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Stability of Symmetries for Equilibrium Configurations of N Particles in Three Dimensions

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We consider equilibrium configurations of n identical particles in three dimensions interacting via two-body potentials depending only on the distance. The symmetry group of a given configuration is defined as the subgroup of isometries which leaves it invariant, up to permutations of the particles. We prove the stability of the symmetry in the following sense: the symmetry group of an equilibrium configuration is the same for the neighboring equilibria arising from any small enough perturbation of the initial potential. Furthermore, for a large class of realistic potentials, the existence of nontrivial symmetries is proved, thus giving a completely geometrical, although partial, approach to the classical crystal problem.

KEY WORDS: Classical crystal theory; crystallographic groups; stability of equilibrium; differential topology; Morse property.

1. INTRODUCTION

The problem of the classical theory of crystals is to show that, for realistic two-body potentials, the corresponding ground states, i.e., configurations with minimal energy per particle, present symmetries of crystal type. Up to now, rigorous results have been obtained essentially for one-dimensional systems.[1-7] To illustrate the specificity of our own work, let us briefly recall these results: Ventevögel and Nijboër[4-6] have studied the 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 one and only one periodic configura-

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tion that minimizes energy per particle (in the set of periodic configurations), this equilibrium being moreover stable with respect to all periodic 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 work with potential energy per particle, the definition of which makes sense only under periodicity assumptions. However, this approach is interesting because the authors draw conclusions about a (whole) class of potentials rather than about a special one: 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. In this way, one is led to work with open sets of potentials, for an adequate topology.

Another possible approach has been used by Radin *et al.*,[1,3] and consists in studying 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 toward a periodic lattice in the limit $n \to \infty$. However, the result is obtained only in the special case of the Lennard-Jones potential.

In a subsequent paper, Hamrick and Radin have dealt with the natural question of the stability of the property of a potential, to produce a lattice. The authors conclude that this ability depends very sensitively on the potential, in the following way: They choose a potential simple enough to clearly give rise to a lattice, and they build an ad hoc perturbation, depending on a small parameter $\epsilon > 0$, such that, for any ϵ, the corresponding equilibrium for the perturbed potential is aperiodic. However, in their counterexample, the perturbation of the potential energy and of its first derivative actually tends to zero with ϵ, but the second derivation remains finite, and therefore the perturbation cannot be considered small for this problem, since the second derivative must be controlled. In other words, the stability of a property of the potential makes sense only once the potential space is given a topology compatible with the physical position of the question.

In a previous paper,[7] we stressed this point of view and developed methods based on functional analysis to study the equilibrium configurations of finite systems in one dimension. We proved that for "almost all" two-body interactions, and for all n, the corresponding n-body energies give rise to nondegenerate equilibria. In mathematical terms, we proved that the set of potentials which yield Morse functions as n-body energies is residual in the space $C^\infty(\mathbb{R}^+, \mathbb{R})$ of the potential. Moreover, the Morse property is precisely the necessary and sufficient condition for a variation $\lambda\psi$ of the potential to give rise to a continuous trajectory of equilibria, for λ small enough. Using this result, we considered the perturbations of equilibria under an arbitrary variation of the potential and showed that a certain symmetry property, namely, the existence of a center of symmetry for the configurations, is stable. Moreover, this stability implies the existence of an open set of potentials such that all the corresponding n-body energies give rise to equilibria having this symmetry.

In the present paper, we give similar results for the three-dimensional case. We first prove, as in the one-dimensional case, that for almost all potential, the corresponding n-body energies are simultaneously Morse functions. As stressed previously, this is the condition to get a continuous trajectory for the equilibrium, under a variation of the potential. We are thus led to study the stability of symmetry properties of the equilibria. More precisely, we show that, if a (nondegenerate) equilibrium configuration is invariant under the action of a finite subgroup of the isometry group of $\mathbb{R}^3$ (e.g., a crystallographic point group), then, the neighboring equilibria corresponding to variations of the potential exhibit the same symmetry. Moreover, we show that, for a large class of realistic interactions, there exist equilibria with such nontrivial symmetry groups.

As a consequence of this approach, it seems that the classical crystal problem splits into two steps: on one hand the existence of symmetry for the equilibrium configurations (which appears to be of geometrical nature) and on the other hand, the particular symmetry of the ground state, which depends on detailed global properties of the potential.

In the next section we present the mathematical framework of our problem. In Section 3 we show how to take into account the invariance with respect to isometries in order to give proper definitions of equilibria and of their nondegeneracy. In Section 4 we prove that for "almost all" interactions the n-body energies are simultaneously Morse functions. This result is obtained through a natural stratification of the configuration space.

In Section 5 we prove our main result concerning the stability of the symmetry of the equilibria. We make use of another stratification of the configuration space, the strata of which are smooth submanifolds corresponding to finite subgroups of the isometries. In the last section we draw some other consequences of our approach. In particular a large class of interactions is proved to yield equilibria with nontrivial symmetries.

2. DEFINITIONS AND NOTATIONS

We first define the configuration space for n particles in three dimensions. We shall assume that the configuration $x = (x_1, \ldots, x_n)$, $x_i \in \mathbb{R}^3$, is actually three dimensional, i.e., there is no 2-plane in $\mathbb{R}^3$ containing all the particles. Besides, we require the particles to have distinct positions. Thus our configuration space $X^{(n)}$ for n particles is the dense open subset of $\mathbb{R}^{3n}$ given by

$$X^{(n)} = \{x = (x_1, \ldots, x_n) \mid x \text{ is 3-dim, and } i \neq j \Rightarrow x_i \neq x_j\} \tag{1}$$

The 2-body potentials are assumed to be smooth functions of the distance given by C^∞ functions φ on $]0, +\infty[$.

For any $n \geqslant 2$, the n-body energies $\varphi^{(n)}$ are C^∞ functions on $X^{(n)}$ defined by

$$\varphi^{(n)}(x) = \sum_{i<j} \varphi(\|x_{ij}\|) \tag{2}$$

where we put $x_{ij} = x_i - x_j$ and $\| \ \|$ is the Euclidean norm in $\mathbb{R}^3$.

Now a configuration $x \in X^{(n)}$ is an equilibrium for the interaction φ, iff all the partial derivatives of $\varphi^{(n)}$ vanish at x, in other words, iff x is a critical point of $\varphi^{(n)}$, that is, the differential satisfies $d\varphi^{(n)}(x) = 0$.

Since $\varphi^{(n)}$ involves the various distances $\|x_{ij}\|$, we introduce the following notations for the differentials:

$$d\|x_{ij}\| = \|x_{ij}\|^{-1}\epsilon_{ij}(x)$$

where $\epsilon_{ij}(x)$ is a one-form on $\mathbb{R}^{3n}$ defined by

$$\epsilon_{ij}(x) \cdot \xi = (x_{ij}, \xi_{ij}) \tag{3}$$

with $\xi = (\xi_1, \ldots, \xi_n)$, $\xi_{ij} = \xi_i - \xi_j$ and where $(\ , \ )$ is the ordinary scalar product in $\mathbb{R}^3$.

Using these notations, the differential of $\varphi^{(n)}$ takes the following form:

$$d\varphi^{(n)}(x) = \sum_{i<j} \varphi'(\|x_{ij}\|)\|x_{ij}\|^{-1}\epsilon_{ij}(x) \tag{4}$$

Now if x is a critical point for $\varphi^{(n)}$, the degeneracy of the equilibrium and its stability are described by the Hessian of $\varphi^{(n)}$ at x which is the symmetric two-form on $\mathbb{R}^{3n}$ given by

$$\begin{aligned} H_x\varphi^{(n)} &= \sum_{i<j} \left[\varphi''(\|x_{ij}\|)\|x_{ij}\|^{-2} - \varphi'(\|x_{ij}\|)\|x_{ij}\|^{-3}\right]\epsilon_{ij}(x) \otimes \epsilon_{ij}(x) \\ &\quad + \sum_{i<j} \varphi'(\|x_{ij}\|)\|x_{ij}\|^{-1}\epsilon_{ij} \end{aligned} \tag{5}$$

where ϵ_{ij} is a two-form on $\mathbb{R}^{3n}$ defined by

$$\epsilon_{ij}(\xi, \zeta) = (\xi_{ij}, \zeta_{ij}) \tag{6}$$

with $\xi = (\xi_1, \ldots, \xi_n)$, $\zeta = (\zeta_1, \ldots, \zeta_n)$, $\xi_{ij} = \xi_i - \xi_j$, $\zeta_{ij} = \zeta_i - \zeta_j$ and where $(\ , \ )$ is the scalar product in $\mathbb{R}^3$.

Actually, since the n-body energies $\varphi^{(n)}$ are invariant with respect to global three-dimensional isometries acting on $X^{(n)}$, we must take into account this Euclidean invariance to give a relevant meaning to the nondegeneracy and positivity property of the Hessians.

