potentials $\bar{\mu}$ there exists a translation invariant probability measure m_L, on the space X of possible packings of the bodies, for which a set of full measure consists of ground state configurations.*

Proof. First we define a function p on X by:

$$p(x) = \begin{cases} c(x), & \text{if the interior of a body } \tilde{b}(x) \text{ of } x \text{ contains } \mathcal{O} \\ 0, & \text{if no body of } x \text{ contains } \mathcal{O} \text{ in its interior} \end{cases} \tag{4}$$

where $\mathcal{O}$ is the origin in $\mathbb{E}^d$ and $c(x) = 1/\text{volume}[\tilde{b}(x)]$. Then we define the function L on X, a density for $\hat{L}$ of (1), by

$$L(x) = p(x)\big[-\mu(x) + \sum_{C\subset x,\ C\ni b(x)} \phi(C)\big] \tag{5}$$

where $b(x)$ is any body in x nearest to $\mathcal{O}$, and $\mu(x)$ is the chemical potential for that species of particle/body. (For completeness, in case one factor in (5) is 0 and the other is $+\infty$ we define the product to be 0, except in those cases where $\mathcal{O}$ is on a boundary of a body in x, in which case we define the product to be $+\infty$.) Note that although $b(x)$ may not specify a particular body, this ambiguity, and therefore that of $\mu(x)$, is irrelevant to $L(x)$ because of the factor $p(x)$; $L(x)$ is nonzero only if some body b of x contains $\mathcal{O}$, and then represents the total energy of interaction of b with the rest of the bodies in x. Note that if $\chi_{_B}$ is the characteristic function for B

$$\int \chi_{_B}(g) L(x-g)\, dg = E[B;(x,x)] - \bar{\mu}\cdot \bar{N}[B;(x,x)]. \tag{6}$$

Let $M(X)$ be the set of Borel probability measures on X in the weak-$*$ topology, which makes $M(X)$ compact, and let $M_I(X)$ be the subset of those measures which are invariant under the natural action of the translation group $\mathcal{G}^d(\approx \mathbb{R}^d)$ of $\mathbb{E}^d$. ($M_I(X)$ is easily seen to be a nonempty closed subset of $M(X)$.)

Lemma 1. *There exists $m_{_L}$ in $M_I(X)$ such that $m_{_L}(L) = \inf\{m(L)\,|\, m\in M_I(X)\}$.*

Proof. We begin by smoothing out a bit the function L. Define $\tilde{L}(x)$ as $\sup\{f(x)\,|\, f$ continuous, and $f(y)\le L(y)$, at all $y\in X\}$. It follows that $\tilde{L}$ is lower semicontinuous on X and bounded below. We consider Borel probability measures as functionals on the space of continuous functions on X, which one extends (with the possible value of $+\infty$) first to over functions and then integrable functions in the usual way [T]. In this sense $\tilde{L}$ is an over function, and, as a function on $M(X)$, and therefore also $M_I(X)$, it is easy to see it is again lower semicontinuous. Therefore by compactness there is some $\tilde{m}\in M_I(X)$ such that $\tilde{m}(\tilde{L}) = \inf\{m(\tilde{L})\,|\, m\in M_I(X)\}$. We claim that $m(L) = m(\tilde{L})$ for all $m\in M_I(X)$. To see this we first note that L and $\tilde{L}$ only differ where L is not lower semicontinuous, and therefore only on the closed set K of packings x such that the origin $\mathcal{O}$ lies on a boundary of a body in x. That this set K has measure zero with respect to any $m\in M_I(X)$ follows easily by applying Birkhoff's pointwise ergodic theorem [W], considered with respect to the action of the translation group on the space X of packings, to the characteristic function of K. This proves the claim, and we can then take $m_{_L} = \tilde{m}$ to complete the proof of Lemma 1. □

Let B_s, for $s>0$, be the cube in $\mathbb{E}^d$ centered at $\mathcal{O}$ and with faces which are distance s from $\mathcal{O}$ and perpendicular to coordinate axes.

