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The Convergence of the One-Dimensional Ground States to an Infinite Lattice

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For one-dimensional systems interacting via a two-body potential, the sequence of ground states is proved to converge to an infinite lattice, for a large open class of interactions, containing in particular the Lennard-Jones potential.

KEY WORDS: Classical crystal theory; ground states; structural stability.

1. INTRODUCTION

This paper is the fourth of a series devoted to the classical theory of crystals, and deals with one-dimensional lattices.[(1-4)]

We consider linear systems of identical particles, interacting via a two-body potential, and the sequence of the ground states for these systems, labeled by the number n of particles. Then we prove that, for a large class of realistic potentials (including the Lennard-Jones potential), this sequence converges to a periodic lattice. Moreover, the class of potential is explicitly defined by sufficient conditions bearing on the potential and its two first derivatives.

Our results thus justify in this case the assumption, usually admitted without proof, that the ground states of such systems are lattices, and provide methods for more general cases.

This work makes use of a precise definition of what is meant by convergence toward a lattice: we shall say that a sequence of equilibria converges to a lattice if the average spacings between particles converge to a limit, while the dispersion of these spacings remains bounded, allowing for boundary deformations which are expected, from a physical point of view, to become independant of the size of the system.

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We introduced this definition in a previous paper,[4] in which we established its physical relevance by proving its structural stability: The property for a potential to give rise to a lattice in the above sense is preserved under perturbation.

The problem of the infinite volume ground state has been recently studied by Gardner and Radin.[5] These authors, dealing with the Lennard-Jones potential, proved by direct calculations that the spacings between neighboring particles tend, in the infinite volume limit, to a unique limit.

The results presented in this work are more general and more precise: more general, because they deal with a whole class of potentials ruled by fairly weak conditions, and more precise, because our definition of the convergence toward a lattice provides a control of the boundary effects.

2. DEFINITIONS AND METHODS

The configuration space of $n+1$ particles in one dimension is given by

$$Q^{(n+1)} = \{q \in \mathbb{R}^{n+1} \mid q_i < q_{i+1}, i = 1,..., n\} \tag{2.1}$$

The translation invariance of the system is taken into account by reducing the configuration space to

$$X^{(n)} = \{x \in \mathbb{R}^n \mid x_i > 0, i = 1,..., n\} \tag{2.2}$$

where $x_i = q_{i+1} - q_i$. Let $\varphi \in C^\infty(]0, \infty[)$ specify the two-body interaction. Then one easily checks that the potential energy $\varphi^{(n)} \in C^\infty(X^{(n)})$ of $n+1$ particles is defined by

$$\varphi^{(n)}(x) = \sum_I{}^{(n)} \varphi(x_I) \tag{2.3}$$

where the summation $\sum_I^{(n)}$ runs over all intervals $I = \{j, j+1,..., k-1, k\}$ in the set $\{1,..., n\}$ and where $x_I = \sum_{i \in I} x_i$, i.e., $x_I = q_{k+1} - q_j$. In the following, $|I|$ denotes the number of elements of I; thus, for instance, $|I| = 1$ corresponds to neighboring particles q_j and q_{j+1}.

A configuration $x \in X^{(n)}$ is an equilibrium iff the differential $d\varphi^{(n)}(x)$ vanishes, i.e., all partial derivatives vanish at x.

The components of $d\varphi^{(n)}(x)$ are easily derived from (2.3):

$$(d\varphi^{(n)}(x))_i = \frac{\partial \varphi^{(n)}}{\partial x_i}(x) = \sum_{I \ni i}{}^{(n)} \varphi'(x_I) \tag{2.4}$$

Let $H_x \varphi^{(n)}$ denote the $n \times n$ symmetric matrix of the second derivatives of $\varphi^{(n)}$ at x.