3. EUCLIDEAN INVARIANCE AND REDUCTION OF THE CONFIGURATION SPACE

Let $I = \mathbb{R}^3 \times O(3)$ be the isometry group of $\mathbb{R}^3$, i.e., the semidirect product of translations and rotations.

If $(\tau, \rho) \in I$, we denote by $(\tau, \rho)^{(n)}$ the natural action on $\mathbb{R}^{3n}$. If $x \in X^{(n)}$ we have

$$(\tau, \rho)^{(n)} x = (\tau, \rho)^{(n)}(x_1, \ldots, x_n) = ((\tau, \rho)x_1, \ldots, (\tau, \rho)x_n) \tag{7}$$

and

$$(\tau, \rho)x_i = \tau + \rho x_i \tag{8}$$

Let $I(x)$ be the orbit of $x \in X^{(n)}$ under the action of I. Then it follows from a theorem of elementary geometry [8] that

$$I(x) = \left\{ y \in X^{(n)} \mid \forall i, j, \|x_{ij}\| = \|y_{ij}\| \right\} \tag{9}$$

For any $x \in X^{(n)}$, $I(x)$ is a submanifold of $X^{(n)}$, and we denote by $\mathcal{I}(x)$ its tangent space at x. One checks that

$$\begin{aligned} \mathcal{I}(x) &= \left\{ \xi \in \mathbb{R}^{3n} \mid \forall i, j, (x_{ij}, \xi_{ij}) = 0 \right\} \\ &= \left\{ \xi \in \mathbb{R}^{3n} \mid \forall i, j, \epsilon_{ij}(x) \cdot \xi = 0 \right\} \end{aligned} \tag{10}$$

The set of one-forms at x, which vanish on $\mathcal{I}(x)$ is a vector subspace $\mathcal{I}(x)^{\perp}$ of the cotangent space $T_x^* X^{(n)}$, and it follows from (10) that

$$\mathcal{I}(x)^{\perp} = \left\{ \theta = \sum_{i<j} a_{ij} \epsilon_{ij}(x) \mid a_{ij} \in \mathbb{R} \right\} \tag{11}$$

Since the two-body potentials φ depend only on the distance, the $\varphi^{(n)}$ are constant on the orbits so that the differentials have the property

$$d\varphi^{(n)}(x) = 0 \qquad \text{on} \quad \mathcal{I}(x) \tag{12}$$

and for any critical point x of $\varphi^{(n)}$ the Hessian satisfies the following equivalent relations:

$$\operatorname{Ker} H_x \varphi^{(n)} \supset \mathcal{I}(x), \qquad \operatorname{Im} H_x \varphi^{(n)} \subset \mathcal{I}(x)^{\perp} \tag{13}$$

Actually, it follows from (5) that the terms

$$\left[\varphi''(\|x_{ij}\|)\|x_{ij}\|^{-2} - \varphi'(\|x_{ij}\|)\|x_{ij}\|^{-3} \right] \epsilon_{ij}(x) \otimes \epsilon_{ij}(x)$$

obviously satisfy (13). If x is a critical point of $\varphi^{(n)}$ we have

$$d\varphi^{(n)}(x)=\sum_{i<j}\varphi'(\|x_{ij}\|)\|x_{ij}\|^{-1}\epsilon_{ij}(x)=0$$

Then $d\varphi^{(n)}$ vanishes on $I(x)$ and by derivation

$$\sum_{i<j}\varphi'(\|x_{ij}\|)\|x_{ij}\|^{-1}\epsilon_{ij}=0 \qquad \text{on} \quad \mathcal{I}(x)$$

which yields (13).

Now, as soon as one deals with mechanical systems with symmetry, one usually proceeds to the reduction of the configuration space in order to get rid of the useless coordinates describing the orbits.

In the present case, since we consider only three-dimensional configurations of distinct particles, the reduced space $X^{(n)}/I$ is a smooth manifold on which we have the usual definitions of nondegenerate critical points and of Morse functions (Hessians of maximal rank at each critical point). However, for the sake of simplicity, we shall not work in the quotient space, but we give the corresponding equivalent "lifted" definitions for the "Morse property" of the n-body energies at a "nondegenerate" critical point:

$$\operatorname{Ker} H_x\varphi^{(n)}=\mathcal{I}(x), \qquad \operatorname{Im} H_x\varphi^{(n)}=\mathcal{I}(x)^{\perp} \tag{14}$$

For instance let h_0 be the following "standard" Hessian at x:

$$h_0=\sum_{i<j}\epsilon_{ij}(x)\otimes\epsilon_{ij}(x) \tag{15}$$

Then $\operatorname{Ker} h_0=\mathcal{I}(x)$ and consequently $\operatorname{Im} h_0=\mathcal{I}(x)^{\perp}$.

The next section is devoted to the proof that for "almost all" 2-body potentials φ, the n-body energies $\varphi^{(n)}$ are "Morse functions" in the previous sense, for all n.

4. GENERICITY OF THE MORSE PROPERTY AND STRATIFICATION BY DISTANCES

As in a previous paper,[7] the Morse property of the n-body energies is the main feature which is used to investigate the effect on critical points, of perturbations of the 2-body potential. In this section we shall prove that this property is generic.

Let us first recall some mathematical definitions (see Refs. 7 and 9 for further details). A property is said to be generic on a given topological space, if it holds for all points in a residual set.

A subset of a topological space is residual if it is presented as the intersection of a countable family of dense open sets.

In our case, the set of potentials $C^{\infty}(]0, \infty[)$ will be endowed with the so-called compact-open (weak) and Whitney (strong) topologies. We recall that $C^{\infty}(]0, \infty[)$ is a Baire space for the strong topology, i.e., the residual sets are dense.[9,11]

Let us mention that the genericity of the "Morse property" for the n-body energies does not follow from the well-known theorems of functional analysis for $C^{\infty}(\mathbb{R}^p)$ (see Ref. 9).

Actually, these theorems use perturbation methods in order to remove the possible degeneracy of critical points. In our case the allowed perturbations of the n-body energies $\varphi^{(n)}$ arise from perturbations of the 2-body potentials φ and therefore are submitted to constraints that do not exist in the general case. Furthermore it is clear that such perturbations step in only by the values they take in the neighborhoods of the distances actually realized by the given equilibrium configuration. Thus it is convenient to split $X^{(n)}$ into classes described by means of equalities of distances between particles, given by the following definition.

Definition. For any $a \in X^{(n)}$ let

$$D_a = \left\{ x \in X^{(n)} \mid \|x_{ij}\| = \|x_{kl}\| \Leftrightarrow \|a_{ij}\| = \|a_{kl}\| \right\} \tag{16}$$

The partition of $X^{(n)}$ arising from (16) will be referred to as the stratification by distances.

It follows from the very definition that each set D_a is a semialgebraic variety, i.e., is defined by a finite family of algebraic equations or inequations.

A classical theorem of Whitney[10] asserts that any connected semialgebraic real variety is a finite disjoint union of smooth manifolds one of them, which is of maximal dimension, being open and dense.

In fact we shall not use the explicit decomposition of D_a but only the following properties of the tangent spaces to its smooth parts:

If Δ is a smooth part of D_a, one checks that Δ is invariant by I and that the tangent spaces $T_x\Delta$ satisfy

$$\mathcal{I}(x) \subset T_x\Delta \subset \mathcal{D}(x) \tag{17}$$

where

$$\mathcal{D}(x) = \left\{ \xi \in \mathbb{R}^{3n} \mid \|x_{ij}\| = \|x_{kl}\| \Rightarrow (x_{ij}, \xi_{ij}) = (x_{kl}, \xi_{kl}) \right\} \tag{18}$$

In particular, if Δ is the open submanifold of D_a, a consequence of Ref. 10 is that

$$\forall x \in \Delta, \qquad T_x\Delta = \mathcal{D}(x) \tag{19}$$

As mentioned above, since the 2-body potentials φ depend only on the distances, the differentials and Hessians of $\varphi^{(n)}$ are submitted to constraints.

We define $\mathcal{E}(x)$ and $\mathcal{H}(x)$, for $x \in X^{(n)}$, as the subspaces of respectively one-forms (4) and symmetric two-forms (5) spanned by differentials and Hessians at x. Then

$$\mathcal{E}(x) = \left\{ \theta = \sum_{i<j} a_{ij}\epsilon_{ij}(x) \mid \|x_{ij}\| = \|x_{kl}\| \Rightarrow a_{ij} = a_{kl} \right\} \tag{20}$$

$$\mathcal{H}(x) = \Big\{ h = \sum_{i<j} \left[b_{ij}\epsilon_{ij}(x) \otimes \epsilon_{ij}(x) + c_{ij}\epsilon_{ij} \right]$$
$$\times \|x_{ij}\| = \|x_{kl}\| \Rightarrow b_{ij} = b_{kl},\ c_{ij} = c_{kl} \text{ and } \sum_{i<j} c_{ij}\epsilon_{ij}(x) = 0 \Big\} \tag{21}$$

It follows from (12) and (20) that $\mathcal{E}(x) \subset \mathcal{I}(x)^{\perp}$.

