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Structural stability of classical lattices in one dimension

by

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ABSTRACT. — We prove the structural stability of the property for a two-body potential to give rise to a one-dimensional lattice in some suitable sense: it is required that a sequence of stable equilibria of n particles exists, such that in the limit $n \to \infty$, the average spacings converge, the dispersions remain bounded and some uniformity of the stability is assumed. Then all neighboring potentials satisfy similar conditions, thus providing open sets of interactions in the Whitney topology, which give rise to lattices in the above sense. Moreover, assuming further realistic conditions on the potential, we prove the structurally stable lattice to be and to remain the ground state.

RÉSUMÉ. — On démontre la stabilité structurelle de la propriété, pour un potentiel à deux corps, de produire un réseau cristallin à une dimension, en un sens convenable : on suppose, pour un potentiel donné, l'existence d'une suite d'équilibres stables de n particules tels que dans la limite $n \to \infty$, les espacements moyens convergent et les dispersions restent bornées, et on suppose une certaine uniformité de la stabilité. Alors tous les potentiels voisins satisfont des conditions similaires, ce qui fournit des ensembles d'interactions, ouverts pour la topologie de Whitney, produisant des réseaux cristallins au sens précédent. En outre, avec des hypothèses supplémentaires réalistes sur les potentiels, on montre que les réseaux cristallins structurellement stables sont et restent les états fondamentaux.

I. INTRODUCTION

This paper is the third of a series devoted to the classical theory of crystals, and deals with one-dimensional lattices. The problem is to show that, for realistic two body potentials, the corresponding ground states, i. e. configurations with minimum energy per particle, present symmetries of crystal type. Up to now, rigorous results have been obtained essentially for one-dimensional systems.

To illustrate the specificity of our own work, let us briefly recall these results: Radin et al. [1], [3], have studied the limit $n \to \infty$ of the sequence of ground states of n particles interacting via a Lennard Jones potential: the authors show that the sequence converges to a periodic lattice when $n \to \infty$. However, it is physically required to discuss the stability of such a convergence property. The point is that, unless the potentials are completely specified by the physical theory, as in the Coulomb case, one usually deals with more or less phenomenological expressions for them. In such a situation, the relevance of the conclusions depends on their stability with respect to physically allowed variations of these potentials, which requires a discussion of topological properties.

This approach is implicit in the work of Ventevögel and Nijboer, [4] [6], who studied the mechanical stability of (one-dimensional) infinite periodic equilibrium configurations, with respect to periodic perturbations of arbitrary length. The authors define a class of potentials such that there is a unique periodic configuration that minimizes the energy per particle (in the set of all periodic configurations), this equilibrium being moreover stable with respect to all perturbations (of arbitrary length) of the positions.

The main difficulty of this approach is that one deals directly with infinite systems: the total potential energy is then infinite and one must consider the energy per particle, the definition of which only makes sense under periodicity assumptions. Moreover, infinite systems do no exist in Nature, and are meaningful only insofar as they allow for a simple description of properties independant of the size of the system.

We have thus been led to the following characterisation of a one-dimensional lattice: we shall say that a potential gives rise to a one-dimensional lattice if there exists a family of equilibrium configurations of n particles ($n \to \infty$), interacting via this potential, such that the average spacings between particles converge to a limit while the dispersion of the spacings remains bounded. Note that we can't expect the dispersion to tend to zero, since it contains at least the boundary deformations of the configurations, which, from a physical point of view, are expected to become independant of the size of the system.

Our results consist mainly in the proof of the stability of the above property, with respect to variations of the potential. This yields *ipso facto* open sets of potentials (in the Whitney topology) that generate lattices: In fact, it is easy to find finite range potentials that obviously generate lattices. Our result asserts the existence of neighborhoods of such potentials containing decreasing infinite range potentials, all of them giving rise to lattices.

However, this framework seems to be too general to insure the structural stability of these lattices being the ground states. In fact, assuming further realistic conditions on the potential, we prove that the sequence of equilibria that converges to the structurally stable lattice corresponds to the ground states.

In a previous paper [7], we developed methods based on functional analysis to study the equilibrium configurations of finite systems in one dimension; the next section is devoted to some recalls of this work, which are used in the sequel. In section III, we obtain a family of estimates which allow us to bound the variations of the average spacing and of the dispersion under a variation of the potential.

In section IV, we prove the stability of the convergence property for the mean spacings, from which our main stability theorem follows. Then, in section V, we discuss the problem of the sequence of ground states converging to a lattice.

II. NOTATIONS AND PREVIOUS RESULTS

The configuration space of $n + 1$ particles with a hard core of diameter $c > 0$, in one dimension, is

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

The interaction is specified by a translation and reflection invariant two-body potential, described by a function $\varphi \in C^\infty([c, \infty[)$.

It is convenient to take into account the translation invariance of the systems by reducing the configuration spaces to

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

where $x_i = q_{i+1} - q_i$. $Q^{(n+1)}$ and $X^{(n)}$ are open submanifolds of $\mathbb{R}^{n+1}$ and $\mathbb{R}^n$ respectively.

Let $\varphi^{(n)} \in C^\infty(X^{(n)})$ denote the potential energy of $n + 1$ particles. Then

$$\varphi^{(n)}(x) = \sum_{I}^{(n)} \varphi(x_I) \tag{2}$$

where the summation $\sum_{\mathrm{I}}^{(n)}$ runs over all intervals $\mathrm{I} = \{j, j+1, \ldots, k-1, k\}$ in the set $\{1, \ldots, n\}$ and where $x_{\mathrm{I}} = \sum_{i \in \mathrm{I}} x_i$.

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

Let $\delta_{i,\mathrm{I}} = 1$ if $i \in \mathrm{I}$ and $\delta_{i,\mathrm{I}} = 0$ otherwise.

Then

$$(d\varphi^{(n)}(x))_i = \frac{\partial \varphi^{(n)}}{\partial x_i}(x) = \sum_{\mathrm{I} \ni i}^{(n)} \varphi'(x_{\mathrm{I}}) = \sum_{\mathrm{I}}^{(n)} \delta_{i,\mathrm{I}} \varphi'(x_{\mathrm{I}}) \tag{3}$$

Let us denote by $\mathrm{H}_x \varphi^{(n)}$ the $n \times n$ symmetric matrix of the second derivatives of $\varphi^{(n)}$ at x. If x is a critical point of $\varphi^{(n)}$ (an equilibrium configuration), $\mathrm{H}_x \varphi^{(n)}$ is just the hessian of $\varphi^{(n)}$ at x, the spectrum of which describes the mechanical stability of the equilibrium. For any $x \in \mathrm{X}^{(n)}$

$$(\mathrm{H}_x \varphi^{(n)})_{ij} = \frac{\partial^2 \varphi^{(n)}}{\partial x_i \partial x_j}(x) = \sum_{\mathrm{I} \ni i,j}^{(n)} \varphi''(x_{\mathrm{I}}) = \sum_{\mathrm{I}}^{(n)} \delta_{i,\mathrm{I}} \delta_{j,\mathrm{I}} \varphi''(x_{\mathrm{I}}) \tag{4}$$

A critical point x of $\varphi^{(n)}$ is non-denegerate if the hessian $\mathrm{H}_x \varphi^{(n)}$ is of maximal rank n, i. e. the n eigenvalues are $\neq 0$.

A non-degenerate critical point is mechanically stable if the hessian is positive definite, as a quadratic form on $\mathbb{R}^n$.

It is commonly assumed without proof that the ground state configurations of classical systems in one, two or three dimensions, are non-degenerate. This property is directly linked to the phonon spectrum of these systems. Actually, the hessian describes exactly the harmonic approximation which is used as the first term of perturbative analysis involving, in particular, anharmonic terms.

