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Topological manifolds and vector bundles with applications to crystal physics

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An adequate description of the phenomena occurring inside a crystal requires an adequate description of the "space" within the crystal characterized by the existence of a regular network of "privileged" points (the equilibrium positions of the atoms of the crystal). The main purpose of this article is to show that this can be done by using a discrete class of "privileged" reference systems and notions such as topological manifold, topological group, vector bundle in a way that extends methods well known in the usual formulation of Classical Mechanics or Special Relativity in terms of Differential Geometry.

In the case of the crystals having the structure of diamond (the corresponding symmetry group is the crystallographic group O_h^7 and it includes semiconductors such as silicon and germanium) each atom has four nearest neighbour atoms and the system of the four corresponding axes is a privileged reference frame. We indicate some O_h^7-invariant mathematical objects in certain numerical O_h^7-spaces and we prove that they can be associated to the crystal by using the class of privileged reference frames in a way that does not depend on the particular reference frame we use. They have physical meaning; an obvious O_h^7-invariant form and their expressions in the descriptions actually used in Crystal Physics are very intricate and difficult to use. From a mathematical point of view, the present paper contains some interesting examples of topological manifolds, vector bundles and representations of O_h^7.

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Introduction

One of the most important methods to study a physical system consists in using a space of mathematical objects as a model. In many cases, this starts by considering the physical space as a set of geometric points $\mathscr{P}$ (as in Solid Geometry) and associating "coordinates" with respect to a reference system to each of these points. An adequate choice of the used coordinates (Cartesian coordinates, spherical coordinates etc.) simplifies the formalism of the model.

The empty space is assumed to be a homogeneous and isotropic space and a particular reference system cannot be chosen in a natural way. The presence of a physical field with a central or axial symmetry allows us to determine a class of "privileged" reference systems. This can also be done in the case of the space within a crystal, where the regular network of the equilibrium positions of the atoms of the crystal can be considered as a subset $\mathcal{R}$ of $\mathcal{P}$ containing "privileged" points.

Each reference system establishes a correspondence between the physical system and the model, but the information about the physical system that we can obtain must be independent of the reference system we choose. Only certain mathematical objects can have physical meaning and we have to find out such objects. In the case of Classical Mechanics or Special Relativity, a formulation in terms of Differential Geometry simplifies the solution of this problem [1].

The main purpose of this article is to prove that an extension of these methods, obtained by using notions such as topological manifold, topological group and vector bundle, are useful in modelling the physical phenomena occurring inside a crystal having the structure of diamond (for example, inside a crystal of silicon or germanium). In this case, the equilibrium position of each atom of the crystal is the centre of the regular tetrahedron formed by the equilibrium positions of its four nearest neighbour atoms.

For each point of $\mathcal{R}$ the directions corresponding to the four nearest points are "privileged" directions and the class of all reference systems whose origins belong to $\mathcal{R}$ and whose axes are "privileged" axes is a class of "privileged" reference systems. Since for each point of $\mathcal{R}$ there are four privileged directions and we cannot choose three of them in natural way, we shall use reference systems having four axes. The term "reference frame" will designate such a reference system together with an indexation of its axes by using the symbols 0, 1, 2, 3. Up to an indexation of its axes, a unique reference frame corresponds to each element of $\mathcal{R}$.

A few mathematical spaces that can be used as models are introduced and for each of them it is shown that each reference frame defines a natural correspondence crystal–model.

A natural representation of O_h^7 as group of transformations is indicated for each of these spaces and the considered O_h^7-invariant mathematical objects can be associated to the crystal by using a reference frame and independently of the reference frame we choose. Possible physical interpretations are suggested.

All the mathematical ideas involved in these developments are well known and our contribution consists in using them in the case of new mathematical spaces. The idea of associating a vector space considered as a fibre to each atom and the idea of considering that in certain physical phenomena only the nearest neighbour atoms are involved and the local symmetry plays an important role are fundamental ideas for our descriptions. Such ideas were previously used in models for quasicrystals [2–5], amorphous solids [6], glasses [7], growth of crystalline and random atomic structures [8,9], dislocations [10], classification of defects [11,12] etc. In most of these cases, the problem considered, the mathematical formalism and the terminology are very different and it is difficult to detail the existing similitudes.