Lemma 2. *For each $j \geq 1$ there exists a function $f_j : X \to X$ such that:*

a) *for every $x \in X$, every $v \in \mathbb{E}^d$ with integer coordinates, and with $B_{j,v}$ defined as $B_j - v(2j+R)$, we have* $\inf_y \{E[B_{j,v}; (y,x)] - \bar{\mu} \cdot \bar{N}[B_{j,v}; (y,x)]\} = E[B_{j,v}; f_j(x), x] - \bar{\mu} \cdot \bar{N}[B_{j,v}; f_j(x), x]$;

b) *f_j commutes with all translations $v(2j+R)$, $v \in \mathbb{E}^d$ having integer coordinates;*

c) *f_j is Borel measurable.*

Proof. Intuitively, what f_j will do to x is replace those bodies of x which are (fully) in any of the regions $B_{j,v}$ by a collection of bodies which minimizes the energy associated with that region, while leaving the other bodies of x as they were. Such an energy minimum exists for a given region because of the continuity of ϕ and N; the only difficulty therefore is to ensure conditions b) and c). We can ensure b) by simply choosing the replacement for B_j for each x and then extending to the translated regions appropriately. It is harder to see how to ensure condition c). An example which illustrates the essence of our difficulty with condition c) is Example 1 above, in which the body is B_1. Take the region $B = B_1$ and let x consist of the single body $B_1 + (2,0)$. The minimum of $E[B; (y,x)] - \bar{\mu} \cdot \bar{N}[B; (y,x)]$ is then $-\mu$, while for the translated packings $x - (\epsilon, 0)$ the minimum would be $-\epsilon\mu$ (for arbitrarily small $\epsilon > 0$). In other words, in choosing how to optimize the bodies in B the dependence on those not in B must be taken into account and condition c) requires that this be done measurably. This is a standard selection problem in optimization. From the lower semicontinuity of $E[B; (y,x)] - \bar{\mu} \cdot \bar{N}[B; (y,x)]$ as a function of $(y,x) \in X \times X$, and the obvious fact that the equation

$$\{(y,x) \,|\, E[B; (y,x)] - \bar{\mu} \cdot \bar{N}[B; (y,x)] = \inf_y E[B; (y,x)] - \bar{\mu} \cdot \bar{N}[B; (y,x)]\} \tag{7}$$

is equivalent to

$$\{(y,x) \,|\, E[B; (y,x)] - \bar{\mu} \cdot \bar{N}[B; (y,x)] \leq \inf_y E[B; (y,x)] - \bar{\mu} \cdot \bar{N}[B; (y,x)]\}, \tag{8}$$

it follows that for given x

$$\{y' \,|\, E[B; (y',x)] - \bar{\mu} \cdot \bar{N}[B; (y',x)] = \inf_y E[B; (y,x)] - \bar{\mu} \cdot \bar{N}[B; (y,x)]\} \tag{9}$$

is closed. It then follows by the theorem of Kuratowski and Ryll-Nardzewski [Ro] that there exists a Borel measurable function (selection) $y = y(x)$ such that

$$E[B; (y(x),x)] - \bar{\mu} \cdot \bar{N}[y(x),x)] = \inf_y E[B; (y,x)] - \bar{\mu} \cdot \bar{N}[B; (y,x)]\}, \tag{10}$$

which gives us condition c). This completes the proof of Lemma 2. $\square$

Returning to the proof of Theorem 1, for each $j \geq 1$ we define the measure $\tilde{m}^j_{{}_L}$, on continuous functions h on X, by $\tilde{m}^j_{{}_L}(h) = m_{{}_L}(h \circ f_j)$ using the composition $(h \circ f_j)[x] = h[f_j(x)]$. We note that $\tilde{m}^j_{{}_L}$ is invariant under the group $\mathcal{G}^d_j$ consisting of translations by $v(2j+R)$ for $v \in \mathbb{E}^d$ with integer coordinates: using the notation $h_g(x) = h(x-g)$, $\tilde{m}^j_{{}_L}(h_g) = \tilde{m}_{{}_L}(h_g \circ f_j) = m_{{}_L}([h \circ (f_j)_g]) = m_{{}_L}(h \circ f_j) = \tilde{m}^j_{{}_L}(h)$ for $g \in \mathcal{G}^d_j$, where we used $(f_j)_g[x] = (f_j[x]) - g$ from b) to get the second equality and the invariance of $m_{_L}$ for the third. Now we define $m^j_{_L}$ by averaging $\tilde{m}^j_{_L}$ over (the flat torus) B_j, which clearly makes $m^j_{_L}$ invariant under all of $\mathcal{G}^d$. We then have