In a first paper [*7*], we proved that in one dimension, the energy potentials $\varphi^{(n)}$ are generically Morse function on $\mathrm{X}^{(n)}$ for any n, i. e. for « almost all » choice of the two-body potential $\varphi \in \mathrm{C}^\infty([c, \infty[)$, all equilibrium configurations of the $\varphi^{(n)}$ are non-degenerate.

We proved later [*8*], that the Morse property of energy potentials in 3 dimensions is generic with respect to the two-body potentials depending only on the distance.

The Morse property is a necessary and sufficient condition to insure the structural stability of critical points. In particular, one can follow the perturbation of a non-degenerate equilibrium under a small but arbitrary variation of the two-body potential.

More precisely, if φ is a generic potential and if $x \in X^{(n)}$ is a critical point of $\varphi^{(n)}$, then for any small enough variation $\psi \in C^{\infty}([c, \infty[)$ and all $t \in [0, 1]$, $(\varphi + t\psi)^{(n)}$ admits a critical point x_t close to x, in such a way that the trajectory $t \to x_t$ is the unique solution of

$$H_{x_t}(\varphi + t\psi)^{(n)} \frac{dx_t}{dt} = - d\psi^{(n)}(x_t) \tag{5}$$

A similar result holds in 3 dimensions and the corresponding equation of the critical points has been used in [8] to prove the structural stability of the possible symmetries of equilibria.

In this paper, we consider sequences of stable equilibrium configurations $x_{(n)}$ of $\varphi^{(n)}$, when $n \to \infty$. We suggest below a definition of the property for a generic potential φ to give rise to a lattice, and we shall prove in the following sections the stability of this property.

As mentionned in the introduction, the definition of the convergence to a lattice involves essentially two sequences of numbers, namely the dispersions of the configurations $x_{(n)}$ and the average spacings between particles.

More precisely, using the underlying vector space structure of $X^{(n)} \subset \mathbb{R}^n$, let P be the projection operator on $X^{(n)}$ (or $\mathbb{R}^n$), given by

$$Px = \bar{x} \qquad \text{and} \qquad \bar{x}_i = n^{-1} \sum_j^{(n)} x_j \tag{6}$$

for any $x \in X^{(n)}$ (or $\mathbb{R}^n$).

Then $\bar{x}$ is the configuration in $X^{(n)}$ with equal spacings, which is the closest to x for the Euclidean norm.

DEFINITION. — For any $n > 0$ and for any $x \in X^{(n)}$ (or $\mathbb{R}^n$), we define the dispersion $\sigma(x)$ and the average spacing $\tau(x)$ by the following:

$$\sigma(x) = \| x - \bar{x} \| = \| (1 - P)x \| \tag{7}$$

$$\tau(x) = n^{-1/2} \| \bar{x} \| = n^{-1/2} \| Px \| \tag{8}$$

Then obviously $\tau(x) = | \bar{x}_i |$, for $i = 1, \ldots, n$ and we have

$$\| x \|^2 = \sigma(x)^2 + n\tau(x)^2 \tag{9}$$

In the following, we shall be concerned with the values of σ and τ for stable equilibria $x_{(n)}$ of $\varphi^{(n)}$, and also for the neighbouring equilibria arising from variations of φ.

The definition stated below, of the property for φ to give rise to a lattice, involves two conditions bearing on the sequences $\{ \sigma(x_{(n)}) \}$ and $\{ \tau(x_{(n)}) \}$.

A convenient way to introduce a uniform estimate on the mechanical stability of the different equilibria $x_{(n)}$, is to require a lower bound on the hessians $H_y\varphi^{(n)}$ in some neighborhood $\Omega(x_{(n)};\alpha,\beta)$ of $x_{(n)}$ where

$$\Omega(x;\alpha,\beta)=\{\, y\in X^{(n)} \mid \sigma(y-x)<\alpha,\ \tau(y-x)<\beta \,\} \tag{10}$$

is an open subset of $X^{(n)}$ for any $x\in X^{(n)}$ and $\alpha, \beta > 0$.

DEFINITION. — Let $\varphi \in C^\infty([c,\infty[)$ be a two-body potential. Then φ is said to give rise to a lattice if there exists a sequence $\{x_{(n)}\}$ of stable equilibrium configurations such that the following conditions hold:

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

$$H_y\varphi^{(n)} > \mu \qquad \text{for any} \qquad y\in\Omega(x_{(n)};\alpha,\beta) \tag{11}$$

where $H_y\varphi^{(n)}$ is the hessian defined by (4).

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

$$\sigma(x_{(n)}) < a \tag{12}$$

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

$$\lim_{n\to\infty} \tau(x_{(n)}) = b \tag{13}$$

We briefly comment these conditions.

First, we don't require $x_{(n)}$ to be the ground state of $\varphi^{(n)}$. Actually the mechanical stability of $x_{(n)}$, implied by L1., is sufficient for structural stability.

Secondly we note that L1. is consistent with the usual phonon spectrum of lattices: for instance, in the case of an harmonic chain with n. n. interaction, $H_x\varphi^{(n)}$ is just equal to the spring constant times the unit matrix. The relation between the phonon spectrum and the spectrum of $H_{x_{(n)}}\varphi^{(n)}$ is even more obvious in the $n\to\infty$ limit, since one checks that the hessian w. r. t. positions q_i is equal to the hessian w. r. t. spacings $x_i = q_{i+1} - q_i$ times the discrete laplacian operator.

The conditions L2. and L3. concern the convergence to a lattice. The uniform bound on $\sigma(x_{(n)})$ allows for boundary effects, the penetration of which is uniformly controlled by (12), thus rejecting a non physical increase in the limit $n\to\infty$.

Finally, we note that no further relations between α, β and a, b are required, but from a physical point of view, the basin $\Omega(x_{(n)};\alpha,\beta)$ of $x_{(n)}$ should not necessarily contain $\bar{x}_{(n)}$, so that $\alpha < a$ is realistic. Similarly, the dispersion bound a may be larger than the limit lattice spacing b. On the other hand, the interval $(\tau(x_{(n)})-\beta,\ \tau(x_{(n)})+\beta)$ allows for the static elastic deformations of the system around the equilibrium configuration.

III. PERTURBATIONS OF THE FINITE SYSTEMS

Let φ be a generic potential and assume x_0 is a non-degenerate critical point of $\varphi^{(n)}$ in $X^{(n)}$.

Then, if $\psi \in C^\infty([c, \infty[)$ is a small enough perturbation ([7]), the trajectory $t \to x_t$ of the critical point of $(\varphi + t\psi)^{(n)}$ for $t \in [0, 1]$, is the unique solution of

$$\xi_t = \frac{dx_t}{dt} = - H_{x_t}^{-1}(\varphi + t\psi)^{(n)} d\psi^{(n)}(x_t) \tag{14}$$

We assume now that φ satisfies the conditions L1. and L2. of the previous section.

Let $\sigma_t = \sigma(x_t - x_{(n)}) = \| (1-P)(x_t - x_{(n)}) \|$. Then if $(1-P)(x_t - x_{(n)}) \neq 0$,

$$\dot{\sigma}_t = \frac{((1 - P)(x_t - x_{(n)}), (1 - P)\xi_t)}{\| (1 - P)(x_t - x_{(n)}) \|} \tag{15}$$

from which follows the uniform bound

$$| \dot{\sigma}_t | \leqslant \| (1 - P)\xi_t \| \tag{16}$$

If $\tau_t = \tau(x_t - x_{(n)}) = n^{-1/2} \| P(x_t - x_{(n)}) \|$, we get in a similar way

$$| \dot{\tau}_t | \leqslant n^{-1/2} \| P\xi_t \| \tag{18}$$

In this section, we derive bounds on $| \dot{\sigma}_t |$ and $| \dot{\tau}_t |$, depending on L1., L2. and on decrease properties of φ and ψ, but independant of n.