Now let Δ be an arbitrary smooth part of the stratification of $X^{(n)}$ and

$$E = \{(x,\theta) \mid x \in \Delta, \theta \in \mathcal{I}(x)^{\perp}\} \tag{22}$$

$$N = \{(x,\theta) \mid x \in \Delta, \theta \in T_x\Delta^{\perp}\} \tag{23}$$

define $F:\Delta \to E$ by $F(x) = (x, d\varphi^{(n)}(x))$. Then we have

Lemma 1. If $x \in \Delta$ is a critical point of $\varphi^{(n)}$, the following conditions are equivalent:

(i) $$H_x(\varphi^{(n)}|_{\Delta})(T_x\Delta) = \mathcal{I}(x)^{\perp}|_{T_x\Delta} \tag{24}$$

i.e., x is "non-degenerate" for the restriction $\varphi^{(n)}|_{\Delta}$.

(ii) $$H_x\varphi^{(n)}(T_x\Delta) + T_x\Delta^{\perp} = \mathcal{I}(x)^{\perp} \tag{25}$$

(iii) F is transverse[9] to N at x: $F \pitchfork_x N$, i.e.

$$\operatorname{Im} T_xF + T_{x,0}N = T_{x,0}E \tag{26}$$

Proof. If $x \in \Delta$ is a critical point of $\varphi^{(n)}$, the Hessian of the restriction $\varphi^{(n)}|_{\Delta}$ is the restriction of the Hessian to $T_x\Delta$ (see Ref. 9, p. 65), and therefore (i)$\Leftrightarrow$(ii).

There is a natural isomorphism of $T_{x,0}E$ onto $T_x\Delta \times \mathcal{I}(x)^{\perp}$ which maps $T_{x,0}N$ onto $T_x\Delta \times T_x\Delta^{\perp}$, and $T_xF(\xi)$ on $(\xi, H_x\varphi^{(n)}(\xi))$ for any $\xi \in T_x\Delta$. Then (iii) reads

$$\{(\xi, H_x\varphi^{(n)}(\xi))\} + T_x\Delta \times T_x\Delta^{\perp} = T_x\Delta \times \mathcal{I}(x)^{\perp}$$

and clearly (ii)$\Leftrightarrow$(iii). ■

Using appropriate perturbations of the potentials we shall prove that the equivalent conditions of Lemma 1 hold densely on $C^{\infty}(]0,+\infty[)$, on suitable compacts of Δ.

Let $\bar{x} \in \Delta$ and $\{\|\bar{x}_{ij}\|\}_{i<j}$ the set of corresponding distances. There exist finite collections $\{U_{ij}\}, \{V_{ij}\}, \{W_{ij}\}$ of relatively compact open sets in $]0, +\infty[$ such that

$$\begin{aligned}
&\text{(i)} && \|\bar{x}_{ij}\| \in U_{ij}, \quad \overline{U}_{ij} \subset V_{ij}, \quad \text{and} \quad \overline{V}_{ij} \subset W_{ij} \\
&\text{(ii)} && \|\bar{x}_{ij}\| = \|\bar{x}_{kl}\| \Rightarrow U_{ij} = U_{kl}, \quad V_{ij} = V_{kl} \quad \text{and} \quad W_{ij} = W_{kl} \\
&\text{(iii)} && \|\bar{x}_{ij}\| \neq \|\bar{x}_{kl}\| \Rightarrow W_{ij} \cap W_{kl} = \emptyset
\end{aligned} \tag{27}$$

The intersections in Δ of the pull-back of $\{U_{ij}\}$, $\{V_{ij}\}$, and $\{W_{ij}\}$ by means of the mappings $x \to \|x_{ij}\|$ contain relatively compact open sets U, V, and W such that $\bar{x} \in U$, $\overline{U} \subset V$ and $\overline{V} \subset W$.

4.1. Local Perturbations on U

For each pair $\{V_{ij}, W_{ij}\}$, one can take an Urysohn function ρ_{ij} on $]0, +\infty[$ such that

$$\rho_{ij} \mid_{V_{ij}} = 1, \qquad \rho_{ij} \mid_{W_{ij}^c} = 0$$

where W_{ij}^c is the complement of W_{ij}.

Let A be the set of $a = \{a_{ij}\}_{i<j}$ in $\mathbb{R}^{n(n-1)/2}$ such that $\|\bar{x}_{ij}\| = \|\bar{x}_{kl}\| \Rightarrow a_{ij} = a_{kl}$. The above construction allows us to associate to any $a \in A$ the "variation" $\psi(a) \in C^\infty(]0, \infty[)$ defined by

$$\psi(a, t) = \frac{1}{2} \sum_{i<j} \rho_{ij}(t) m_{ij}^{-1} a_{ij} t^2 \tag{28}$$

where m_{ij} is the number of pairs $k < l$ such that $\|\bar{x}_{ij}\| = \|\bar{x}_{kl}\|$.

This definition is justified by the following property of the corresponding n-body energy $\psi(a)^{(n)}$: For $x \in V$,

$$\psi^{(n)}(a, x) = \frac{1}{2} \sum_{i<j} a_{ij} \|x_{ij}\|^2 \tag{29}$$

$$d\psi^{(n)}(a, x) = \sum_{i<j} a_{ij} \epsilon_{ij}(x) \tag{30}$$

Define G: $\Delta \times A \to E$, [see (22)], by

$$G(x, a) = \big(x, d(\varphi + \psi(a))^{(n)}(x)\big) \tag{31}$$

Let

$$\Gamma = \{(x, a) \in V \times A \mid G(x, a) = (x, 0)\} \tag{32}$$

that is $(x, a) \in \Gamma \Leftrightarrow x$ is a critical point of the perturbed n-body energy $(\varphi + \psi(a))^{(n)}$ in V.

$$\Gamma_0 = \{x \in V \mid G(x, 0) = (x, 0)\} \tag{33}$$

Then $\Gamma_0 = \Gamma \cap (V \times \{0\})$ is the set of critical points of $\varphi^{(n)}$ lying in V.

Lemma 2. If $(x,a) \in \Gamma$, the following conditions are equivalent:

(i) $H_x(\varphi + \psi(a))^{(n)}|_{\Delta}(T_x\Delta) + T_a(d\psi^{(n)})(T_aA, x) = \mathcal{G}(x)^{\perp}|_{T_x\Delta}$

$$\tag{34}$$

(ii) $H_x(\varphi + \psi(a))^{(n)}(T_x\Delta) + T_a(d\psi^{(n)})(T_aA, x) + T_x\Delta^{\perp} = \mathcal{G}(x)^{\perp}$

$$\tag{35}$$

(iii) G is transverse to N at $(x,a): G \pitchfork_{x,a} N$, i.e.,

$$\operatorname{Im} T_{x,a}G + T_{x,0}N = T_{x,0}E \tag{36}$$

Proof. The equivalence of (i) and (ii) follows from the same argument as in Lemma 1. The isomorphism mentioned above maps $T_{x,a}G(\xi,\alpha)$ on $(\xi, H_x(\varphi + \psi(a))^{(n)}(\xi) + T_a\psi^{(n)}(\alpha, x))$ for any $(\xi,\alpha) \in T_x\Delta \times T_aA$ and clearly (ii)$\Leftrightarrow$(iii). ■

We now prove that the set of variations associated with A is large enough to insure the equivalent conditions of Lemma 2.

Actually, in view of (35), it is sufficient to prove the following.

Lemma 3. Let A and ψ be defined as above. Then

$$T_a(d\psi^{(n)})(T_aA, x) + T_x\Delta^{\perp} = \mathcal{G}(x)^{\perp} \tag{37}$$

Proof. Since A is a linear subspace of $\mathbb{R}^{n(n-1)/2}$, we can identify the tangent spaces T_aA with A itself. Using (30), one gets the following expression for the partial derivative with respect to $a \in A$:

$$T_a(d\psi^{(n)})(\alpha, x) = \sum_{i<j} \alpha_{ij}\epsilon_{ij}(x) \tag{38}$$

where $\|\bar{x}_{ij}\| = \|\bar{x}_{kl}\| \Rightarrow \alpha_{ij} = \alpha_{kl}$.

Comparing with (20), it is equivalent to check that

$$\mathcal{E}(x) + T_x\Delta^{\perp} = \mathcal{G}(x)^{\perp}$$

It follows from the definition (15) of the "standard" Hessian at x and of (17) that $h_0(T_x\Delta) \subset \mathcal{E}(x)$, and it is sufficient to prove that

$$h_0(T_x\Delta) + T_x\Delta^{\perp} = \mathcal{G}(x)^{\perp}$$

But $h_0(T_x\Delta)$ and $T_x\Delta^{\perp}$ are supplementary subspaces of $\mathcal{G}(x)^{\perp}$: if $\theta \in h_0(T_x\Delta) \cap T_x\Delta^{\perp}$ then $\theta = h_0(\xi)$ for some $\xi \in T_x\Delta$; then $\theta \cdot \xi = 0$, i.e., $h_0(\xi,\xi) = 0$, which implies $\xi \in \mathcal{G}(x)^{\perp}$ and therefore $\theta = h_0(\xi) = 0$.