1. The diamond structure and the space group O_h^7

Let $\mathbb{R}$ be the field of all real numbers and W_0 be the subspace $\{(\alpha, \alpha, \alpha, \alpha) | \alpha \in \mathbb{R}\}$ of the vector space $(\mathbb{R}^4 = \{x = (x_0, x_1, x_2, x_3) | x_0, x_1, x_2, x_3 \in \mathbb{R}\}, +, \cdot)$ considered with the usual structure

$$(x_0, x_1, x_2, x_3) + (y_0, y_1, y_2, y_3) = (x_0 + y_0, x_1 + y_1, x_2 + y_2, x_3 + y_3) ,$$
$$\lambda(x_0, x_1, x_2, x_3) = (\lambda x_0, \lambda x_1, \lambda x_2, \lambda x_3) . \tag{1.1}$$

The symbol $[x_0, x_1, x_2, x_3]$ will be used for the coset

$$(x_0, x_1, x_2, x_3) + W_0 = \{(x_0 + \alpha, x_1 + \alpha, x_2 + \alpha, x_3 + \alpha) | \alpha \in \mathbb{R}\}$$

corresponding to the element $(x_0, x_1, x_2, x_3) \in \mathbb{R}^4$ in the factor vector space $(\mathbb{R}^4 / W_0, +, \cdot)$. This vector space will be denoted by $\mathbb{P}$ and we note that its structure is given by

$$[x_0, x_1, x_2, x_3] + [y_0, y_1, y_2, y_3] = [x_0 + y_0, x_1 + y_1, x_2 + y_2, x_3 + y_3] ,$$
$$\lambda[x_0, x_1, x_2, x_3] = [\lambda x_0, \lambda x_1, \lambda x_2, \lambda x_3] . \tag{1.2}$$

Let Σ_4 be the group of all permutations, $\sigma: \{0, 1, 2, 3\} \to \{0, 1, 2, 3\}$, of the set $\{0, 1, 2, 3\}$, let $\Lambda: \mathbb{P} \to \mathbb{P}$ be the bijection $\Lambda[x_0, x_1, x_2, x_3] = [-x_0 + 1, -x_1, -x_2, -x_3]$, and let $\Lambda_\sigma: \mathbb{P} \to \mathbb{P}$ be the linear isomorphism $\Lambda_\sigma[x_0, x_1, x_2, x_3] = [x_{\sigma(0)}, x_{\sigma(1)}, x_{\sigma(2)}, x_{\sigma(3)}]$ for all $\sigma \in \Sigma_4$. The subset

$$T_d = \{\Lambda_\sigma: \mathbb{P} \to \mathbb{P} | \sigma \in \Sigma_4\}$$

of the group $GL(\mathbb{P})$ of all linear isomorphisms of $\mathbb{P}$ can be considered as a subgroup and $\Sigma_4 \to T_d$, $\sigma \mapsto \Lambda_\sigma$ is a group isomorphism.

The linear isomorphism $\eta: \mathbb{P} \to \mathbb{R}^3$,

$$\eta[x_0, x_1, x_2, x_3]$$
$$= (-x_0 - x_1 + x_2 + x_3, -x_0 + x_1 - x_2 + x_3, -x_0 + x_1 + x_2 - x_3) , \tag{1.3}$$

and its inverse $\eta^{-1}: \mathbb{R}^3 \to \mathbb{P}$,

$$\eta^{-1}(x, y, z) = [0, (y+z)/2, (x+z)/2, (x+y)/2] , \tag{1.4}$$

allow us to identify these two vector spaces and to bring the mathematical structures we usually consider on $\mathbb{R}^3$ to the space $\mathbb{P}$. For example,

$$\langle [x_0, x_1, x_2, x_3], [y_0, y_1, y_2, y_3] \rangle = 3 \sum_{j=0}^{3} x_j y_j - \sum_{j \neq k} x_j y_k \tag{1.5}$$

is the usual scalar product and

$$d([x_0, x_1, x_2, x_3], [y_0, y_1, y_2, y_3]) = \left(3 \sum_{j=0}^{3} (x_j - y_j)^2 - \sum_{j \neq k} (x_j - y_j)(x_k - y_k) \right)^{1/2} \tag{1.6}$$

is the usual distance on $\mathbb{P}$.

One verifies easily that Λ and Λ_σ are isometries of $\mathbb{P}$, that is, $d(x, y) = d(\Lambda(x), \Lambda(y))$, $d(x, y) = d(\Lambda_\sigma(x), \Lambda_\sigma(y))$ for all $x, y \in \mathbb{P}$ and $\sigma \in \Sigma_4$. We denote by $\mathbb{G}$ the subgroup generated by $\{\Lambda\} \cup \{\Lambda_\sigma | \sigma \in \Sigma_4\}$ of the group Isom$(\mathbb{P})$ of all isometries of $\mathbb{P}$.