If x is an equilibrium configuration for $\varphi^{(n)}$, $H_x\varphi^{(n)}$ is just the Hessian of $\varphi^{(n)}$ at x, which describes the mechanical stability of the given equilibrium. For any $x \in X^{(n)}$

$$(H_x\varphi^{(n)})_{ij} = \frac{\partial^2\varphi^{(n)}}{\partial x_i\,\partial x_j}(x) = \sum_{I \ni i,j}^{(n)} \varphi''(x_I) \tag{2.5}$$

which is equivalent to

$$H_x\varphi^{(n)} = \sum_{i,j}^{(n)} \sum_{I \ni i,j}^{(n)} \varphi''(x_I)\, dx_i \otimes dx_j$$

If $H_x\varphi^{(n)}$ is of maximal rank, then the equilibrium configuration x is mechanically stable iff the Hessian is positive definite, as a quadratic form on $\mathbb{R}^n$. Moreover, the spectrum of $H_x\varphi^{(n)}$ is directly linked to the phonon spectrum of the system which is derived from the Hessian of the energy with respect to absolute positions q_i, $i = 1,\dots, n+1$.

In a previous paper,[4] we proposed a definition of the property for an interaction φ to give rise to a lattice, as a limit of finite equilibrium configurations.

We proved then that this property is structurally stable, i.e., if a given interaction φ gives rise to a lattice according to this definition, then all neighboring interactions share the same property.

Let P be the projection operator on $\mathbb{R}^n$, given by

$$Px = \bar{x} \qquad \text{with} \quad \bar{x}_i = n^{-1} \sum_j^{(n)} x_j \tag{2.6}$$

Then $\bar{x}$ is a configuration with a constant spacing equal to the mean spacing of x.

Definition 2.1. For any $n \geqslant 1$ and $x \in X^{(n)}$, we define the dispersion $\sigma(x)$ and the mean spacing $\tau(x)$ by

$$\sigma(x) = \|x - \bar{x}\| = \|(1-P)x\| \tag{2.7}$$

$$\tau(x) = n^{-1/2}\,\|\bar{x}\| = n^{-1/2}\,\|Px\| \tag{2.8}$$

Then obviously $\|x\|^2 = \sigma(x)^2 + n\tau(x)^2$ and $\tau(x) = |\bar{x}_i|$.

The mechanical stability of an equilbrium configuration x implies a lower bound on the Hessian, holding in some neighborhood of x.

A convenient basis of such neighborhoods is given by

$$\Omega(x;\alpha,\beta) = \{y \in X^{(n)} \mid \sigma(y-x) < \alpha,\ \tau(y-x) < \beta\} \tag{2.9}$$

for any $\alpha, \beta > 0$.

Definition 2.2. Let $\varphi \in C^\infty(]0, \infty[)$ be a two-body interaction. Then φ is said to give rise to a lattice if there exists a sequence $\{x_{(n)}\}$ of stable equilibrium configurations of $n+1$ particles such that the following conditions hold:

L1. There exist constants $\alpha, \beta > 0$ and $\mu > 0$, such that for n large enough

$$H_y \varphi^{(n)} > \mu, \text{ for any } y \in \Omega(x_{(n)}; \alpha, \beta) \tag{2.10}$$

where $H_y \varphi^{(n)}$ is the Hessian of $\varphi^{(n)}$ at y.

L2. There exists a constant $s > 0$ such that for n large enough

$$\sigma(x_{(n)}) < s$$

L3. There exists a constant $a > 0$ such that

$$\lim \tau(x_{(n)}) = a$$

The physical meaning of this definition is discussed in (4) where its structural stability is proved.

In this paper we are exclusively concerned with the ground state problem. The main result consists in the proof that for a large class of two-body interactions $\mathscr{C}$, the corresponding ground-states $x_{(n)}$ converge to a lattice according to the above definition.

The conditions defining the class $\mathscr{C}$ will be introduced in the following sections: In Section 3 we give sufficient conditions on the interaction φ implying that any equilibrium configuration $x_{(n)}$ of $\varphi^{(n)}$ satisfies an uniform estimate of the form $r_0 < x_i < r_1$, $i = 1,..., n$, where r_0 and r_1 only depend on φ.