We define below different moduli for potentials in $C^\infty([c, \infty[)$, which are linked to our problem of bounding $| \dot{\sigma}_t |$ and $| \dot{\tau}_t |$.

One can easily check [9] that these definitions correspond to open subsets of $C^\infty([c, \infty[)$ for the Whitney topology.

For any strictly positive decreasing function $\delta \in C^\infty([c,\infty[)$ and any $j \in \mathbb{N}$, let

$$M^j(\delta) = \sum_{k \in \mathbb{N}} k^j \delta(kc) \in \mathbb{R} \cup \{ + \infty \} \tag{19}$$

Then for any potential $\varphi \in C^\infty([c, \infty[)$ and any $i \in \mathbb{N}$, we define D_i^j as the lower bound of $M^j(\delta)$, for δ such that the i^{th} derivative $| \varphi^{[i]} | \leqslant \delta$:

$$D_i^j = \operatorname{Inf} \{ M^j(\delta) \mid \delta' \leqslant 0 \quad \text{and} \quad | \varphi^{[i]} | \leqslant \delta \} \tag{20}$$

Similarly, for any perturbation $\psi \in C^\infty([c, \infty[)$ and any $i, j \in \mathbb{N}$, we define

$$E_i^j = \operatorname{Inf} \{ M^j(\varepsilon) \mid \varepsilon' \leqslant 0 \quad \text{and} \quad | \psi^{[i]} | \leqslant \varepsilon \} \tag{21}$$

Then, for any $i, j \in \mathbb{N}$ and $\eta > 0$, the set $\{ \psi \in C^\infty([c, \infty[) \mid E_i^j < \eta \}$ is open for the Whitney topology.

Variation of the dispersion.

We obtain here *a priori* estimates on $|\dot{\sigma}_t|$ assuming that the initial potential φ satisfies L1. and L2. and that the critical point x_t of $(\varphi + t\psi)^{(n)}$ remains in $\Omega(x_{(n)}, \alpha, \beta)$ for $t \in [0, 1]$.

Using (14) and (16) we obtain

$$|\dot{\sigma}_t| \leqslant \|(1 - \mathrm{P})h_t^{-1} d\psi^{(n)}(x_t)\|$$

where

$$h_t = \mathrm{H}_{x_t}(\varphi + t\psi)^{(n)} = \mathrm{H}_{x_t}\varphi^{(n)} + t\mathrm{H}_{x_t}\psi^{(n)}$$

$$\begin{aligned}(1 - \mathrm{P})h_t^{-1} &= h_t^{-1} - [\mathrm{P}, h_t^{-1}] - h_t^{-1}\mathrm{P} \\ &= h_t^{-1}(1 - \mathrm{P}) + h_t^{-1}[\mathrm{P}, h_t]h_t^{-1}\end{aligned}$$

Thus

$$|\dot{\sigma}_t| \leqslant \|h_t^{-1}\| \, \|(1-\mathrm{P})d\psi^{(n)}(x_t)\| + \|h_t^{-1}\|^2 \, \|[\mathrm{P}, h_t]\| \, \|d\psi^{(n)}(x_t)\| \quad (22)$$

The different terms of the r. h. s. of (22) are now investigated in the following lemmas.

LEMMA 1. — Let φ satisfy L1. and L2. Then for any $\psi \in \mathrm{C}^\infty([c, \infty[)$ such that $\mathrm{E}_2^2 < \mu$, (see (21)), the following holds for any $t \in [0, 1]$ and any $y \in \Omega(x_{(n)}; \alpha, \beta)$:

$$\|\mathrm{H}_y^{-1}(\varphi + t\psi)^{(n)}\| \leqslant (\mu - t\mathrm{E}_2^2)^{-1} \quad (23)$$

Proof. — Since $\mathrm{H}_y\varphi^{(n)} > \mu$, we have

$$\begin{aligned}\|\mathrm{H}_y^{-1}(\varphi + t\psi)^{(n)}\| &\leqslant \mu^{-1} \sum_{p \in \mathbb{N}} (t\mu^{-1}\|\mathrm{H}_y\psi^{(n)}\|)^p \\ &\leqslant (\mu - t\|\mathrm{H}_y\psi^{(n)}\|)^{-1} \quad (24)\end{aligned}$$

of course (24) holds only if $t\|\mathrm{H}_y\psi^{(n)}\| < \mu$.

Let $$\mathrm{K}_{ij} = (\mathrm{H}_y\psi^{(n)})_{ij} = \sum_{\mathrm{I}}^{(n)} \delta_{i,\mathrm{I}}\delta_{j,\mathrm{I}}\psi''(y_\mathrm{I})$$

Then $$\mathrm{K}_{ij} = \sum_{p \geqslant 1} \mathrm{K}_{ij}^{(p)} \quad \text{and} \quad \|\mathrm{K}\| \leqslant \sum_{p \geqslant 1} \|\mathrm{K}^{(p)}\|$$

where

$$\mathrm{K}_{ij}^{(p)} = \sum_{|\mathrm{I}| = p}^{(n)} \delta_{i,\mathrm{I}}\delta_{j,\mathrm{I}}\psi''(y_\mathrm{I})$$

Since $y \in X^{(n)}$, $y_i > c$ for $i = 1, \ldots, n$ and therefore, if ε is a positive decreasing function such that $|\psi''| \leqslant \varepsilon$, we have

$$|K_{ij}^{(p)}| \leqslant \sum_{|I|=p} \delta_{i,I}\delta_{j,I}\varepsilon(pc)$$

A bound for $\| K^{(p)} \|$ is now obtained using a splitting of $K^{(p)}$ corresponding to the different diagonals ($i-j=k$ constant) of this $n \times n$ matrix. One easily checks that the norm of such a « diagonal » matrix is bounded by the supremum of the absolute values of its terms. Thus

$$\begin{aligned} \| K^{(p)} \| &\leqslant \sum_{k\in\mathbb{Z}} \sum_{|I|=p} \delta_{0,I}\delta_{k,I}\varepsilon(pc) \\ &\leqslant \varepsilon(pc) \sum_{k\in\mathbb{Z}} \sum_{|I|=p} \delta_{0,I}\delta_{k,I} \end{aligned}$$

The summation can be restricted to $|k| \leqslant p - 1$, otherwise $\delta_{0,I}\delta_{k,I} = 0$. Then, the number of intervals I with $|I| = p$, containing 0 and k is $p - |k|$, and therefore

$$\begin{aligned} \| K^{(p)} \| &\leqslant \varepsilon(pc) \sum_{k=-p+1}^{p-1} (p - |k|) \\ &\leqslant p^2\varepsilon(pc) \end{aligned}$$

Finally, $\| K \| \leqslant \sum_{p\geqslant 1} p^2\varepsilon(pc)$ and according to the definition (21) of the modulus

$$\| H_y\psi^{(n)} \| \leqslant E_2^2 \qquad \text{for any} \qquad y \in X^{(n)}.$$

which completes the proof of lemma 1. Q. E. D.

The next term of (22) we investigate is $\| d\psi^{(n)}(x_t) \|$. We have

LEMMA 2. — For any $\psi \in C^\infty([c, \infty[)$ and any $y \in X^{(n)}$, the following bound holds

$$\| d\psi^{(n)}(y) \| \leqslant n^{1/2}E_1^1 \tag{26}$$

Proof. — One easily checks from the definition of the euclidean norm that

$$\| d\psi^{(n)}(y) \| \leqslant n^{1/2} \operatorname{Sup} |(d\psi^{(n)}(y))_i|$$

where

$$(d\psi^{(n)}(y))_i = \sum_{I}^{(n)} \delta_{i,I}\psi'(y_I)$$

If ε is a positive decreasing function such that $|\psi'| \leqslant \varepsilon$, we have

$$| d\psi^{(n)}(y))_i | \leqslant \sum_{\mathrm{I}} \delta_{i,\mathrm{I}}\varepsilon(|\mathrm{I}|c) \leqslant \sum_{p\geqslant 1} p\varepsilon(pc)$$

from which follows (26). Q. E. D.