A mapping $f: \mathbb{R} \to \mathbb{P}$ is called differentiable if the mapping $\eta \circ f: \mathbb{R} \to \mathbb{R}^3$ is differentiable and we define

$$\mathrm{d}f/\mathrm{d}t = \eta^{-1}((\mathrm{d}/\mathrm{d}t)(\eta \circ f)) . \tag{1.7}$$

A mapping $f: \mathbb{P} \to \mathbb{P}$ is said to be C^r-differentiable if $\eta \circ f \circ \eta^{-1}: \mathbb{R}^3 \to \mathbb{R}^3$ is C^r-differentiable.

Let $\mathbb{Z} = \{..., -3, -2, -1, 0, 1, 2, 3, ...\}$ be the set of all integers and $\mathbb{S}$ be the set

$$\{n = (n_0, n_1, n_2, n_3) \in \mathbb{Z}^4 | n_0 + n_1 + n_2 + n_3 \in \{0; 1\}\} .$$

The injective mapping $\mathbb{S} \to \mathbb{P}$, $(n_0, n_1, n_2, n_3) \mapsto [n_0, n_1, n_2, n_3]$ allows us to identify the set $\mathbb{S}$ with the subset $\{[n_0, n_1, n_2, n_3] | (n_0, n_1, n_2, n_3) \in \mathbb{S}\}$ of $\mathbb{P}$. One can easily see that $\mathbb{S}$ is a $\mathbb{G}$-invariant subset of $\mathbb{P}$, that is, $g(n) \in \mathbb{S}$ for all $n \in \mathbb{S}$ and $g \in \mathbb{G}$. More than that, the group $\mathbb{G}$ and the group $\mathbb{G}' = \{g|_{\mathbb{S}}: \mathbb{S} \to \mathbb{S} | g \in \mathbb{G}\}$ are isomorphic.

Let $\mathbb{N} = \{0, 1, 2, 3, ...,\}$ be the set of all natural numbers, $0! = 1$, $1! = 1$ and $k! = 1 \cdot 2 \cdot 3 \cdots k$ for all $k \in \mathbb{N}$, $k > 1$. The mapping

$$\delta: \mathbb{S} \times \mathbb{S} \to \mathbb{N}, \delta((n_0, n_1, n_2, n_3), (n'_0, n'_1, n'_2, n'_3)) = \sum_{j=0}^{3} |n_j - n'_j| , \tag{1.8}$$

is a distance on the set $\mathbb{S}$ and one can easily see that it is $\mathbb{G}$-invariant, that is, $\delta(n, n') = \delta(g(n), g(n'))$ for all $n, n' \in \mathbb{S}$ and $g \in \mathbb{G}$. We call it the intrinsic distance on $\mathbb{S}$. The mapping

$$N: \mathbb{S} \times \mathbb{S} \to \mathbb{N} ,$$

$$N((n_0, n_1, n_2, n_3), (n'_0, n'_1, n'_2, n'_3)) = \frac{(\sum_{n'_j > n_j} (n'_j - n_j))! (\sum_{n'_j < n_j} (n_j - n'_j))!}{|n_0 - n'_0|! \, |n_1 - n'_1|! \, |n_2 - n'_2|! \, |n_3 - n'_3|!} \tag{1.9}$$

is another example of a $\mathbb{G}$-invariant mapping.

Let A, A_0, A_1, A_2, A_3 be elements of $\mathscr{P}$ such that A is the centre of the regular tetrahedron $A_0A_1A_2A_3$. We denote by e_0, e_1, e_2, e_3 the vectors corresponding to the oriented segments $\overrightarrow{AA_0}$, $\overrightarrow{AA_1}$, $\overrightarrow{AA_2}$, $\overrightarrow{AA_3}$, respectively, and $\bar{e}_0=-e_0$, $\bar{e}_1=-e_1$, $\bar{e}_2=-e_2$, $\bar{e}_3=-e_3$. The diamond structure is a subset $\mathscr{R}$ of $\mathscr{P}$ that can be generated as follows. The points A, A_0, A_1, A_2, A_3 belong to $\mathscr{R}$. At each of the points A_0, A_1, A_2, A_3 taken as initial point we construct representatives of the vectors $\bar{e}_0$, $\bar{e}_1$, $\bar{e}_2$, $\bar{e}_3$. The terminal points of these segments belong to $\mathscr{R}$. Then at each of the terminal points thus obtained considered as initial point we construct representatives of the vectors e_0, e_1, e_2, e_3. The terminal points of the last constructed segments belong to $\mathscr{R}$ and by choosing each of them as initial point we construct representatives of the vectors $\bar{e}_0$, $\bar{e}_1$, $\bar{e}_2$, $\bar{e}_3$ and so on (we construct alternatively representatives of e_0, e_1, e_2, e_3 and representatives of $\bar{e}_0$, $\bar{e}_1$, $\bar{e}_2$, $\bar{e}_3$ by choosing as initial point each of the last obtained points).