As we shall see, a divergence as low as $\varphi(r) \simeq r^{-1}$ is possible at the origin. In Section 4, we obtain sufficient conditions for $\varphi^{(n)}$ to be a strictly convex function in given neighborhoods of the form

$$K^{(n)}(s_0, s_1) = \{x \in X^{(n)} \mid s_0 < x_i < s_1, i = 1,..., n\}$$

The class $\mathscr{C}$ is defined in such a way that the convexity of $\varphi^{(n)}$ holds at least in $K^{(n)}(r_0, r_1)$, which contains therefore the unique equilibrium configuration of the system.

Then in Section 5 we prove that the sequence of ground states thus obtained, converges to the one-dimensional lattice of spacing a, corresponding to the absolute minimum of the energy per particle $e(r) = \sum_{p \geqslant 1} \varphi(pr)$.

The different conditions are proved to be satisfied in particular by the Lennard-Jones potential $\varphi_{LJ}(r) = r^{-12} - r^{-6}$, which therefore belongs to $\mathscr{C}$.

3. BOUNDS ON THE SPACINGS OF EQUILIBRIUM CONFIGURATIONS

In this section we derive upper and lower bounds on the spacings x_i of any equilibrium configuration $x_{(n)} = (x_1,..., x_n)$, for an interaction φ satisfying the conditions given in the following definition.

Definition 3.1. Let $\mathscr{C}_0$ be the class of interactions $\varphi \in C^\infty(]0, \infty[)$ such that the following conditions hold:

(1) $\exists r_1 > 0$ such that

$$\varphi'(r) < 0 \quad \text{for} \quad 0 < r < r_1 \qquad \text{and} \qquad \varphi'(r) > 0 \quad \text{for } r > r_1 \tag{3.1}$$

(2) $\exists r_2 > 0$ such that

$$\varphi''(r) > 0 \quad \text{for } 0 < r < r_2 \qquad \text{and} \qquad \varphi''(r) \leqslant 0 \quad \text{for} \quad r \geqslant r_2 \tag{3.2}$$

(3) The series $e'(r) = \sum_{p \geqslant 1} p\varphi'(pr)$ is convergent for $r > 0$ and $\exists r_0 > 0$ such that $0 < r < r_0$ implies

$$e'(r) + \sum_{1 < p \leqslant N} p(\varphi'(r_2) - \varphi'(pr)) < 0 \tag{3.3}$$

where $N = E(r_2/r)$ is the integer part of r_2/r and where the sum stands for zero if $N \leqslant 1$.

These conditions define a large class of interactions, actually an open one for the Whitney topology of $C^\infty(]0, \infty])$,[6] which contains for instance the Lennard-Jones potential $\varphi_{LJ}(r) = r^{-12} - r^{-6}$.

In this case, $r_1 \simeq 1.122$, $r_2 \simeq 1.244$ and one checks that $r_0 = 1.119$ satisfies the third condition. More generally, we have

Lemma 3.1. For any $\varphi \in \mathscr{C}_0$, the following holds:

$$0 < r_0 \leqslant a_0 < r_1 < r_2 \tag{3.4}$$

where a_0 is the first root of $e'(r) = 0$.

Proof. Since $\varphi'(r_2) = \int_{r_1}^{r_2} \varphi''(r)\, dr$, (3.1) and (3.2) are compatible only if $r_1 < r_2$.

Now, $e'(r) > 0$ for $r \geqslant r_1$, thus $e'(a_0) = 0$ implies $a_0 < r_1$. Finally, it follows from (3.3) that $r_0 \leqslant a$ for any root of $e'(r) = 0$. ∎

Actually, in the Lennard-Jones case, r_0 is equal to the unique solution $a \simeq 1.119$ of $e'(r) = 0$. Notice that for $r > r_2/2$, (3.3) reduces to $e'(r) < 0$. If $N = E(r_2/r) \geqslant 2$, (3.3) then reads

$$\varphi'(r) + [N(N+1)/2 - 1]\, \varphi'(r_2) + \sum_{p \geqslant N+1} p\varphi'(pr) < 0 \tag{3.5}$$

One easily checks that the second and third terms of (3.5) diverge as r^{-2} at the origin. It follows then that $r_0 = a_0$, first root of $e'(r) = 0$, will satisfy condition (3.3), if φ' diverges fast enough at the origin.