We consider now the term $\| (1 - \mathrm{P})d\psi^{(n)}(x_t) \|$.

LEMMA 3. — For any $\psi \in \mathrm{C}^\infty([\mathrm{C}, \infty[)$ and any $y \in \mathrm{X}^{(n)}$, the following bound holds:

$$\| (1 - \mathrm{P})d\psi^{(n)}(y) \| \leqslant 2(\mathrm{E}_1^1\mathrm{E}_1^2)^{1/2} + \mathrm{E}_2^2\sigma(y) \tag{27}$$

where $\sigma(y) = \| (1 - \mathrm{P})y \|$ is the dispersion of y.

Proof. — Let $\bar{y} = \mathrm{P}y$. Then

$$\| (1 - \mathrm{P})d\psi^{(n)}(y) \| \leqslant \| d\psi^{(n)}(y) - d\psi^{(n)}(\bar{y}) \| + \| (1 - \mathrm{P})d\psi^{(n)}(\bar{y}) \| \tag{28}$$

The first term of the r. h. s. of (28) can be bounded using the mean value theorem.

Actually,

$$(d\psi^{(n)}(y) - d\psi^{(n)}(\bar{y}))_i = \sum_{\mathrm{I}}^{(n)} \delta_{i,\mathrm{I}}(\psi'(y_\mathrm{I}) - \psi'(\bar{y}_\mathrm{I})) = \sum_{\mathrm{I}}^{(n)} \delta_{i,\mathrm{I}}\psi''(z_\mathrm{I})(y_\mathrm{I} - \bar{y}_\mathrm{I})$$

where the collection of z_I does not correspond necessarily to a configuration in $\mathrm{X}^{(n)}$, but certainly $\min(y_\mathrm{I}, \bar{y}_\mathrm{I}) \leqslant z_\mathrm{I} \leqslant \max(y_\mathrm{I}, \bar{y}_\mathrm{I})$ holds and therefore $z_\mathrm{I} > |\mathrm{I}|c$.

Let $\mathrm{K}_{ij} = \sum_{\mathrm{I}}^{(n)} \delta_{i,\mathrm{I}}\delta_{j,\mathrm{I}}\psi''(z_\mathrm{I})$. Then

$$d\psi^{(n)}(y) - d\psi^{(n)}(\bar{y}) = \mathrm{K}(y - \bar{y}) = \mathrm{K}(1 - \mathrm{P})y$$

One easily checks that the bound on $\| \mathrm{H}_y\psi^{(n)} \|$ derived in the proof of lemma 1 applies to the present situation and thus

$$\| d\psi^{(n)}(y) - d\psi^{(n)}(\bar{y}) \| \leqslant \mathrm{E}_2^2\sigma(y) \tag{29}$$

The second term $\| (1 - \mathrm{P})d\psi^{(n)}(\bar{y}) \|$ of (28) requires a more carefull analysis since we expect $\| d\psi^{(n)}(\bar{y}) \|$ to be of order $n^{1/2}$ (see lemma 2).

The point is that $\bar{y} = \mathrm{P}y$ is a piece of lattice and that $1 - \mathrm{P}$ projects orthogonally to the image of P. Actually we have

$$\begin{aligned}
\| (1 - \mathrm{P}) d\psi^{(n)}(\bar{y}) \|^2 &= \| d\psi^{(n)}(\bar{y}) \|^2 - \| \mathrm{P} d\psi^{(n}(\bar{y}) \|^2 \\
&= \sum_i \Big(\sum_{\mathrm{I}}^{(n)} \delta_{i,\mathrm{I}} \psi'(\bar{y}_{\mathrm{I}}) \Big)^2 \\
&\quad - n^{-1} \Big(\sum_i \sum_{\mathrm{I}}^{(n)} \delta_{i,\mathrm{I}} \psi'(\bar{y}_{\mathrm{I}}) \Big)^2 \\
&= \sum_i \sum_{\mathrm{I},\mathrm{J}}^{(n)} \delta_{i,\mathrm{I}} \delta_{i,\mathrm{J}} \psi'(\bar{y}_{\mathrm{I}}) \psi'(\bar{y}_{\mathrm{J}}) \\
&\quad - n^{-1} \sum_{i,j} \sum_{\mathrm{I},\mathrm{J}}^{(n)} \delta_{i,\mathrm{I}} \delta_{j,\mathrm{J}} \psi'(\bar{y}_{\mathrm{I}}) \psi'(\bar{y}_{\mathrm{J}}) \\
&= n^{-1} \sum_{i,j} \sum_{\mathrm{I},\mathrm{J}}^{(n)} (\delta_{i,\mathrm{I}} \delta_{i,\mathrm{J}} - \delta_{i,\mathrm{I}} \delta_{j,\mathrm{J}}) \psi'(\bar{y}_{\mathrm{I}}) \psi'(\bar{y}_{\mathrm{J}})
\end{aligned}$$

We can split the summation over I, J with respect to their length $|\mathrm{I}| = p$ and $|\mathrm{J}| = q$. Thus

$$\begin{aligned}
\| (1 - \mathrm{P}) d\psi^{(n)}(\bar{y}) \|^2 &= n^{-1} \sum_{p,q} \sum_{i,j} \sum_{|\mathrm{I}|=p}^{(n)} \delta_{i,\mathrm{I}} \psi'(\bar{y}_{\mathrm{I}}) \\
&\quad \times \sum_{|\mathrm{J}|=q}^{(n)} (\delta_{i,\mathrm{J}} - \delta_{j,\mathrm{J}}) \psi'(\bar{y}_{\mathrm{J}})
\end{aligned}$$

Since $\bar{y}$ is a configuration with equal spacing $\tau(y)$,

$$\psi'(\bar{y}_{\mathrm{I}}) = \psi'(|\mathrm{I}|\,\tau(y))$$

and

$$\begin{aligned}
\| (1 - \mathrm{P}) d\psi^{(n)}(\bar{y}) \|^2 &= n^{-1} \sum_{p,q} \psi'(p\tau(y)) \psi'(q\tau(y)) \\
&\quad \times \sum_{i,j} \sum_{|\mathrm{I}|=p}^{(n)} \delta_{i,\mathrm{I}} \sum_{|\mathrm{J}|=q}^{(n)} (\delta_{i,\mathrm{J}} - \delta_{j,\mathrm{J}}) \qquad (30)
\end{aligned}$$

Now $\sum_{|\mathrm{I}|=p}^{(n)} \delta_{i,\mathrm{I}}$ is just the number of intervals I in $\{1, \ldots, n\}$ with $|\mathrm{I}| = p$, that contain the point i. If $i \geqslant p$ or $i \leqslant n - p + 1$, this number is exactly p. Otherwise it is lower than p. The same remark holds for $\sum_{|\mathrm{J}|=q}^{(n)} \delta_{i,\mathrm{J}}$ and

$\sum_{|J|=q}^{(n)} \delta_{j,J}$ which are bounded by q in such a way that for $i, j \geqslant q$ and $i, j \leqslant n - q + 1$, $\sum_{|J|=q}^{(n)} (\delta_{i,J} - \delta_{j,J}) = 0$.