$$
\begin{aligned}
m^j_{_L}(L) &= \int \Big[\frac{\int \chi_{_{B_j}}(g) L_g(x)\, d\nu(g)}{\int \chi_{_{B_j}}(g)\, d\nu(g)}\Big]\, d\tilde{m}^j_{_L}(x) \\
&= \int \Big[\frac{\int \chi_{_{B_j}}(g) (L_g \circ f_j)(x)\, d\nu(g)}{\int \chi_{_{B_j}}(g)\, d\nu(g)}\Big]\, dm_{_L}(x).
\end{aligned} \tag{11}
$$

Let $U_{j,n}$ be the set of packings x for which

$$
\inf_y \{E[B_j; (y,x)] - \bar{\mu} \cdot \bar{N}[B_j; (y,x)]\} \le E[B_j; (x,x)] - \bar{\mu} \cdot \bar{N}[B_j; (x,x)] - \frac{1}{n}. \tag{12}
$$

Then

$$
\begin{aligned}
m^j_{_L}(L) &= \int \Big[\frac{\int \chi_{_{B_j}}(g) (L_g \circ f_j)(x)\, d\nu(g)}{\int \chi_{_{B_j}}(g)\, d\nu(g)}\Big] \chi_{_{U_{j,n}}}(x)\, dm_{_L}(x) \\
&\quad + \int \Big[\frac{\int \chi_{_{B_j}}(g) (L_g \circ f_j)(x)\, d\nu(g)}{\int \chi_{_{B_j}}(g)\, d\nu(g)}\Big] \chi_{_{U^c_{j,n}}}(x)\, dm_{_L}(x) \\
&\le \int \Big[\frac{\int \chi_{_{B_j}}(g) L_g(x)\, d\nu(g) - \frac{1}{n}}{\int \chi_{_{B_j}}(g)\, d\nu(g)}\Big] \chi_{_{U_{j,n}}}(x)\, dm_{_L}(x) \\
&\quad + \int \Big[\frac{\int \chi_{_{B_j}}(g) (L_g \circ f_j)(x)\, d\nu(g)}{\int \chi_{_{B_j}}(g)\, d\nu(g)}\Big] \chi_{_{U^c_{j,n}}}(x)\, dm_{_L}(x) \\
&\le m_{_L}(L) - \frac{m_{_L}(\chi_{_{U_{j,n}}})}{n \int \chi_{_{B_j}}(g)\, dg}.
\end{aligned} \tag{13}
$$

Therefore from the optimum property of $m_{_L}$ it follows that $m_{_L}(\chi_{_{U_{j,n}}}) = 0$. But then $m_{_L}(\chi_{_U}) = 0$ for $U = \cup_{j,n} U_{j,n}$, the set of configurations which are not ground states. $\square$

3. Summary

In lattice gas models the sets S_j, of configurations satisfying energy minimization with respect to the cubes B_j, are compact, nonempty, and decreasing as j increases, and therefore have a nonempty intersection. This is the structure of the simple proof for the existence of ground state configurations in lattice gas models [Sc]. However such sets S_j are not compact in some of our continuum models, for instance Example 1. Instead (following Bowen [B]), we get existence of ground state configurations as the countable intersection of sets which are of full measure for $m_{_L}$.

One motivation of this paper is the analysis of the symmetry of low temperature matter, often analyzed as a perturbation of the ground state [Ru], [I], [Si]. Since the discovery of quasicrystals it has been necessary to look within a broader setting than the crystallographic groups for a general understanding of the geometric symmetry of solids [Ra1]-[Ra4], [BHRS]. Coupled with this is the tantalizing, but unsatisfactory, well-known argument [Pi] to explain the experimental nonexistence of a critical point separating the solid and fluid phases of matter, based on a supposed geometric symmetry for solids. There are indeed many ways in which the symmetry of ground state configurations are significant, for which the above existence theorem should be a useful step.

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