Theorem 3.1. For any $\varphi \in \mathscr{C}_0$ and all $n \geqslant 2$, any equilibrium configuration $x_{(n)} = (x_1,..., x_n)$ of $\varphi^{(n)}$ satisfies $r_0 < x_i \leqslant r_1$ for $i = 1,..., n$.

Proof. The upper bound is trivial since the interaction is supposed to be attractive for all $r > r_1$.

Let $x_{(n)} = (x_1,..., x_n)$ be an equilibrium configuration for $\varphi^{(n)}$ and let $r = \operatorname{Inf}\{x_i\} = x_k$ for some k.

Then, using (2.4), the equilibrium condition $d\varphi^{(n)}(x_{(n)}) = 0$ implies

$$0 = \varphi'(r) + \sum_{\substack{I \ni k \\ |I| > 1}}^{(n)} \varphi'(x_I)$$

$$0 = \varphi'(r) + \sum_{\substack{I \ni k \\ 1 < |I| \leqslant N}}^{(n)} \varphi'(x_I) + \sum_{\substack{I \ni k \\ |I| \geqslant N+1}}^{(n)} \varphi'(x_I) \tag{3.6}$$

Let $N = E(r_2/r)$, so that $N \leqslant r_2/r < N + 1$.

The first sum of (3.6) is certainly bounded by $[N(N + 1)/2 - 1]\, \varphi'(r_2)$. For any term in the second sum, we have $x_I \geqslant |I|\, r \geqslant (N + 1)r > r_2$, and therefore, using (3.2), $\varphi'(x_I) \leqslant \varphi'(|I|\, r)$. Thus

$$0 \leqslant \varphi'(r) + [N(N + 1)/2 - 1]\, \varphi'(r_2) + \sum_{p \geqslant N+1} p\varphi'(pr)$$

In view of (3.3), such a condition implies $r > r_0$, which achieves the proof. ∎

In the case of the Lennard-Jones potential, the accuracy of the bounds $1.119 < x_i \leqslant 1.122$ is almost unexpected, and suggests that boundary effects can be very small. But as precise as the estimate is, the existence of many equilibrium configurations is not ruled out, and the convergence to a simple lattice is not yet ensured. This is the purpose of the following sections.

4. CONVEXITY OF THE N-BODY POTENTIAL AND MECHANICAL STABILITY

In this section we give sufficient conditions on the interaction φ, for the n-body potential $\varphi^{(n)}$ to satisfy a certain convexity property in the configuration space.

The convexity of $\varphi^{(n)}$, as a function of $x = (x_1,..., x_n)$, is directly connected to the Hessian $H_x\varphi^{(n)}$ defined in Section 2. A positive definite Hessian in a convex domain implies the convexity of $\varphi^{(n)}$ and the existence of at most one equilibrium configuration in that domain, which is therefore mechanically stable.

The sufficient conditions given in this section express the idea that the nearest-neighbour terms of the Hessian dominate the others, which seems to be the rule as well for real three-dimensional lattices. Let $H_x\varphi^{(n)} = h^{(n)} = \sum_{p=1}^{n} h^{(n,p)}$ with

$$h^{(n,p)} = \sum_{i,j}^{(n)} \sum_{\substack{I \ni i,j \\ |I|=p}}^{(n)} \varphi''(x_I)\, dx_i \otimes dx_j \tag{4.2}$$

Then we have the following.

Lemma 4.1. For any $x \in X^{(n)}$, and $p = 1,\dots, n$ the following bounds hold:

$$-p^2 \sup_{|I|=p} \{|\varphi''(x_I)|\}\, Id \leqslant h^{(n,p)} \leqslant p^2 \sup_{|I|=p} \{|\varphi''(x_I)|\}\, Id \tag{4.3}$$

where the inequality is that of symmetric operators on $\mathbb{R}^n$ and Id is the unit operator.