Thus, for fixed p, q, the partial sum over i, j in (30) is bounded by $4npq^2$.
Now, if ε is a positive decreasing function such that $|\psi'| \leqslant \varepsilon$

$$\| (1 - P)d\psi^{(n)}(\bar{y}) \|^2 \leqslant 4 \sum_{p,q} p \, . \, q^2 \varepsilon(pc)\varepsilon(qc)$$
$$\leqslant 4E_1^1E_1^2 \tag{31}$$

Finally, it follows from (28), (29) and (31) that

$$\| (1 - P)d\psi^{(n)}(y) \| \leqslant 2(E_1^1E_1^2)^{1/2} + E_2^2\sigma(y) \qquad \text{Q. E. D.}$$

The last term of (22) to be bounded is $\| [P, h_t] \|$.

LEMMA 4. — Let φ satisfy L1 and L2. Then for any $\psi \in C^\infty([c, \infty[)$, the following bound holds for any $t \in [0, 1]$ and $y \in \Omega(x_{(n)}; \alpha, \beta)$:

$$\| [h, P] \| \leqslant n^{-1/2} \{ 2(D_2^2 + tE_2^2)^{1/2}(D_2^3 + tE_2^3)^{1/2} + (D_3^3 + tE_3^3)\sigma(y) \} \tag{32}$$

where $h = H_y(\varphi + t\psi)^{(n)}$ and D_i^j, E_i^j are defined by (20) and (21) respectively, and are supposed to be finite.

Proof. — It follows from (6) that all matrix elements $P_{i,j}$ of P are equal to n^{-1}. Thus

$$P = n^{-1}\mathbb{1} \otimes \mathbb{1} \tag{33}$$

where $\mathbb{1} = (1, \ldots, 1)$ is the n-vector with all components equal to 1.

Now, since P and h are symmetric,

$$[h, P] = hP - (h.P)^t \tag{34}$$

For any i, j

$$(h.P)_{ij} = n^{-1} \sum_k^{(n)} h_{ik}(\mathbb{1} \otimes \mathbb{1})_{kj}$$
$$= n^{-1} \sum_k^{(n)} h_{ik} \tag{35}$$

Let $v \in \mathbb{R}^n$ be defined by

$$v_i = \sum_k^{(n)} h_{ik} = \sum_k^{(n)} \sum_I^{(n)} \delta_{i,I}\delta_{k,I}(\varphi + t\psi)''(y_I)$$
$$= \sum_I^{(n)} \delta_{i,I} |I| (\varphi + t\psi)''(y_I) \tag{36}$$

Then, it follows from (35) and (36) that

$$[h, \mathrm{P}] = n^{-1}(v \otimes \mathbb{1} - \mathbb{1} \otimes v)$$

Since $\mathrm{P}v = n^{-1}(\mathbb{1}, v)\mathbb{1}$,

$$[h, \mathrm{P}] = n^{-1}(u \otimes \mathbb{1} - \mathbb{1} \otimes u)$$

where $u = (1 - \mathrm{P})v$. Now the norm of $u \otimes \mathbb{1} - \mathbb{1} \otimes u$ can be computed explicitely and one finds $n^{-1/2} \| u \|$. Therefore

$$\| [h, \mathrm{P}] \| = n^{-1/2} \| (1 - \mathrm{P})v \| \tag{37}$$

Finally, $\| (1 - \mathrm{P})v \|$ can be bounded using the proof of Lemma 3 for $\| (1-\mathrm{P})d\psi^{(n)}(y) \|$, replacing $\psi'(y_\mathrm{I})$ with $|\mathrm{I}| (\varphi + t\psi)''(y_\mathrm{I})$. Then, using (20) and (21), one checks easily that E_1^1, E_1^2 and E_2^2 are respectively replaced with $\mathrm{D}_2^2 + t\mathrm{E}_2^2$, $\mathrm{D}_2^3 + t\mathrm{E}_2^3$, which yields (32). Q. E. D.

The results of the previous lemmas imply a bound on $|\dot{\sigma}_t|$ given by

THEOREM 1. — Let φ satisfy L1 and L2 and assume that D_2^2, D_2^3 and D_3^3 are finite. Then for any $\psi \in \mathrm{C}^\infty([c, \infty[)$ such that $\mathrm{E}_2^2 < \mu$ the following bound holds for the derivative of $\sigma_t = \sigma(x_t - x_{(n)})$, where the critical point x_t of $(\varphi + t\psi)^{(n)}$ arising from the perturbation of $x_0 = x_{(n)}$ is supposed to be in $\Omega(x_{(n)}; \alpha, \beta)$:

$$\begin{aligned} |\dot{\sigma}_t| \leqslant\ & (\mu - t\mathrm{E}_2^2)^{-1} [2(\mathrm{E}_1^1\mathrm{E}_1^2)^{1/2} + \mathrm{E}_2^2\sigma(x_t)] \\ & + (\mu - t\mathrm{E}_2^2)^{-2}\mathrm{E}_1^1 [2(\mathrm{D}_2^2 + t\mathrm{E}_2^2)^{1/2}(\mathrm{D}_2^3 + t\mathrm{E}_2^3)^{1/2} + (\mathrm{D}_3^3 + t\mathrm{E}_3^3)\sigma(x_t)] \end{aligned} \tag{38}$$

Proof. — The result follows from Lemmas 1-4. Q. E. D.

Variation of the average spacing.

In the following, we use this *a priori* estimate of $|\dot{\sigma}_t|$ to prove that if ψ is small enough, the critical points x_t all lie in $\Omega(x_{(n)}; \alpha, \beta)$ for $t \in [0, 1]$. This requires of course a bound on $|\dot{\tau}_t|$ which is derived now.

THEOREM 2. — Let φ satisfy L1 and L2. For any $\psi \in \mathrm{C}^\infty([c, \infty[)$ such that $\mathrm{E}_2^2 < \mu$, and for n large enough the following bound holds, assuming that

$$x_t \in \Omega(x_{(n)}; \alpha, \beta) \qquad \text{for} \qquad t \in [0, 1]:$$

$$|\dot{\tau}_t| \leqslant 2(\mu - t\mathrm{E}_2^2)^{-1}\mathrm{E}_1^1 \tag{39}$$

Proof. — Using (14), we have

$$\mathrm{P}\xi_t = -[\mathrm{P}, h_t^{-1}]d\psi^{(n)}(x_t) - h_t^{-1}\mathrm{P}d\psi^{(n)}(x_t)$$

where $h_t = \mathrm{H}_{x_t}(\varphi + t\psi)^{(n)}$. Then, using (18),

$$|\dot{\tau}_t| \leqslant n^{-1/2}(\| h_t^{-1} \| + \| h_t^{-1} \|^2 \| [\mathrm{P}, h_t] \|) \| d\psi^{(n)}(x_t) \|$$

Since the conditions of lemmas 1, 2 and 4 are satisfied, we obtain

$$|\dot{\tau}_t| \leqslant (\mu - t\mathrm{E}_2^2)^{-1}\mathrm{E}_1^1 + n^{-1/2}(\mu - t\mathrm{E}_2^2)^{-2}\mathrm{C}\mathrm{E}_1^1$$

where C stands for the bracket in the r.h.s. of (32) which gives a bound for $\| [h_t, \mathrm{P}] \|$.

Then (39) follows for n large enough. Q. E. D.

The bounds for $|\dot{\sigma}_t|$ and $|\dot{\tau}_t|$ given in theorem 1 and theorem 2 are submitted to the condition that $x_t \in \Omega(x_{(n)}; \alpha, \beta)$ for all $t \in [0, 1]$.