Now, $\dim h_0(T_x\Delta) = \dim T_x\Delta - \dim \mathcal{G}(x)$, and we obtain the stronger result:

$$h_0(T_x\Delta) \oplus T_x\Delta^{\perp} = \mathcal{G}(x)^{\perp} \quad ■ \tag{39}$$

Lemmas 1 and 2 imply that G is transverse to N on Γ. A classical theorem of transversality theory asserts the existence of an open neighborhood $\mathcal{V}(\Gamma)$ of Γ in $V \times A$ such that G is transverse to N on $\mathcal{V}(\Gamma)$.

Since Γ_0 is closed and $\bar{U}$ is compact in V, $\bar{U} \cap \Gamma_0 \times \{0\}$ is compact in $V \times A$ and is contained in Γ. Then there exist open neighborhoods $\mathcal{V}(\bar{U} \cap \Gamma_0)$ in V and $\mathcal{W}'(0)$ in A, such that $\mathcal{V}(\bar{U} \cap \Gamma_0) \times \mathcal{W}'(0) \subset \mathcal{V}(\Gamma)$.

An important result of transversality theory (Ref. 9, Lemma 4.6) claims that for almost all $a \in \mathcal{W}'(0)$, the partial mappings $G_a\colon x \to G(x, a)$, are transverse to N on $\mathcal{V}(\bar{U} \cap \Gamma_0)$. It follows then from Lemma 1 that for almost all $a \in \mathcal{W}'(0)$, the critical points of $(\varphi + \psi(a))^{(n)}$ lying in $\mathcal{V}(\bar{U} \cap \Gamma_0)$, are "nondegenerate" for the restriction to Δ.

On the other hand $d\varphi^{(n)}$ does not vanish on $\bar{U} \backslash \Gamma_0$, and *a fortiori* on $\bar{U} \backslash \mathcal{V}(\bar{U} \cap \Gamma_0)$, a compact subset of V. Then, there exists an open neighborhood $\mathcal{W}''(0)$ in A such that $d(\varphi + \psi(a))^{(n)} \neq 0$ on $\bar{U} \backslash \mathcal{V}(\bar{U} \cap \Gamma_0)$ for any $a \in \mathcal{W}''(0)$.

Finally, for almost all $a \in \mathcal{W}(0) = \mathcal{W}'(0) \cap \mathcal{W}''(0)$ and any $x \in \bar{U}$, one has either (i) $x \in \mathcal{V}(\bar{U} \cap \Gamma_0)$. Then if x is a critical point of $(\varphi + \psi(a))^{(n)}$, it is nondegenerate for the restriction to Δ. or (ii) $x \in \bar{U} \backslash \mathcal{V}(\bar{U} \cap \Gamma_0)$ and x is not critical for $(\varphi + \psi(a))^{(n)}$.

Now, it follows from the definition of the strong (Whitney) topology on $C^\infty(]0, \infty[)$ that the "variation mapping" $\psi\colon A \to C^\infty(]0, \infty[)$, defined by (28) is continuous. The above remarks yield the following corollary.

Corollary 1. Let Δ be any smooth part of the stratification by distances, and U an open set arising from the construction (27), and let $\varphi \in C^\infty(]0, \infty[)$.

Then any strong neighborhood of φ contains a potential φ_0 such that the critical points of $\varphi_0^{(n)}$ in $\bar{U}$ are "nondegenerate" for the restriction to Δ. Since the n-body energies are invariant with respect to isometries, any critical point x gives rise to a critical orbit $I(x)$.[9] Then, a modified version of a classical theorem (Ref. 9, Proposition 6.3) gives the following corollary.

Corollary 2. Let Δ, U, φ, and φ_0 be as above. If $x \in \bar{U}$ is a critical point of $\varphi_0^{(n)}$, the "nondegeneracy" at x of the Hessian of the restriction $\varphi_0^{(n)}|_\Delta$ implies that the critical orbit $I(x)$ is isolated from other critical orbits of $\varphi_0^{(n)}$ intersecting $\bar{U}$. Therefore there are finitely many such orbits which intersect $\bar{U}$.

4.2. Density of the "Morse Property" on Δ

Notice that the critical points of $\varphi_0^{(n)}$ in $\bar{U}$ can be degenerate in directions transverse to Δ.

We now prove that if φ_0 is as above, any strong neighborhood of φ_0 contains a potential φ_k such that the critical points of $\varphi_k^{(n)}$ in $\bar{U}$ are "nondegenerate" in $X^{(n)}$, i.e., $\varphi_k^{(n)}$ is a "Morse function" on $\bar{U}$.

Let $x_1, \ldots, x_k$ be critical points of $\varphi_0^{(n)}$ in $\overline{U}$ such that $I(x_1), \ldots, I(x_k)$ are the different critical orbits of $\varphi_0^{(n)}$ intersecting $\overline{U}$. Corollary 2 asserts that there exist relatively compact neighborhoods Ω_i in Δ with $I(x_i) \cap \overline{U} \subset \Omega_i$, such that no other critical orbit intersects $\overline{\Omega}_i$. We claim that for $i = 1, \ldots, k$, there exist open neighborhoods $\mathcal{V}_i$ of φ_0 for the weak topology of $C^\infty(]0, \infty[)$, such that $\forall \psi \in \mathcal{V}_i$, $\psi^{(n)}|_\Delta$ is a "Morse function" on $\overline{\Omega}_i$ with a unique critical orbit in Ω_i.

Actually, this follows from (1) The mapping of $C^\infty(]0, \infty[)$ to $C^\infty(\Delta)$ given by $\varphi \to \varphi^{(n)}|_\Delta$ is continuous for the weak topology. (2) A general theorem of transversality theory (Ref. 9, p. 52) implies that in $C^\infty(\Delta)$, the set of "Morse functions" on $\overline{\Omega}_i$ is open for the strong or weak topology.

On the other hand, $\varphi_0^{(n)}$ has no critical point in $\overline{U} \backslash (\bigcup_{i=1}^k \Omega_i)$, a compact subset. The continuity of $\varphi \to \varphi^{(n)}|_\Delta$ yields an open neighborhood $\mathcal{V}_0$ of φ_0, such that $\forall \psi \in \mathcal{V}_0$, $\psi^{(n)}$ has no critical point in $\overline{U} \backslash (\bigcup_{i=1}^k \Omega_i)$.

Now, if $\psi \in \mathcal{V}^{(0)} = \bigcup_{i=0}^k \mathcal{V}_i$, $\psi^{(n)}$ has at most k critical orbits in $\overline{U}$, each of them being "nondegenerate" for the restriction.

The possible degeneracy of the Hessians in directions out of Δ will be removed with the help of the following "variations" centered on critical orbits. If $y \in V$, we define $\chi_y \in C^\infty(]0, \infty[)$ [see (28)] by

$$\chi_y(t) = \frac{1}{2} \sum_{i<j} \rho_{ij}(t) m_{ij}^{-1} (t - \|y_{ij}\|)^2 \tag{40}$$

Then, the corresponding n-body energy satisfies, for $x \in V$,

$$\chi_y^{(n)}(x) = \frac{1}{2} \sum_{i<j} (\|x_{ij}\| - \|y_{ij}\|)^2 \tag{41}$$

$$d\chi_y^{(n)}(x) = \sum_{i<j} (\|x_{ij}\| - \|y_{ij}\|) \|x_{ij}\|^{-1} \epsilon_{ij}(x) \tag{42}$$

$$H_y \chi_y^{(n)} = \sum_{i<j} \|y_{ij}\|^{-2} \epsilon_{ij}(y) \otimes \epsilon_{ij}(y) \tag{43}$$

Let us remark that the Hessians $H_y \chi_y^{(n)}$ are of maximal rank, i.e., satisfy (14).

Lemma 4. Let $\varphi_0, \Omega_1, \ldots, \Omega_k$ and $\mathcal{V}^{(0)}$ be as above. Then any neighborhood of φ_0 intersects the open subset $\mathcal{V}^{(1)} = \mathcal{V}^{(0)} \cap \mathcal{V}_1'$ where $\mathcal{V}_1'$ is the open set of ψ such that $\psi^{(n)}$ is a "Morse function" on $\overline{\Omega}_1$.