Proof. For any $p = 1,\dots, n$ and $\varepsilon = \pm 1$ define

$$M_\varepsilon^{(n,p)} = p^2 \sup_{|I|=p} \{|\varphi''(x_I)|\}\, Id + \varepsilon h^{(n,p)} \tag{4.4}$$

Then $M_\varepsilon^{(n,p)}$ is a symmetric operator and a classical theorem asserts that $M_\varepsilon^{(n,p)}$ is positive as soon as its matrix elements satisfy

$$(M_\varepsilon^{(n,p)})_{ii} \geqslant \sum_{j \neq i} |(M_\varepsilon^{(n,p)})_{ij}| \qquad \text{for} \quad i = 1,\dots, n$$

Consider the diagonal term

$$\begin{aligned}(M_\varepsilon^{(n,p)})_{ii} &= p^2 \sup_{|I|=p} \{|\varphi''(x_I)|\} + \varepsilon \sum_{\substack{I \ni i \\ |I|=p}}^{(n)} \varphi''(x_I) \\ &\geqslant (p^2 - p) \sup_{|I|=p} \{|\varphi''(x_I)|\} \end{aligned} \tag{4.5}$$

Consider now an off-diagonal term

$$|(M_\varepsilon^{(n,p)})_{ij}| \leqslant \sum_{\substack{I \ni i,j \\ |I|=p}}^{(n)} |\varphi''(x_I)|$$

If $p < |i-j|$, then no interval I of p points can connect i and j, so that $(M_\varepsilon^{(n,p)})_{ij} = 0$.

If $p \geqslant |i-j|$, there exist at most $p-|i-j|$ such intervals and $|(M_\varepsilon^{(n,p)})_{ij} \leqslant (p-|i-j|) \sup_{|I|=p}\{|\varphi''(x_I)|\}$. Therefore

$$\sum_{j\neq i} |(M_\varepsilon^{(n,p)})_{ij}| \leqslant \sum_{j=i-p}^{i+p} (p-|i-j|) \sup_{|I|=p} \{|\varphi''(x_I)|\}$$

$$\leqslant 2 \sum_{k=1}^{p} (p-k) \sup_{|I|=p} \{|\varphi''(x_I)|\}$$

$$\leqslant (p^2-p) \sup_{|I|=p} \{|\varphi''(x_I)|\} \tag{4.6}$$

It follows from (4.5) and (4.6) that $M_\varepsilon^{(n,p)} \geqslant 0$ for $\varepsilon = \pm 1$, and thus

$$-p^2 \sup_{|I|=p} \{|\varphi''(x_I)|\}\, Id \leqslant h^{(n,p)} \leqslant p^2 \sup_{|I|=p} \{|\varphi''(x_I)|\}\, Id$$

which completes the proof. ∎

Now, using this lemma, we derive an upper and a lower bound for the Hessian $H_x\varphi^{(n)}$ in domains of the form

$$K^{(n)}(s_0, s_1) = \{x \in X^{(n)} \mid s_0 < x_i < s_1, i = 1,..., n\}$$

Theorem 4.1. For any $\varphi \in C^\infty(]0,\infty[)$ and any $0 < s_0 < s_1$, the following bounds hold for all $x \in K^{(n)}(s_0, s_1)$:

$$\{\inf_{(s_0,s_1)} \{\varphi''(r)\} - \sum_{p>1} p^2 \sup_{(s_0,s_1)} \{|\varphi''(pr)|\}\}\, Id \leqslant H_x\varphi^{(n)}$$

$$\leqslant \{\sup_{(s_0,s_1)} \{\varphi''(r)\} + \sum_{p>1} p^2 \sup_{(s_0,s_1)} \{|\varphi''(pr)|\}\}\, Id \tag{4.7}$$

Proof. The first term of the decomposition of $H_x\varphi^{(n)}$ defined by (4.2), is given by

$$h^{(n,1)} = \sum_i{}^{(n)} \varphi''(x_i)\, dx_i \otimes dx_i \tag{4.8}$$

Then $h^{(n,1)}$ is clearly a diagonal operator which corresponds exactly to the nearest-neighbour terms of the total Hessian. Therefore

$$\inf_{(s_0,s_1)} \{\varphi''(r)\}\, Id \leqslant h^{(n,1)} \leqslant \sup_{(s_0,s_1)} \{\varphi''(r)\}\, Id \tag{4.9}$$