A unique point $B\in\mathscr{R}$ satisfying the condition

$$\overrightarrow{AB}=e_{i_1}+\bar{e}_{i_2}+e_{i_3}+\bar{e}_{i_4}+\cdots+e'_{ik} \tag{1.10}$$

can in a natural way be associated to each finite sequence

$$e_{i_1}\bar{e}_{i_2}e_{i_3}\bar{e}_{i_4}\cdots e'_{ik}\,, \tag{1.11}$$

where $i_j\in\{0,1,2,3\}$, $e'_{ik}=e_{ik}$ for k odd and $e'_{ik}=\bar{e}_{ik}$ for k even (barred symbols and non-barred symbols alternate and each sequence starts by a non-barred symbol).

Two such sequences are said to be equivalent if one of them can be obtained from the other one by using operations such as:

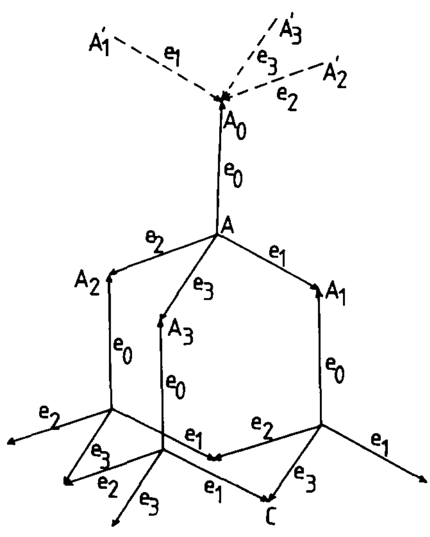

Fig. 1. The diamond structure.

$$\cdots e_i \bar{e}_j e_k \cdots \to \cdots e_k \bar{e}_j e_i \cdots \tag{1.12}$$

(permutation of two neighbouring non-barred components),

$$\cdots \bar{e}_i e_j \bar{e}_k \cdots \to \cdots \bar{e}_k e_j \bar{e}_i \cdots \tag{1.13}$$

(permutation of two neighbouring barred components),

$$\cdots e_i \bar{e}_j e_j \bar{e}_k \cdots \to \cdots e_i \bar{e}_k \cdots \quad \text{or} \quad \cdots \bar{e}_i e_j \bar{e}_j e_k \cdots \to \cdots \bar{e}_i e_k \cdots \tag{1.14}$$

(elimination of a sequence of the form $\bar{e}_j e_j$ or $e_j \bar{e}_j$),

$$\cdots e_i \bar{e}_k \cdots \to \cdots e_i \bar{e}_j e_j \bar{e}_k \cdots \quad \text{or} \quad \cdots \bar{e}_i e_k \cdots \to \cdots \bar{e}_i e_j \bar{e}_j e_k \cdots \tag{1.15}$$

(insertion of a sequence of the form $\bar{e}_j e_j$ or $e_j \bar{e}_j$). This is an equivalence relation and we can divide the set of all sequences (1.11) into equivalence classes. One can see that two sequences (1.11) describe the same point if and only if they are equivalent and $\mathscr{R}$ can be identified with the set of all the equivalence classes thus obtained.

We associate to each sequence (1.11) the element $(n_0, n_1, n_2, n_3) \in \mathbb{Z}^4$, where n_i is the number of appearances of e_i inside it minus the number of appearances of $\bar{e}_i$, for any $i \in \{0, 1, 2, 3\}$. One sees immediately that we obtain a bijection $\psi: \mathscr{R} \mapsto \mathbb{S}$. The equivalence class corresponding to point C in fig. 1 contains sequences such as $e_3\bar{e}_0e_1$, $e_1\bar{e}_0e_3$, $e_3\bar{e}_0e_2\bar{e}_2e_1$, $e_2\bar{e}_0e_3\bar{e}_2e_1$, etc. and $\psi(\mathrm{C}) = (-1, 1, 0, 1)$.