Therefore the self consistency of the proofs requires $\sigma(x_t - x_{(n)}) < \beta$. As mentionned above, this is achieved as soon as the perturbation ψ is small enough. More precisely, we have

THEOREM 3. — Let ψ satisfy L1 and L2 and assume D_2^2, D_2^3 and D_3^3 are finite. For any $\psi \in \mathrm{C}^\infty([c, \infty[)$ such that the moduli E_1^1, E_1^2, E_2^2, E_2^3 and E_3^3 are small enough, and for n large enough, the critical point x_t of $(\varphi + t\psi)^{(n)}$ arising from the perturbation of $x_0 = x_{(n)}$, lies in $\Omega(x_{(n)}; \alpha, \beta)$ for all $t \in [0, 1]$.

Proof. — Since $\sigma(x_{(n)}) < \alpha$ for all n, $\sigma(x_t) \leqslant \alpha + \sigma_t$. Then the inequations (38) and (39) can be written in the following from

$$|\dot{\sigma}_t| \leqslant \mathrm{A}(t, \mu, \alpha, \{ \mathrm{D}_i^j \}, \{ \mathrm{E}_i^j \}) + \mathrm{B}(t, \mu, \{ \mathrm{D}_i^j \}, \{ \mathrm{E}_i^j \})\sigma_t \tag{42}$$

$$|\dot{\tau}_t| \leqslant \mathrm{C}(t, \mu, \{ \mathrm{E}_i^j \}) \tag{43}$$

The important point is that A, B and C vanish when $\mathrm{E}_1^1 = \mathrm{E}_2^2 = 0$ and are continuous functions of $\{ \mathrm{E}_i^j \}$ in a neighborhood of $\mathrm{E}_i^j = 0$.

Now consider the following differential equations

$$\dot{u}(t) = \mathrm{A}(t) + \mathrm{B}(t)u(t) \tag{44}$$

$$\dot{v}(t) = \mathrm{C}(t) \tag{45}$$

with initial conditions $u(0) = v(0) = 0$.

Then it follows from the theory of differential equations and the previous remarks, that if the moduli E_1^1, E_1^2, E_2^2, E_2^3 and E_3^3 are small enough, we certainly have $u(t) < \alpha$ and $v(t) < \beta$ for all $t \in [0, 1]$.

Consequently $\sigma_t = \sigma(x_t - x_{(n)}) < \alpha$ and $\tau_t = \tau(x_t - x_{(n)})) < \beta$, and therefore $x_t \in \Omega(x_{(n)}; \alpha, \beta)$ for all $t \in [0, 1]$. Q. E. D.

The differential equations (44) and (45) are independant of n. The sufficient condition given above on the moduli E_i^j is also independant of n. Therefore the conclusion of theorem 3 applies uniformly for all n large enough. In other words, the critical points $x'_{(n)}$ of $(\varphi + \psi)^{(n)}$ arising from the perturbation of $x_{(n)}$, all lie in $\Omega(x_{(n)}; \alpha, \beta)$.

IV. STRUCTURAL STABILITY

In this section we investigate the structural stability of conditions L1, L2 and L3, taken as a definition for the existence of a lattice in the infinite volume limit.

Actually, the conditions L1 and L2 can easily be proved to be stable using the results of the previous section.

The condition L3, convergence of the average spacings, requires a more detailed analysis. We prove below that the limit average spacing ℓ, corresponding to φ, can be identified with the lattice spacing which gives a local minimum to the energy per particle.

For any $\ell' > c$ the energy per particle for the corresponding infinite lattice with interaction φ, is given by

$$e(\varphi, \ell') = \sum_{k \geqslant 1} \varphi(k\ell')$$

Then, when $e(\varphi, \ell')$ is a local minimum with respect to ℓ', we certainly have

$$\frac{\partial e}{\partial \ell}(\varphi, \ell') = \sum_{k \geqslant 1} k\varphi'(k\ell') = 0 \tag{46}$$

Using conditions L1, L2 and L3, we check now that ℓ (given by L3) is the unique solution of (46) in the interval $]\ell-\beta, \ell+\beta[$, and corresponds to a local minimum of $e(\varphi,.)$.

THEOREM 4. — Let φ satisfy L1, L2, L3, and assume D_2^2, D_2^3, $D_3^3 < \infty$. Then $e(\varphi,.)$ is a convex function in the interval $]\ell-\beta, \ell+\beta[$, and the following bound holds:

$$\frac{\partial^2 e}{\partial \ell^2}(\varphi, \ell') = \sum_{k \geqslant 1} k^2\varphi''(k\ell') > \mu \tag{47}$$

The proof is given below in lemmas 5 and 6 where the actual equilibrium configurations $x_{(n)}$ are compared to finite pieces of lattice.

LEMMA 5. — Let φ satisfy the conditions of Theorem 4. Then for any $\ell' \in]\ell-\beta, \ell+\beta[$ and for any large enough n, there exists a configuration $y \in \Omega(x_{(n)}; \alpha, \beta)$ such that $\tau(y) = \ell'$.

Proof. — First we remark that if $\ell' \in]\ell - \beta, \ell + \beta[$ then, using L3,

$\ell' \in]\tau(x_{(n)})-\beta, \tau(x_{(n)})+\beta[$ for n large enough. Let then $y_t = x_{(n)} + t\mathrm{P}x_{(n)}$.

$$\sigma(y_t - x_{(n)}) = \| (1 - \mathrm{P})(y_t - x_{(n)}) \| = 0$$
$$\tau(y_t - x_{(n)}) = n^{-1/2} \| \mathrm{P}(y_t - x_{(n)}) \| = |t| \, \tau(x_{(n)})$$

Thus, if $t = (\ell' - \tau(x_{(n)}))/\tau(x_{(n)})$, we have $y_t \in \Omega(x_{(n)}; \alpha, \beta)$ and $\tau(y_t) = \ell'$.

Q. E. D.

Using this result, we prove now that under the same conditions, some configurations in $\Omega(x_{(n)}; \alpha, \beta)$ contain a piece of lattice with spacing ℓ'.

LEMMA 6. — Let φ satisfy the conditions of theorem 4. Let

$$\ell' \in]\ell - \beta, \quad \ell + \beta[\,.$$

Then for any $n_0 \geqslant 1$, there exists $n = mn_0$, ($m \in \mathbb{N}$) such that

1) $\exists y \in \Omega(x_{(n)}; \alpha, \beta)$ with $\sigma(y - x_{(n)}) = 0$ and $\tau(y) = \ell'$.

2) Let $y = (y_1, \ldots, y_m)$ be the splitting of y into m pieces of length n_0. Then $\exists k \leqslant m$ such that

$$y' = (y_1, \ldots, y_{k-1}, z, y_{k+1}, \ldots, y_m) \in \Omega(x_{(n)}; \alpha, \beta),$$

where z is a piece of lattice of length n_0, with spacing ℓ'.

Proof. — The first conclusion follows directly from lemma 5.

Let $y' = (y_1, \ldots, y_{k-1}, z, y_{k+1}, \ldots, y_m)$ defined as above, for some arbitrary $k \leqslant m$.

$$\begin{aligned}\sigma(y' - x_{(n)}) &= \| (1 - \mathrm{P})(y' - x_{(n)}) \| \\ &\leqslant \| (1 - \mathrm{P})(y' - y) \| + \| (1 - \mathrm{P})(y - x_{(n)}) \|\end{aligned}$$

Since $\sigma(y - x_{(n)}) = 0$, we have

$$\sigma(y' - x_{(n)}) \leqslant \| z - y_k \| \qquad (\text{in } \mathbb{R}^{n_0})$$

Besides, since $\sigma(y - x_{(n)}) = 0, (1 - \mathrm{P})y = (1 - \mathrm{P})x_{(n)}$ and $\mathrm{P}y = (z, \ldots, z)$ (m times); thus

$$\sigma(x_{(n)})^2 = \sum_{l=1}^{m} \| y_l - z \|^2$$

Since $\sigma(x_{(n)}) < a$ by L1, there exists at least one $k \leqslant m$ such that

$$\| y_k - z \| < a/\sqrt{m}\,.$$

Then, for the corresponding y', we have $\sigma(y' - x_{(n)}) < a/\sqrt{m}$, which is smaller than α for m large enough.