Proof. Consider the set of perturbed potentials $\varphi_0 + \lambda \chi_{x_1}$ where $\lambda \in \mathbb{R}$ and χ_{x_1} is the variation defined by (40) and centered on $I(x_1)$. Since $d\chi_{x_1}^{(n)}(x_1) = 0$, $I(x_1)$ is a critical orbit of $(\varphi_0 + \lambda \chi_{x_1})^{(n)}$ for any λ. The corresponding Hessian which is simply $H_{x_1} \varphi_0^{(n)} + \lambda H_{x_1} \chi_{x_1}^{(n)}$, will be of maximal rank except for a finite number of λ, zeros of a certain determinant.

On the other hand, for λ small enough the perturbed potential $\varphi_0 + \lambda\chi_{x_1}$ belongs to $\mathcal{V}^{(0)}$. Finally, there exist arbitrarily small λ's such that the perturbed n-point energy $(\varphi_0 + \lambda\chi_{x_1})^{(n)}$ is a "Morse function" on $\overline{\Omega}_1$. In other words, any (weak or strong) neighborhood $\mathcal{U}$ of φ_0 intersects $\mathcal{V}^{(1)}$. ∎

In such an arbitrary neighborhood $\mathcal{U}$ of φ_0, one can pick up a φ_1 in $\mathcal{V}^{(1)}$ and iterate the previous construction in order to remove the possible degeneracy of the next critical orbit.

After at most k steps, one gets a potential φ_k in an arbitrary (weak or strong) neighborhood of φ_0 such that $\varphi_k^{(n)}$ is a "Morse function" on $\overline{U}$. Since φ_0 is taken arbitrarily close to the initial potential φ (cf. Corollary 1), we can conclude the following:

Lemma 5. For any Δ of the stratification by distances, and any open set U arising from the construction (27), the set of $\varphi \in C^{\infty}(]0, \infty[)$ such that $\varphi^{(n)}$ is a "Morse function" on $\overline{U}$, is dense in $C^{\infty}(]0, \infty[)$ for both weak and strong topologies.

4.3. Genericity of the Morse Property on $X^{(n)}$

One can easily check that the continuity of $\varphi \to \varphi^{(n)}$ for the weak topology (but not for the strong one) implies that for any compact K of $X^{(n)}$, the set of φ such that $\varphi^{(n)}$ is "Morse" on K, is an open subset of $C^{\infty}(]0, \infty[)$ for the weak, and consequently for the strong topology. Then, on account of Lemma 5, we have the following lemma.

Lemma 6. For any Δ of the stratification by distances, and any open set U arising from the construction (27), the set of $\varphi \in C^{\infty}(]0, \infty[)$ such that $\varphi^{(n)}$ is a "Morse function" on $\overline{U}$, is open and dense in $C^{\infty}(]0, \infty[)$ for both weak and strong topologies.

Now, we proceed to the globalization of this result on $X^{(n)}$. This is achieved in the following way. The construction (27) associates to any $\bar{x}$ in Δ an open neighborhood U of $\bar{x}$ in Δ. The collection of these open subsets covers the paracompact manifold Δ. Therefore, one can pick up a countable collection $\{U_\alpha\}_{\alpha \in \mathbb{N}}$, which covers Δ. On the other hand, the stratification of $X^{(n)}$ by distances gives rise to a finite partition of $X^{(n)}$ by smooth manifolds Δ. Consequently, for any n, the set of $\varphi \in C^{\infty}(]0, \infty[)$ such that $\varphi^{(n)}$ is "Morse" on $X^{(n)}$ is a countable intersection of (weak or strong) open dense subsets of $C^{\infty}(]0, \infty[)$.

The intersection over n does not change this result, and therefore the set of $\varphi \in C^{\infty}(]0, \infty[)$ such that for all n, $\varphi^{(n)}$ is "Morse" on $X^{(n)}$, is residual as well. In other words, the "Morse property" of $\varphi^{(n)}$ on $X^{(n)}$ for all $n \geqslant 2$, is generic in $C^{\infty}(]0, \infty[)$ for both weak and strong topologies.

Now, a nice property of the strong topology is that it makes a Baire space of $C^\infty(]0,\infty[)$ (see Ref. 11, Theorem 4.4), i.e., any residual subset is dense. Finally, we obtain the following theorem.

Theorem 1. The set of $\varphi \in C^\infty(]0,\infty[)$ such that $\varphi^{(n)}$ is "Morse" on $X^{(n)}$ for all n, is residual and therefore dense in $C^\infty(]0,\infty[)$ for both weak and strong topologies.

Let us remark that the density for the strong topology is a rather strong result. For instance if $\varphi \in C^\infty(]0,\infty[)$ is any given potential and δ is any (strictly) positive function on $]0,\infty[$, there exists $\psi \in C^\infty(]0,\infty[)$ with $|\varphi - \psi| < \delta$, such that $\psi^{(n)}$ is "Morse" on $X^{(n)}$ for all n.

The methods developed in this section to remove the possible degeneracy of critical points can be used to give the following consequence of physical interest:

Any point $x \in X^{(n)}$ is a stable nondegenerate equilibrium for some potential φ in $C^\infty(]0,\infty[)$. Moreover, for a given x the set of such potentials is dense in $C^\infty(]0,\infty[)$ for the C^0 strong topology: if $\varphi \in C^\infty(]0,\infty[)$ is any given potential and δ is any (strictly) positive function on $]0,\infty[$, there exists $\psi \in C^\infty(]0,\infty[)$ with $|\varphi - \psi| < \delta$ and x is a stable "nondegenerate" equilibrium for $\psi^{(n)}$.

Actually for any x and φ, a perturbation (28), with a support as small as required by δ, can be used to make x into a critical point. Then, in the same conditions, a perturbation (40) will make this equilibrium stable and nondegenerate.

Let us conclude this section by giving the following local and direct consequence of Lemma 6: for any compact subset K of $X^{(n)}$, the set of $\varphi \in C^\infty(]0,\infty[)$ such that $\varphi^{(n)}$ is "Morse" on K is open and dense in $C^\infty(]0,\infty[)$ for both weak and strong topologies.

5. STRATIFICATION WITH RESPECT TO SYMMETRIES AND STABILITY PROPERTIES

In this section we are concerned with the symmetry properties of equilibrium configurations in $X^{(n)}$.

To be more specific, we have a natural action of the direct product $I \times \Sigma^{(n)}$ of the isometry group and the permutation group of n elements: for $(\tau,\rho) \in I$ and $\sigma \in \Sigma^{(n)}$, define

$$\forall x \in X^{(n)}, \qquad (\tau,\rho,\sigma)^{(n)}x = y, \qquad y_i = \tau + \rho x_{\sigma^{-1}(i)} \tag{44}$$

The symmetry group of a configuration x is defined as the isotropy group of x for the action (44):

$$G_x = \left\{(\tau,\rho,\sigma) \in I \times \Sigma^{(n)} \mid x_i = \tau + \rho x_{\sigma^{-1}(i)}\right\} \tag{45}$$

One can check from the definition (1) of $X^{(n)}$ that the correspondence between isometries and permutations defined by (45) is one to one. Actually, G_x is isomorphic to each of its projections I_x on I and Σ_x on $\Sigma^{(n)}$. Moreover, I_x is isomorphic to its projection R_x on $O(3)$, and we have

$$I_x = \left\{(\tau, \rho) \in I \,|\, \exists \sigma \in \Sigma^{(n)} \tau + \rho x_i = x_{\sigma(i)}\right\} \tag{46}$$

$$\Sigma_x = \left\{\sigma \in \Sigma^{(n)} \,|\, \forall i, j \; \|x_{ij}\| = \|x_{\sigma(i)\sigma(j)}\|\right\} \tag{47}$$

The isomorphism between G_x and Σ_x comes from a general theorem of Euclidean geometry.[8]

Since the elements of G_x are diffeomorphisms keeping x fixed, the corresponding tangent maps are automorphisms of $T_x X^{(n)}$. They actually define a subgroup $\mathcal{G}_x$ of $\operatorname{Aut} T_x X^{(n)}$ which is isomorphic to G_x, and if $T_x X^{(n)}$ is identified with $\mathbb{R}^{3n} \supset X^{(n)}$, $\mathcal{G}_x$ is simply the projection of G_x on $O(3) \times \Sigma^{(n)}$, with the following equivalent definition:

$$\mathcal{G}_x = \left\{(\rho, \sigma) \in O(3) \times \Sigma^{(n)} \,|\, \rho x_{ij} = x_{\sigma(i)\sigma(j)}\right\} \tag{48}$$

In order to apply a general result stated below on the action of compact Lie groups, we consider the linear submanifold $\check{X}^{(n)} \subset X^{(n)}$ of "centered" configurations, defined by

$$\check{X}^{(n)} = \left\{x \in X^{(n)} \,|\, \sum_{i=1}^{n} x_i = 0\right\} \tag{49}$$

Then $\check{X}^{(n)}$ is invariant for the action (44) restricted to the subgroup $O(3) \times \Sigma^{(n)}$, since

$$\forall x \in \check{X}^{(n)}, \qquad (\rho, \sigma)^{(n)} x = y, \qquad y_i = \rho x_{\sigma^{-1}(i)} \tag{50}$$

and $\sum_{i=1}^{n} x_i = 0$ implies $\sum_{i=1}^{n} y_i = 0$.