For any $x \in K^{(n)}(s_0, s_1)$, $|I|\, s_0 < x_I < |I|\, s_1$, and (4.7) follows from (4.9) and Lemma 4.1. ∎

In Section 3, we proved that for any $\varphi \in \mathscr{C}_0$ and for all $n \geqslant 2$, the possible equilibrium configurations of $\varphi^{(n)}$, all belong to $K^{(n)}(r_0, r_1)$ where r_0, r_1 are independent of n. It is therefore natural to investigate the convexity of $\varphi^{(n)}$ is this domain. We now define a class of interactions for which the lower bound given in the above theorem reads in a very simple way.

Definition 4.1. Let $\mathscr{C}$ be the class of interactions $\varphi \in \mathscr{C}_0$ (see Section 3), such that the following conditions hold:

(1) The first root r_2 of $\varphi''(r) = 0$, and r_0, defined by (3.3), are such that

$$r_2 < 2r_0 \tag{4.10}$$

(2) φ'' is decreasing in $]r_0, r_1[$ and increasing in $]2r_0, \infty[$.

(3) The series $e''(r) = \sum_{p \geqslant 1} p^2 \varphi''(pr)$ is convergent for $r > 0$ and

$$\mu(\varphi) = e''(r_0) + \varphi''(r_1) - \varphi''(r_0) > 0 \tag{4.11}$$

(4) The series $\sum_{p>1} p^2 |\varphi'(pr)|$ is convergent for $r > 0$.

These conditions define an open class of interactions for the Whitney topology of $C^\infty(]0, \infty[)$, which contains the Lennard-Jones potential. In this particular case, $r_0 \simeq 1.119$ and $r_2 \simeq 1.244$ satisfy (4.10); φ'''_{LJ} has a unique root $r_3 \simeq 1.366$ and this insures condition (2). Finally, $\mu(\varphi_{LJ}) \simeq 14$.

We observed in Lemma 3.1 that for any $\varphi \in \mathscr{C}_0$, the possible roots of $e'(r) = 0$ all belong to (r_0, r_1). A consequence of the following theorem is that for $\varphi \in \mathscr{C}$, $e(r)$ is convex in (r_0, r_1), but the most important result concerns the ground state.

Theorem 4.2. For any $\varphi \in \mathscr{C}$, and all $n \geqslant 2$, $\varphi^{(n)}$ has a unique equilibrium configuration $x_{(n)}$ in $X^{(n)}$, therefore its ground-state, which lies in $K^{(n)}(r_0, r_1) = \{x \in X^{(n)} \mid r_0 < x_i < r_1;\ i = 1,\dots, n\}$.

Proof. Since $\mathscr{C} \subset \mathscr{C}_0$, we already know, from Theorem 3.1 that all equilibrium configurations of $\varphi^{(n)}$ belong to $K^{(n)}(r_0, r_1)$. The uniqueness will follow from the convexity of $\varphi^{(n)}$ in this domain. In view of Theorem 4.1, it is sufficient to prove that

$$\inf_{(r_0, r_1)} \{\varphi''(r)\} - \sum_{p>1} p^2 \sup_{(r_0, r_1)} \{|\varphi''(pr)|\} > 0 \tag{4.12}$$

Now, since φ'' is decreasing in $]r_0, r_1[$, $\inf_{(r_0, r_1)}\{\varphi''(r)\} = \varphi''(r_1)$.

For any term in the sum, $pr \geqslant 2r_0 \geqslant r_2$. Thus $|\varphi''(pr)| = -\varphi''(pr)$ and since $-\varphi''$ is assumed to decrease, $\sup_{(r_0, r_1)}\{|\varphi''(pr)|\} = -\varphi''(pr_0)$.