We consider now the condition $\tau(y' - x_{(n)}) < \beta$.

$$\begin{aligned}\tau(y' - x_{(n)}) &= n^{-1/2} \| \mathrm{P}(y' - x_{(n)}) \| \\ &\leqslant n^{-1/2} \| \mathrm{P}(y' - y) \| + n^{-1/2} \| \mathrm{P}(y - x_{(n)}) \| \\ &\leqslant n^{-1/2} \| y_k - z \| + | \ell' - \tau(x_{(n)}) |\end{aligned}$$

The above choice of k yields

$$\tau(y' - x_{(n)}) \leqslant a(mn)^{-1/2} + |\ell' - \tau(x_{(n)})|$$

Therefore $\tau(y' - x_{(n)}) < \beta$ for m large enough, which completes the proofs.
Q. E. D.

Now, the convexity of $e(\varphi, .)$ can be derived from L1, using the approximation by finite pieces of lattice given in the above lemma.

Actually, under the conditions of theorem 4, for any n_0 and m large enough, the condition L1 implies $H_{y'}\varphi^{(n)} > \mu$ where y' is given by lemma 6.

Let i be the integer part of $\left(k - \frac{1}{2}\right)n_0$, so that the index i is in the « middle » of the k^{th} section of $y' = (y_1, \ldots, y_{k-1}, z, y_{k+1}, \ldots, y_n)$.

Then $(H_{y'} \varphi^{(n)})_{ii} > \mu$ with

$$\begin{aligned}(H_{y'}\varphi^{(n)})_{ii} &= \sum_{I}^{(n)} \delta_{i,I} |I| \varphi''(y'_I) \\ &= \sum_{I}^{(n_0)} \delta_{i,I} |I| \varphi''(|I|\ell') + \sum_{I}^{(n)\backslash(n_0)} \delta_{i,I} |I| \varphi''(y'_I)\end{aligned}$$

where the first sum stands for the intervals $I \subset \{(k-1)n_0+1, kn_0\}$ and the second one, for the remaining I's in $\{1, \ldots, n\}$.

Since $D_2^2 < \infty$ if we let $n_0 \to \infty$, the first sum converges to $\sum_{k\geqslant 1} k^2\varphi''(k\ell')$ and the second one vanishes. Therefore $\sum_{k\geqslant 1} k^2\varphi''(k, \ell') > \mu$ and the proof of theorem 4 is achieved.

The convexity of $e(\varphi, .)$ implies that the energy per particle has at most one minimum in $]\ell - \beta, \ell + \beta[$.

We prove below that the existence of the sequence of equilibria $x_{(n)}$ insures the existence of a minimum $e(\varphi, \ell)$. This result establishes the relation between the limit average spacing ℓ and the minimum energy per particle for the infinite lattices.

LEMMA 7. — Let φ satisfy the conditions of theorem 4, and assume $D_1^1 < \infty$. Then

$$\frac{\partial e}{\partial \ell}(\varphi, \ell) = \sum_{k\geqslant 1} \varphi'(k\ell) = 0$$

where ℓ is the limit average spacing given by L3.

Proof. — Using the methods of lemma 5 and 6, one easily checks that for any n_0 and for $n = mn_0$ large enough,

$$x' = (x_1, \ldots, x_{k-1}, z, x_{k+1}, \ldots, x_{(n)}) \in \Omega(x_{(n)}; \alpha, \beta),$$

where $x_{(n)} = (x_1, \ldots, x_m)$ is the splitting of $x_{(n)}$ into m sections of length n_0, and where z is a piece of lattice with spacing ℓ.

Moreover, we have $\| x' - x_{(n)} \| < a/\sqrt{m}$.

In particular, if i is the integer part of $\left(k - \frac{1}{2}\right)n_0$, and since $x_{(n)}$ is an equilibrium configuration, $| (d\varphi^{(n)}(x'))_i | < D_2^2\, a/\sqrt{m}$ with

$$(d\varphi^{(n)}(x'))_i = \sum_{I}^{(n)} \delta_{i,I}\varphi'(x'_I)$$
$$= \sum_{I}^{(n_0)} \delta_{i,I}\varphi'(|I|\ell) + \sum_{I}^{(n)\setminus(n_0)} \delta_{i,I}\varphi'(x'_I)$$

where the splitting of the sum is the same as in lemma 6. The proof is achieved is a similar way, the convergence following from $D_1^1 < \infty$. Q. E. D.

We prove now that the property of φ to give rise to a lattice in the limit $n \to \infty$, as stated by conditions L1, L2 and L3, is stable under appropriate assumptions on φ, already given in the previous theorems.

More precisely, there exists a neighborhood of φ defined through the moduli E_i^j of the perturbations ψ, such that $\varphi + \psi$ satisfies conditions L1, L2 and L3 (with possibly different constants).

THEOREM 5. — Let φ satisfy conditions L1, L2, L3 and assume D_1^1, D_2^2, D_2^3, D_3^3, defined by (20) are finite.

Then there exists a neighborhood $\mathcal{N}(\varphi)$ of the origin in $C^\infty([c, \infty[)$, such that for all $\psi \in \mathcal{N}(\varphi)$, $\varphi + \psi$ has the following properties:

There exists a sequence $\{ x'_{(n)} \}$ of stable equilibrium configurations for $(\varphi + \psi)^{(n)}$ with

L1 : $\exists \alpha_1, \beta_1, \mu_1 > 0$ such that for n large enough

$$H_y(\varphi + \psi)^{(n)} > \mu_1, \qquad \forall y \in \Omega(x'_{(n)}, \alpha_1, \beta_1)$$

L2 : $\exists a_1 > 0$ such that $\sigma(x'_{(n)}) < a_1$ for n large enough

L3 : $\exists \ell_1 > c$ such that $\lim_{n\to\infty} \tau(x'_{(n)}) = \ell_1$.

Proof.

1) Stability of L1.

Using the proof of theorem 3, we check easily that if the moduli E_1^1, E_1^2, E_2^2, E_3^3 are small enough, the solutions of (44) and (45) satisfy $u(1) < \alpha/2$ and $v(1) < \beta/2$.

Then, $\sigma(x'_{(n)} - x_{(n)}) < \alpha/2$ and $\tau(x'_{(n)} - x_{(n)}) < \beta/2$.

Now let $\alpha_1 = \alpha/2$, $\beta_1 = \beta/2$ and $\mu_1 = \mu = E_2^2 > 0$.

For any $y \in \Omega(x'_{(n)}; \alpha_1, \beta_1)$, we have

$$\sigma(y - x_{(n)}) \leqslant \sigma(y - x'_{(n)}) + \sigma(x'_{(n)} - x_{(n)}) < \alpha$$
$$\tau(y - x_{(n)}) \leqslant \tau(y - x'_{(n)}) + \tau(x'_{(n)} - x_{(n)}) < \beta$$

Thus $\Omega(x'_{(n)}; \alpha_1, \beta_1) \subset \Omega(x_{(n)}; \alpha, \beta)$ and L1 follows immediatly for $(\varphi + \psi)$ with $\mu_1 = \mu - E_2^2$.

2) Stability of L2.

Under the same conditions, $\sigma(x'_{(n)}) \leqslant \sigma(x_{(n)}) + \mathscr{u}(1) < \mathscr{a} + \alpha/2$. Then L2 holds for $(\varphi + \psi)$ with $\mathscr{a}_1 = \mathscr{a} + \alpha/2$.

3) Stability of L3.