Moreover, if $x \in \check{X}^{(n)}$, the symmetry group G_x can be identified with the isotropy group of x for the action (50).

The main purpose of this paper is to study the stability of the symmetry groups of equilibrium configurations (under small variations of the potential). Thus it is necessary to investigate the smoothness properties of the subsets of $X^{(n)}$ corresponding to a given symmetry group, or to its class of conjugation in $O(3) \times \Sigma^{(n)}$.

We give now a relevant theorem in the general form stated in Ref. 12 (Theorem 3.3, p. 182, and Corollary 2.5, p. 309):

Theorem 2. Let G be a compact Lie group acting smoothly on a manifold X. Let H be a subgroup of G and let

$$S_H = \{x \in X \,|\, G_x \text{ conjugate to } H \text{ in } G\}$$

where G_x is the isotropy group of x. Then S_H is a smooth submanifold of X and its topological boundary is the union of S_K for K strictly larger than H.

This theorem asserts that the subsets

$$\check{S}_x = \left\{ y \in \check{X}^{(n)} \mid G_x \text{ conjugate to } G_y \text{ in } O(3) \times \Sigma^{(n)} \right\} \tag{51}$$

are smooth submanifolds of $\check{X}^{(n)}$.

Now, for any $x \in X^{(n)}$, define

$$S_x = \left\{ y \in X^{(n)} \mid G_x \text{ conjugate to } G_y \text{ in } I \times \Sigma^{(n)} \right\} \tag{52}$$

Then, S_x is the orbit of $\check{S}_y$, for some $y \in \check{X}^{(n)}$, under the action of translations, and clearly S_x is a smooth submanifold of $X^{(n)}$.

On the other hand, we have the following continuity of Σ_x with respect to x:

Lemma 7. For any $x \in X^{(n)}$, there exists a neighborhood $\mathcal{V}(x)$ in $X^{(n)}$ such that $\forall y \in \mathcal{V}(x)$, Σ_y is a subgroup of Σ_x.

Proof. Suppose the result is false. For some $x \in X^{(n)}$ there exists a sequence $\{y^{(p)}\}$ such that

(1) $$\lim_{p \to \infty} y^{(p)} = x$$

(2) $\Sigma_{y^{(p)}}$ is not a subgroup of Σ_x, for any p.

Since the set $\Sigma^{(n)} \backslash \Sigma_x$ is finite, we can take a subsequence $\{z^{(q)}\}$ such that

(1) $$\lim_{q \to \infty} z^{(q)} = x$$

(2) $\exists \sigma \in \Sigma^{(n)} \backslash \Sigma_x$ with $\sigma \in \Sigma_{z^{(q)}}$ for any q.

Then, we have by (47)

$$\forall i, j \qquad \|z_{ij}^{(q)}\| = \|z_{\sigma(i)\sigma(j)}^{(q)}\|$$

and letting $q \to \infty$, $\forall i, j$ $\|x_{ij}\| = \|x_{\sigma(i)\sigma(j)}\|$, a contradiction. ∎

It follows from this lemma that in any submanifold S_x, the subgroups Σ_x are locally constant. Thus if $\mathcal{V}(x)$ is a neighborhood which satisfies the conclusion of Lemma 7:

$$S_x \cap \mathcal{V}(x) = \left\{ y \in \mathcal{V}(x) \mid I_x \text{ conjugate to } I_y \text{ in } I \text{ and } \Sigma_x = \Sigma_y \right\} \tag{53}$$

For any given n, the number of finite symmetry groups (up to a conjugation), is obviously finite, and consequently there are only finitely many submanifolds S_x covering $X^{(n)}$.

The partition of $X^{(n)}$ thus defined will be referred to as the stratification with respect to symmetries. It is convenient to consider the following submanifold S_x^0 of S_x:

$$S_x^0 = \left\{ y \in X^{(n)} \mid G_x = G_y \right\} \tag{54}$$

In fact, if $y = (\tau, \rho, \sigma)^{(n)} x$ we have obviously $G_y = (\tau, \rho, \sigma) G_x (\tau, \rho, \sigma)^{-1}$

and one checks easily that S_x is the orbit of S_x^0 under the action of $I \times \Sigma^{(n)}$. Moreover, it follows from (53) that S_x is "locally" the orbit of S_x^0 under the subgroup I of isometries.

Now, we have clearly the following equation for the closure $\overline{S_x^0}$ of S_x^0 in $X^{(n)}$:

$$\overline{S_x^0} = \left\{ y \in X^{(n)} \mid \forall (\tau, \rho, \sigma) \in G_x : \tau + \rho y_i = y_{\sigma(i)} \right\} \tag{55}$$

and the tangent space $\mathbb{S}^0(x) = T_x S_x^0$ is given by

$$\mathbb{S}^0(x) = \left\{ \xi \in \mathbb{R}^{3n} \mid \forall (\rho, \sigma) \in \mathcal{G}_x \,,\, \rho \xi_i = \xi_{\sigma(i)} \right\} \tag{56}$$

Lemma 8. For any $x \in X^{(n)}$, the tangent space $T_x S_x$ is equal to $\mathbb{S}^0(x) + \mathcal{I}(x) = \mathbb{S}(x)$, where

$$\mathbb{S}(x) = \left\{ \xi \in \mathbb{R}^{3n} \mid \forall \sigma \in \Sigma_x \,,\, (x_{ij}, \xi_{ij}) = \left(x_{\sigma(i)\sigma(j)}, \xi_{\sigma(i)\sigma(j)} \right) \right\} \tag{57}$$

Proof. First, since S_x is locally the orbit of S_x^0 under the isometries, we have $T_x S_x = \mathbb{S}^0(x) + \mathcal{I}(x)$. Obviously (10) implies $\mathcal{I}(x) \subset \mathbb{S}(x)$. Moreover, if $\xi \in \mathbb{S}^0(x)$, $(x_{ij}, \xi_{ij}) = (\rho x_{ij}, \rho \xi_{ij}) = (x_{\sigma(i)\sigma(j)}, \xi_{\sigma(i)\sigma(j)})$ and $\xi \in \mathbb{S}(x)$. Thus $\mathbb{S}^0(x) + \mathcal{I}(x) \subset \mathbb{S}(x)$.

Conversely, if $\xi \in \mathbb{S}(x)$ let $\bar{\xi}$ be defined by

$$\bar{\xi}_i = |G_x|^{-1} \sum_{G_x} \rho \xi_{\sigma^{-1}(i)}$$

Then $\bar{\xi}$ clearly belongs to $\mathbb{S}^0(x)$. Besides, $\xi - \bar{\xi}$ belongs to $\mathcal{I}(x)$ since we have

$$\left(x_{ij}, \xi_{ij} - \bar{\xi}_{ij} \right) = |G_x|^{-1} \sum_{G_x} \left(x_{ij}, \xi_{ij} - \rho \xi_{\sigma^{-1}(i)\sigma^{-1}(j)} \right)$$

and using (48) and (57) the right-hand-side vanishes. ∎

5.1. Trajectories of Critical Points

Let $\tilde{X}^{(n)} = X^{(n)}/I$ be the quotient space of $X^{(n)}$ by the isometries and denote by π the projection of $X^{(n)}$ on $\tilde{X}^{(n)}$. The definition (14) of the "Morse property" for the n-body energies was stated in Section 3. This definition is equivalent to the true Morse property for the projection $\tilde{\varphi}^{(n)}$ of $\varphi^{(n)}$ on $\tilde{X}^{(n)}$.

On account of Section 4, we can define the trajectory of a nongenerate critical point, arising from a perturbation of the potential φ.

Actually for any nondegenerate critical point $\tilde{x}$ of $\tilde{\varphi}^{(n)}$, the final remark of Section 4 asserts the existence of a convex neighborhood $\mathcal{V}(0)$ in

$C^\infty(]0,\infty[)$ and a compact neighborhood $\tilde{K}$ of $\tilde{x}$ such that, for any $\psi \in \mathcal{V}(0)$ and any $\lambda \in [0,1], \tilde{\varphi}^{(n)} + \lambda\tilde{\psi}^{(n)}$ is a Morse function in $\tilde{K}$ with a unique critical point. Using similar arguments as in one dimension,[7] we obtain the equation for the trajectory of the critical point $\tilde{x}$ which is given by

$$\begin{gathered} d(\tilde{\varphi}^{(n)} + \lambda\tilde{\psi}^{(n)})(\tilde{x}_\lambda) = 0 \\ H_{\tilde{x}_\lambda}(\tilde{\varphi}^{(n)} + \lambda\tilde{\psi}^{(n)}) \cdot \frac{d\tilde{x}_\lambda}{d\lambda} + d\tilde{\psi}^{(n)}(\tilde{x}_\lambda) = 0 \end{gathered} \tag{58}$$

Notice that the Morse property for the n-body energies is the main condition required for the existence of a trajectory, since the degeneracy of the Hessian allows bifurcations.