Therefore, the lower bound for the Hessian reads $\varphi''(r_1) + \sum_{p>1} p^2\varphi''(pr_0)$, which is clearly equal to $\mu(\varphi)$ defined by (4.11), and condition (3) insures the convexity, which achieves the proof. ∎

Notice that the conditions (1), (2), and (3) of Definition 4.1 are sufficient but not necessary to insure the convexity of $\varphi^{(n)}$ in $K^{(n)}(r_0, r_1)$. Actually, they have the advantage of involving φ and e in a very simply way.

In a classical series of papers, M. Born and coworkers[7] derived the mechanical stability of an infinite lattice with respect to infinitesimal periodic perturbations, using an elementary version of the conditions of Definition 4.1. The above theorem improves this particular result in two directions: first, the mechanical stability holds in an open neighborhood of the equilibrium configuration, and second, this property is satisfied uniformly for all finite systems.

As a final remark, we observe that the convexity of $\varphi^{(n)}$ may hold in a larger domain than $K^{(n)}(r_0, r_1)$. Actually, if s_0, s_1 are such that $0 < s_0 < s_1$, with $r_2 < 2s_0$, if φ'' is decreasing in $]s_0, s_1[$ and increasing in $]2s_0, \infty[$, then a uniform lower bound of $H_x\varphi^{(n)}$, for $x \in K^{(n)}(s_0, s_1)$, is given by $e''(s_0) + \varphi''(s_1) - \varphi''(s_0)$.

In the case of the Lennard-Jones potential, for instance, this lower bound is strictly positive for $s_0 = 1$ and $s_1 = 1.22$.

5. CONVERGENCE OF FINITE EQUILIBRIUM CONFIGURATIONS TO AN INFINITE LATTICE

In this last section, we prove that for any $\varphi \in \mathscr{C}$, the sequence of ground states $x_{(n)}$ of $\varphi^{(n)}$ converges to an infinite lattice, according to an appropriate definition given in Section 2.

Recall that $\mathscr{C}$ is the set of interactions $\varphi \in C^\infty(]0, \infty[)$ such that the following conditions hold:

(1) $\exists r_1 > 0$ such that $\varphi' < 0$ in $]0, r_1[$ and $\varphi' > 0$ in $]r_1, \infty[$.

(2) $\exists r_2 > 0$ such that $\varphi'' > 0$ in $]0, r_2[$ and $\varphi'' \leqslant 0$ in $[r_2, \infty[$.

(3) The series $e'(r) = \sum_{p \geqslant 1} p\varphi'(pr)$, $e''(r) = \sum_{p \geqslant 1} p^2\varphi''(pr)$ and $\sum_{p>1} p^2 |\varphi'(pr)|$ are convergent for $r > 0$.

(4) $\exists r_0 > r_2/2$ such that φ'' is decreasing in $]r_0, r_1[$, increasing in $]2r_0, \infty[$; moreover $e''(r_0) + \varphi''(r_1) - \varphi''(r_0) > 0$ and $r < r_0$ implies $e'(r) + \sum_{1<p\leqslant N} p(\varphi'(r_2) - \varphi'(pr)) < 0$, where $N = E(r_2/r)$ is the integer part of r_2/r.

Under the above conditions, the ground states $x_{(n)}$ of $\varphi^{(n)}$ have been proved to belong to $K^{(n)}(r_0, r_1) = \{x \in X^{(n)} \mid r_0 < x_i < r_1,\ i = 1,..., n\}$. But so far, the convergence of the ground states to a complex or even to an incommensurate lattice is not yet ruled out. This is the purpose of the following theorem.

Theorem 5.1. For any $\varphi \in \mathscr{C}$, the sequence of ground states $x_{(n)}$ of $\varphi^{(n)}$ satisfies the following bound:

$$\|x_{(n)} - a_{(n)}\| \leqslant [e''(r_0) + \varphi''(r_1) - \varphi''(r_0)]^{-1}(2D_1D_2)^{1/2} \tag{5.1}$$

where $a_{(n)} = (a,..., a)$, a is the unique root of $e'(r) = 0$ and

$$D_1 = \sum_{p>1} p\,|\varphi'(pa)| \tag{5.2}$$

$$D_2 = \sum_{p>1} p^2\,|\varphi'(pa)| \tag{5.3}$$

Proof. We prove in Lemma 3.1 that $r_0 \leqslant a < r_1$ thus $a_{(n)}$ belongs to the closure of $K^{(n)}(r_0, r_1)$.