In a similar way, the critical points $x'_{(n)}$ satisfy

$$\tau(x_{(n)}) - \beta/2 < \tau(x'_{(n)}) < \tau(x_{(n)}) + \beta/2 .$$

Since the sequence $\{ \tau(x_{(n)}) \}$ converges to ℓ, for n large enough, we certainly have

$$\tau(x'_{(n)}) \in [\ell - 2\beta/3, \ell + 2\beta/3] .$$

Using the proofs of theorem 4 and lemma 7, we show now that the sequence $\{ \tau(x'_{(n)}) \}$ has a unique limit point $\ell' \in [\ell - \beta/2, \ell + \beta/2]$.

Actually, it follows from lemma 7 that for any limit point ℓ' of

$$\{ \tau(x'_{(n)}) \}, \qquad \frac{\partial e}{\partial \ell}(\varphi + \psi, \ell') = 0 .$$

On the other hand, theorem 4 implies that $e(\varphi + \psi, .)$ is a convex function on $]\ell - \beta, \ell + \beta[$ satisfying $\frac{\partial^2 e}{\partial \ell^2}(\varphi + \psi, \ell') > \mu - E_2^2$.

Then the derivative has at most one zero ℓ' in this interval, and one checks easily that $\ell' = \lim_{n \to \infty} \tau(x'_{(n)}) \in [\ell - \beta/2, \ell + \beta/2]$. Q. E. D.

Thus the properties L1, L2 and L3 are structurally stable as soon as one requires decrease properties on the potential given by the conditions D_1^1, D_2^2, D_2^3 and $D_3^3 < \infty$. If φ decreases like $r^{-\chi}$ at infinity, these conditions are satisfied as soon as $\chi > 2$.

V. THE GROUND STATE CASE

Notice that, in the previous section, the equilibrium configurations $x_{(n)}$ were not assumed to give the ground state of $\varphi^{(n)}$: the structural stability L1, L2, L3 holds under the weaker assumption of mechanical stability.

Actually, the property for $x_{(n)}$ to be the ground state of $\varphi^{(n)}$ could be lost for $x'_{(n)}$ (and $(\varphi + \psi)^n$).

Although it seems difficult, from an experimental point of view, to decide wether a given sample is in its ground state and/or is a crystal free of defect, the theorical problem of identifying the ground state to a lattice is an interesting one.

In this section, we specify regularity conditions for the potential, such that the structural stability preserves the property of the ground state to be a lattice.

One can easily find a potential, the ground state of which is a lattice: consider the case of a $n-n$ interaction with finite range $< 2c$, and which has a unique non-degenerate minimum at $b \in]c, 2c[$. The sequence of the ground states $x_{(n)}$: $x_i = b \forall i$ obviously satisfies conditions L1 L2 L3, and theorem 5 insures the existence of an open neighborhood of potentials giving rise to lattices.

The intersection $\mathcal{V}$ of this neighborhood and of the open class defined below has the further property that the lattices thus obtained remain the ground states.

Let $\mathcal{C}$ be the class of hard core potentials $\varphi \in C^\infty [c, +\infty[$ such that:

$\exists r_1, r_2, r_3, \quad 2c > r_3,$

$$\begin{array}{llll} \varphi'(r) < 0 & \forall r \in [c, r_1[, & \varphi'(r) > 0 & \forall r > r_1 \\ \varphi''(r) > 0 & \forall r \in [c, r_2[, & \varphi''(r) < 0 & \forall r > r_2 \\ \varphi'''(r) < 0 & \forall r \in [c, r_3[, & \varphi'''(r) > 0 & \forall r > r_3 \end{array}$$

and such that

$$e''(c) + \varphi''(r_1) - \varphi''(c) > 0 \tag{48}$$

where $e(r)$ is the energy per particle for the lattice spacing r:

$$e(r) = \sum_{k>0} \varphi(kr) \tag{49}$$

One can check that these conditions are non-contradictory only if

$$c < r_1 < r_2 < r_3$$

These monotonicity conditions are satisfied, for instance, by any Lennard-Jones type potential with an hard core.

Observe that $\mathcal{C}$ is obviously an open set in the Whitney topology, and that the boundary of $\mathcal{C}$ contains finite range potentials of the type just mentionned, in such a way that their stability neighborhood intersect $\mathcal{C}$.

The lattices obtained by perturbation into $\mathcal{C}$ are proved to be the ground states by the following theorem:

THEOREM 6. — For any $\varphi \in \mathcal{C}$, for any n, and for any configuration $y = (y_1, \ldots, y_n)$ such that $\forall i$, $c < y_i < r_1$, the following bound holds:

$$H_y \varphi^{(n)} \geqslant (e''(c) + \varphi''(r_1) - \varphi''(c)) \mathrm{Id} > 0$$

Proof. — Recall that for any real symmetric matrix h to be positive definite, it is sufficient that:

$$h_{ii} - \sum_{i \neq j} | h_{ij} | > 0$$

We check now that this condition holds for $H_y \varphi^{(n)}$ with $\varphi \in \mathscr{C}$. In fact, the matrix elements of $H_y \varphi^{(n)}$ are given by (4):

$$(H_y \varphi^{(n)})_{ij} = \sum_{I \ni i,j} \varphi''(y_I)$$

We get:

$$(H_y \varphi^{(n)})_{ii} = \varphi''(y_i) + \sum_{\substack{I \ni i \\ |I| > 1}} \varphi''(y_I)$$

Using the definition of $\mathscr{C}$:

$$(H_y \varphi^{(n)})_{ii} > \varphi''(r_1) + \sum_{I \ni i,j} \varphi''(|I| c)$$

$$> \varphi''(r_1) + \sum_{k>1} k\varphi''(kc)$$

And for $i \neq j$

$$|(H_y \varphi^{(n)})_{ij}| \leqslant - \sum_{I \ni i,j} \varphi''(|I| c)$$

Then

$$\sum_{j \neq i} |(H_y \varphi^{(n)})_{ij}| \leqslant - \sum_{j \neq i} \sum_{I \ni i,j} \varphi''(|I| c)$$

$$\leqslant - \sum_{k>1} k(k-1)\varphi''(kc)$$

Thus

$$(H_y \varphi^{(n)})_{ii} - \sum_{j \neq i} |(H_y \varphi^{(n)})_{ij}| \geqslant \varphi''(r_1) + \sum_{k>1} k^2 \varphi''(kc) \tag{50}$$

The r. h. s. of (50) is equal to

$$\varphi''(r_1) - \varphi''(c) + e''(c) > 0 \qquad \text{Q. E. D.}$$

On the other hand, for $\varphi \in \mathscr{C}$, any equilibrium configuration $x_{(n)}$ is such that $\forall i,\ x_i < r_1$. But in the hypercube $\{ x_i < r_1 \}$, the convexity of $\varphi^{(n)}$ just proved implies that there is at most one equilibrium configuration.

For any $\varphi \in \mathscr{V}$, the equilibria $x_{(n)}$, on one hand exists and converges to a lattice (by structural stability) and, on the other hand, (by unicity), corresponds to the ground state.

As a final remark, notice that the assumption (48) is only slightly stronger than $e''(b) > 0$, (where $b \in]c, r_1[$ is the spacing of the limit lattice), which is an obviously necessary condition for the lattice to be stable.

CONCLUSION

It is clear that the main grounds for working on one dimensional systems are to provide a basis for the more physical three dimensional problem. Of course, the one-dimensional case is much simpler but we hope that the methods used in this paper can extend to the 3-dimensional case.

On this grounds, one could approach more physically relevant questions, such as the structural stability of lattices with a basis, or of the large class of non spherically invariant potentials, which concern most of the molecular lattices. The three dimensional stability problem will be investigated in a subsequent paper.

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