5.2. Statement of the Stability Property

It is clear that the stratification by symmetries (53) is invariant with respect to isometries. Thus the image $\pi(S_x) = \tilde{S}_x$ of any stratum is a submanifold of $\tilde{X}^{(n)}$, in such a way that we get a stratification of $\tilde{X}^{(n)}$.

Definition. A submanifold $\tilde{Y}$ of $\tilde{X}^{(n)}$ is stable iff for any potential φ yielding a nondegenerate critical point in $\tilde{Y}$, and for any small enough perturbation of this potential, the corresponding trajectories [defined by (58)] remain in $\tilde{Y}$.

Since it is more convenient to deal with $X^{(n)}$ than with $\tilde{X}^{(n)}$, we give the following equivalent statement:

Lemma 9. A submanifold $\tilde{Y}$ of $\tilde{X}^{(n)}$ is stable iff the submanifold $Y = \pi^{-1}(\tilde{Y})$ of $X^{(n)}$ satisfies the following condition:

$$\forall x \in Y, \qquad \forall h \in \mathcal{H}^*(x), \qquad \mathcal{E}(x) \subset h(T_x Y) \tag{59}$$

where $\mathcal{E}(x)$ is given by (20) and $\mathcal{H}^*(x) \subset \mathcal{H}(x)$ is the subset of Hessians (21) satisfying (14), i.e., of maximal rank.

Proof. Let $x \in Y$ be a "nondegenerate" critical point of $\varphi^{(n)}$. For any perturbation ψ the following properties are clearly equivalent:

(i) $\exists\tilde{\xi} \in T_{\tilde{x}}\tilde{Y}$ with $H_{\tilde{x}}\tilde{\varphi}^{(n)}(\tilde{\xi}) + d\tilde{\psi}^{(n)}(\tilde{x}) = 0$

(ii) $\exists\xi \in T_x Y$ with $H_x\varphi^{(n)}(\xi) + d\psi^{(n)}(x) = 0$

Thus, using (58), the stability condition is equivalent to

$$\forall h \in \mathcal{H}^*(x), \qquad \mathcal{E}(x) \subset h(T_x Y)$$

since $\mathcal{E}(x)$ is spanned by the differentials $d\psi^{(n)}(x)$. ∎

5.3. Symmetry Properties of $\mathcal{E}(x)$ and $\mathcal{H}(x)$

The existence of nontrivial symmetry groups implies corresponding symmetry properties for the differentials and Hessians:

Lemma 10. For any $x \in X^{(n)}$ we have

(i) $\mathcal{E}(x) \subset \mathcal{S}'(x)$, where

$$\mathcal{S}'(x) = \left\{\theta \in \mathcal{G}(x)^{\perp} \,|\, \forall(\rho,\sigma) \in \mathcal{G}_x\,,\ \theta(\rho,\sigma)^{(n)} = \theta\right\} \tag{60}$$

(ii) $\forall(\rho,\sigma) \in \mathcal{G}_x\,,\ \forall h \in \mathcal{H}(x)$

$$h\left((\rho,\sigma)^{(n)}\xi, (\rho,\sigma)^{(n)}\zeta\right) = h(\xi,\zeta) \tag{61}$$

for any $\xi, \zeta \in \mathbb{R}^{3n}$.

Proof. First let $\theta = \sum_{i<j} a_{ij}\epsilon_{ij}(x) \in \mathcal{E}(x)$ with $\|x_{ij}\| = \|x_{kl}\| \Rightarrow a_{ij} = a_{kl}$. Then, using (48)

$$\begin{aligned}
\theta \cdot (\rho,\sigma)^{(n)}(\xi) &= \sum_{i<j} a_{ij}\left(x_{ij}\,, \rho\xi_{\sigma^{-1}(i)\sigma^{-1}(j)}\right) \\
&= \sum_{i<j} a_{ij}\left(\rho^{-1}x_{ij}\,, \xi_{\sigma^{-1}(i)\sigma^{-1}(j)}\right) \\
&= \sum_{i<j} a_{ij}\left(x_{\sigma^{-1}(i)\sigma^{-1}(j)}\,, \xi_{\sigma^{-1}(i)\sigma^{-1}(j)}\right)
\end{aligned}$$

Since $\|x_{ij}\| = \|x_{\sigma^{-1}(i)\sigma^{-1}(j)}\|$ by (47), we have $a_{ij} = (a_{\sigma(i)\sigma(j)}$ or $a_{\sigma(j)\sigma(i)})$ and a relabeling of the indices yields $\theta \cdot (\rho,\sigma)^{(n)}(\xi) = \theta \cdot \xi$. Secondly, using the expression (21) for h we have

$$\begin{aligned}
h\left((\rho,\sigma)^{(n)}\xi, (\rho,\sigma)^{(n)}\zeta\right) &= \sum_{i<j} b_{ij}\left(x_{ij}\,, \rho\xi_{\sigma^{-1}(i)\sigma^{-1}(j)}\right)\left(x_{ij}\,, \rho\zeta_{\sigma^{-1}(i)\sigma^{-1}(j)}\right) \\
&\quad + \sum_{i<j} c_{ij}\left(\rho\xi_{\sigma^{-1}(i)\sigma^{-1}(j)}\,, \rho\zeta_{\sigma^{-1}(i)\sigma^{-1}(j)}\right)
\end{aligned}$$

Using similar arguments we have $b_{ij} = (b_{\sigma(i)\sigma(j)}$ or $b_{\sigma(j)\sigma(i)})$ and $c_{ij} = (c_{\sigma(i)\sigma(j)}$ or $c_{\sigma(j)\sigma(i)})$ so that a relabeling of the indices completes the proof. ■

5.4. Stability of the Stratification by Symmetries

The symmetry properties of differentials and Hessians, given above, yield, on account of Lemma 10, the stability of the symmetry groups:

Theorem 3. Let φ be any potential in $C^{\infty}(]0,\infty[)$ and assume $x \in X^{(n)}$ is a "nondegenerate" equilibrium configuration of n particles interacting through φ. Then for any small enough perturbation ψ of φ, the corresponding new equilibria have the same symmetry group as x, up to a conjugation.

Proof. The stability of the stratification by symmetries is equivalent by Lemma 9 to the following property: $\forall x \in X^{(n)}$, $\forall h \in \mathcal{H}^*(x)$, $\mathcal{G}(x) \subset h(\mathbb{S}(x))$, where $\mathbb{S}(x)$ is the tangent space (57) of the stratum S_x at x. By Lemma 10, we have $\mathcal{G}(x) \subset \mathbb{S}'(x)$, so that is sufficient to prove $\mathbb{S}'(x) \subset h(\mathbb{S}(x))$ for any $h \in \mathcal{H}^*(x)$. Actually we can check that $\mathbb{S}'(x) = h(\mathbb{S}(x))$:

(1) For any $\xi \in \mathbb{S}(x)$, there exists $\bar{\xi} \in \mathbb{S}^0(x)$, by Lemma 8 such that $\xi - \bar{\xi} \in \mathbb{S}(x)$. Then, for any $h \in \mathcal{H}(x)$, $h(\xi) = h(\bar{\xi})$. Now for any $(\rho, \sigma) \in \mathcal{G}_x$ and any $\zeta \in \mathbb{R}^{3n}$, Lemma 10 gives

$$h(\xi, \zeta) = h(\bar{\xi}, \zeta) = h\big((\rho,\sigma)^{(n)}\bar{\xi}, (\rho,\sigma)^{(n)}\zeta\big)$$
$$= h\big(\bar{\xi}, (\rho,\sigma)^{(n)}\zeta\big)$$

and $h(\xi) \in \mathbb{S}'(x)$, i.e., $h(\mathbb{S}(x)) \subset \mathbb{S}'(x)$.

(2) Conversely let $\theta \in \mathbb{S}'(x) \subset \mathcal{I}(x)^{\perp} = \operatorname{Im} h$ [for any $h \in \mathcal{H}^*(x)$]. Then $\theta = h(\xi)$ for some $\xi \in \mathbb{R}^{3n}$. Now for any $(\rho,\sigma) \in \mathcal{G}_x$ and any $\zeta \in \mathbb{R}^{3n}$, $\theta \in \mathbb{S}'(x)$ implies, using Lemma 10, that

$$h(\xi, \zeta) = h\big((\rho,\sigma)^{(n)}\xi, (\rho,\sigma)^{(n)}\zeta\big)$$
$$= h\big((\rho,\sigma)^{(n)}\xi, \zeta\big)$$

Thus $h(\xi) = h((\rho,\sigma)^{(n)}\xi) = h(\bar{\xi})$ where $\bar{\xi} = |G_x|^{-1}\sum_{G_x}(\rho,\sigma)^{(n)}\xi$ obviously belongs to $\mathbb{S}^0(x) \subset \mathbb{S}(x)$ (56). In other words, we have $\mathbb{S}'(x) \subset h(\mathbb{S}^0(x)) = h(\mathbb{S}(x))$ and finally

$$\forall h \in \mathcal{H}^*(x), \qquad \mathbb{S}'(x) = h(\mathbb{S}(x)) \quad \blacksquare$$

Now, the following natural question arises: are the strata of the symmetry the smallest stable subsets of $X^{(n)}$? Actually the answer is positive, at least on open dense subsets of each stratum. More precisely, we have

Theorem 4. In any stratum S of the stratification by symmetries, there exists an open dense subset of points x such that

$$\forall h \in \mathcal{H}^*(x), \qquad \mathcal{G}(x) = h(\mathbb{S}(x)) \tag{62}$$

In other words, if such a point projects on a nondegenerate critical point $\pi(x)$ in $\tilde{X}^{(n)}$, the set of trajectories arising from all possible perturbations of the potential, locally covers the stratum $\pi(S)$.