Let $x_\lambda = \lambda a_{(n)} + (1-\lambda)\,x_{(n)}$ for $\lambda \in [0, 1]$. Then

$$d\varphi^{(n)}(a_{(n)}) - d\varphi^{(n)}(x_{(n)}) = \int_0^1 d\lambda\,\frac{\partial}{\partial\lambda}\,(d\varphi^{(n)}(x_\lambda))$$

which reads

$$d\varphi^{(n)}(a_{(n)}) = \int_0^1 d\lambda\,H_{x_\lambda}\varphi^{(n)}(a_{(n)} - x_{(n)}) \tag{5.4}$$

Since the whole path x_λ, $\lambda \in [0, 1]$ is in the closure of $K^{(n)}(r_0, r_1)$ the lower bound $e''(r_0) + \varphi''(r_1) - \varphi''(r_0)$ for $H_{x_\lambda}\varphi^{(n)}$ holds. Therefore $\int_0^1 d\lambda\,H_{x_\lambda}\varphi^{(n)}$ is positive definite and

$$a_{(n)} - x_{(n)} = \left[\int_0^1 d\lambda\,H_{x_\lambda}\varphi^{(n)}\right]^{-1} d\varphi^{(n)}(a_{(n)}) \tag{5.5}$$

which implies

$$\|x_{(n)} - a_{(n)}\| \leqslant [e''(r_0) + \varphi''(r_1) - \varphi''(r_0)]^{-1}\,\|d\varphi^{(n)}(a_{(n)})\| \tag{5.6}$$

Now $d\varphi^{(n)}(a_{(n)}) = \sum_i^{(n)}[\sum_{I\ni i}^{(n)}\varphi'(|I|\,a)]\,dx_i$ and since $e'(a) = \sum_{p\geqslant 1} p\varphi'(pa) = 0$, we have for any component i, $1 \leqslant i \leqslant n$:

$$\sum_{I\ni i}^{(n)}\varphi'(|I|\,a) = -\sum_{\substack{I\ni i\\ I\not\subset\{1,...,n\}}}\varphi'(|I|\,a)$$

where the second sum extends to all intervals I containing i but not included in $\{1,..., n\}$. Therefore

$$\left| \sum_{I \ni i}^{(n)} \varphi'(|I|\, a) \right| \leqslant \sum_{p > \inf\{i, n-i+1\}} p\, |\varphi'(pa)|$$

Then

$$\begin{aligned} \|d\varphi^{(n)}(a_{(n)})\|^2 &\leqslant 2 \sum_{i \geqslant 1} \left(\sum_{p > i} p\, |\varphi'(pa)| \right)^2 \\ &\leqslant 2 \left(\sum_{p > 1} p\, |\varphi'(pa)| \right) \sum_{i \geqslant 1} \sum_{p > i} p\, |\varphi'(pa)| \\ &\leqslant 2 \left(\sum_{p > 1} p\, |\varphi'(pa)| \right) \left(\sum_{p > 1} p^2\, |\varphi'(pa)| \right) \end{aligned}$$

The bound (5.1) follows then from (5.6) and the definitions (5.2) and (5.3). ∎

The proof of the convergence of the sequence of ground states to a lattice, according to definition (2.2), is now straightforward:

The mechanical stability is already insured by $\varphi \in \mathscr{C}$. Now, one easily checks that $\|x_{(n)} - a_{(n)}\|^2 = \sigma(x_{(n)})^2 + n[\tau(x_{(n)} - a)]^2$, where σ and τ are the dispersion and mean spacing defined by (2.7) and (2.8). The uniform bound on $\|x_{(n)} - a_{(n)}\|$ given in the above theorem implies a similar bound for the dispersion $\sigma(x_{(n)})$, and the convergence of the mean spacings $\tau(x_{(n)})$ to a.

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