Proof. For any $x \in X^{(n)}$, we have

$$\forall \sigma \in \Sigma_x, \qquad \|x_{ij}\| = \|x_{\sigma(i)\sigma(j)}\|$$

Then, using (17), (18), and (57) we obtain

$$T_x\Delta \subset \mathcal{D}(x) \subset \mathbb{S}(x) \tag{63}$$

However, it follows from a theorem of Whitney[10] mentioned in Section 4, that $X^{(n)}$ is covered by a finite number of submanifolds Δ. The inclusion (63) of the tangent spaces implies that, at least locally, any stratum Δ intersecting S is contained in S. Consequently the finiteness of the stratification by distances implies that $T_x\Delta \neq \mathbb{S}(x)$ holds only on a finite union of closed submanifolds Δ of nonzero codimension in S. Thus we have on an open dense subset of S:

$$T_x\Delta = \mathcal{D}(x) = \mathbb{S}(x) \tag{64}$$

Moreover, using the "standard" Hessian (15) at x, Theorem 3 implies

$$\mathcal{E}(x) \subset h_0(\mathbb{S}(x)) = h_0(\mathcal{D}(x))$$

On the other hand, one checks that for any x, $h_0(\mathcal{D}(x)) \subset \mathcal{E}(x)$. Thus $\mathcal{E}(x) = h_0(\mathbb{S}(x))$ (on an open dense subset of S). Since for any $h \in \mathcal{H}^*(x)$, $\operatorname{Ker} h = \operatorname{Ker} h_0 = \mathcal{T}(x)$, we have $\mathcal{E}(x) = h(\mathbb{S}(x))$ on the same subset.

Finally, it follows from Eq. (58) of critical points in $\tilde{X}^{(n)}$, that the set of trajectories covers a neighborhood of $\pi(x)$ in $\pi(S)$. ■

We conclude this section by giving a direct consequence of the stability property: if a perturbation gives rise to a change of the symmetry group of an equilibrium configuration, then, necessarily, this change occurs through a degeneracy of the Hessian.

Conversely, even for large perturbations, as long as the corresponding Hessians are nondegenerate, the symmetry group is preserved.

6. PHYSICAL CONSEQUENCES

In the previous sections, we have proved, first, that for almost all potentials, the n-body energies are "Morse functions" for all n, and secondly, that the possible symmetries of the critical points are stable.

However, the stratum associated with the trivial group (which consist of configuration with no particular symmetry), is open and dense in $X^{(n)}$ for all n. On the other hand, we have seen, at the end of Section 4, that any configuration in $X^{(n)}$ is a nondegenerate equilibrium for some potential. Thus, one may ask if the class of potentials giving rise to nontrivial symmetries is large enough to contain realistic interactions.

In this section, we prove that this is actually the case.

The first step in this direction is given by the following lemma.

Lemma 11. Let $S \subset X^{(n)}$ be any stratum of the stratification by symmetries. Let φ be any potential in $C^\infty(]0,\infty[)$. Then any critical point for the restriction of $\varphi^{(n)}$ to S is a critical point for $\varphi^{(n)}$.

Proof. Let $x \in S$ be a critical point of $\varphi^{(n)}|_S$. The stability property of S gives in particular $\mathcal{E}(x) \subset h_0(\mathbb{S}(x))$, where h_0 is the "standard" Hessian (14). (See the proof of Theorem 3.) Thus $d\varphi^{(n)}(x) = h_0(\xi)$ for some ξ in $\mathbb{S}(x)$. Since $d\varphi^{(n)}(x)$ vanishes on $\mathbb{S}(x)$, we have $h_0(\xi, \xi) = 0$, which implies $\xi \in \mathcal{I}(x)$, and consequently $d\varphi^{(n)}(x) = h_0(\xi) = 0$. ■

Let us now consider the following class $\mathcal{C}$ of realistic potentials:

$$\mathcal{C} = \left\{ \varphi \in C^\infty(]0, \infty[) \,|\, \lim_{t \to 0} \varphi(t) = +\infty, \exists r > 0 \text{ such that } t \geqslant r \Rightarrow \varphi'(t) > 0 \right\} \tag{65}$$

Remark that $\mathcal{C}$ is open for the strong topology and consists of the potentials which are divergent at the origin and attractive at large distances.

An elementary argument of Euclidean geometry implies that if $\varphi \in \mathcal{C}$, any critical point of $\varphi^{(n)}$ satisfies for any i, j: $\|x_{ij}\| < (n-1)r$.

Now we claim that for any stratum $S \subset X^{(n)}$ of the stratification by symmetries, the lower bound of $\varphi^{(n)}$ in S is reached in S^* where

$$S^* = \left\{ x \in \bar{S} \,|\, i \neq j \Rightarrow x_i \neq x_j \right\} \tag{66}$$

and the closure $\bar{S}$ is taken in $\mathbb{R}^{3n}$.

Actually this follows from the continuity of $\varphi^{(n)}$ and the definition (65) of $\mathcal{C}$.

It is clear that points in $S^* \backslash S$, either belong to strata S' with strictly larger symmetry groups, or correspond to planar configurations in $\mathbb{R}^{3n} \backslash X^{(n)}$.

In other words, for any symmetry group G, we have for the corresponding stratum S either $S^* \subset X^{(n)}$ for any n (with possibly $S = \varnothing$), or S^* contains planar configurations for some n. One easily checks that the trivial group, the cyclic groups and dihedrals groups fall in the second class, and a more careful analysis shows that the first class consists of the groups such that any invariant plane is a symmetry plane, i.e., in the Hermann–Mauguin notations:[13]

mmm (orthorhombic system);

$4/m$ and $4/mmm$ (tetragonal system);

$\bar{6}, 6/m, \bar{6}2m, 6/mmm$ (hexagonal system);

$m3$ and $m3m$ (cubic system);

the two icosahedron groups.

For any of these groups, one of the three following cases holds, depending on n:

(i) $S = \varnothing$: the corresponding symmetry is not realized in $X^{(n)}$.

(ii) $S^* = S \neq \varnothing$: there is no strictly larger group than G realized in $X^{(n)}$.

(iii) $S^* \backslash S \neq \varnothing$: the corresponding symmetry is not maximal.

Finally, using Lemma 11, we can state the final result:

Theorem 5. Let G and n be such that the corresponding stratum S satisfies (ii). Then for any $\varphi \in \mathcal{C}$, $\varphi^{(n)}$ admits at least an equilibrium configuration in S with symmetry group G. Moreover, for almost all φ in $\mathcal{C}$ (in the Baire sense; see Theorem 1), this previous equilibrium is nondegenerate.

Remarks. (1) Even if x is a local minimum for $\varphi^{(n)}|_S$, nothing can be said, up to now, about the mechanical stability of this equilibrium in $X^{(n)}$. (2) The necessary existence of equilibria with different symmetries (for a given n) implies in particular that for any φ in $\mathcal{C}$, $\varphi^{(n)}$ cannot be convex on $X^{(n)}$, as opposed to the situation in one dimension.

7. CONCLUSION

As a conclusion, we stress the fact that the existence of equilibria with nontrivial symmetries is essentially of geometrical nature and does not depend on detailed properties of the potential.

Actually, such nontrivial symmetries arise, for any number of particles, for a large class of realistic potentials, namely, those which are infinitely repulsive at the origin and attractive at large distances.

However, the study of the symmetry of the ground states seems to require a more precise knowledge of the interaction, since they may have no symmetry at all.

In fact one may ask if some other properties of the interaction, such as convexity, could imply symmetry properties for the ground state, as is the case in one dimension.

Nevertheless, there exist potentials giving rise to a ground state of n particles with any arbitrary symmetry consistent with n. The stability property of the symmetry asserts the existence of a strongly open neighborhood for any of these potentials, such that the corresponding ground states have the same symmetry. For instance, ground states with icosahedron symmetry are obtained for strongly open sets of interactions, thus giving a theoretical basis to experimental observations.

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