One verifies easily that a bijection $\Psi: \mathscr{P} \to \mathbb{P}$ is obtained if we associate a point B to each element $(x_0, x_1, x_2, x_3) \in \mathbb{R}^4$ satisfying the condition $\overrightarrow{\mathrm{AB}} = x_0 e_0 + x_1 e_1 + x_2 e_2 + x_3 e_3$.

Let $\mathscr{F}$ be the set of all elements $(\mathrm{D}, \mathrm{D}_0, \mathrm{D}_1, \mathrm{D}_2, \mathrm{D}_3) \in \mathscr{R}^5$ such that $\mathrm{D}_0, \mathrm{D}_1, \mathrm{D}_2, \mathrm{D}_3$ are the four nearest neighbour points of D. We obtain a bijection between $\mathscr{F}$ and the set of all reference frames if to each $(\mathrm{D}, \mathrm{D}_0, \mathrm{D}_1, \mathrm{D}_2, \mathrm{D}_3) \in \mathscr{F}$ we associate the reference frame having D as origin and whose j-axis is directed to D_j for all $j \in \{0, 1, 2, 3\}$. We can start from any element $\gamma = (\mathrm{D}, \mathrm{D}_0, \mathrm{D}_1, \mathrm{D}_2, \mathrm{D}_3) \in \mathscr{F}$ and regenerate the set $\mathscr{R}$ by using the method presented above with $\mathrm{D}, \mathrm{D}_0, \mathrm{D}_1, \mathrm{D}_2, \mathrm{D}_3$ instead of $\mathrm{A}, \mathrm{A}_0, \mathrm{A}_1, \mathrm{A}_2, \mathrm{A}_3$, respectively. Let $\psi_\gamma: \mathscr{R} \to \mathbb{S}$ and $\Psi_\gamma: \mathscr{P} \to \mathbb{P}$ be the corresponding bijections.

Let $\alpha = (\mathrm{A}, \mathrm{A}_0, \mathrm{A}_1, \mathrm{A}_2, \mathrm{A}_3) \in \mathscr{F}$ and let $\mathrm{A}'_1, \mathrm{A}'_2, \mathrm{A}'_3$ be points of $\mathscr{R}$ such that $\overrightarrow{\mathrm{A}_0\mathrm{A}'_1}, \overrightarrow{\mathrm{A}_0\mathrm{A}'_2}, \overrightarrow{\mathrm{A}_0\mathrm{A}'_3}$ are representatives of the vectors $\bar{e}_1, \bar{e}_2, \bar{e}_3$, respectively (see fig. 1). If $e_{i_1}\bar{e}_{i_2}e_{i_3}\bar{e}_{i_4}\cdots e'_{ik}$ describes a point $\mathrm{B} \in \mathscr{R}$ with respect to $(\mathrm{A}, \mathrm{A}_0, \mathrm{A}_1, \mathrm{A}_2, \mathrm{A}_3)$, then $e_0\bar{e}_{i_1}e_{i_2}\bar{e}_{i_3}e_{i_4}\cdots e''_{ik}$ describes the same point with respect to $\beta = (\mathrm{A}_0, \mathrm{A}, \mathrm{A}'_1, \mathrm{A}'_2, \mathrm{A}'_3)$ and $e_{\sigma^{-1}(i_1)}\bar{e}_{\sigma^{-1}(i_2)}e_{\sigma^{-1}(i_3)}\cdots e'_{\sigma^{-1}(ik)}$ describes the same point with respect to $\alpha_\sigma = (\mathrm{A}, \mathrm{A}_{\sigma(0)}, \mathrm{A}_{\sigma(1)}, \mathrm{A}_{\sigma(2)}, \mathrm{A}_{\sigma(3)})$ for any $\sigma \in \Sigma_4$ ($e''_{ik} = e_{ik}$ for k even and $e''_{ik} = \bar{e}_{ik}$ for k odd). One can easily verify that

$$\psi_\beta \circ \psi_\alpha^{-1}(n_0, n_1, n_2, n_3) = (-n_0 + 1, -n_1, -n_2, -n_3)\,,$$

$$\psi_{\alpha_\sigma} \circ \psi_\alpha^{-1}(n_0, n_1, n_2, n_3) = (n_{\sigma(0)}, n_{\sigma(1)}, n_{\sigma(2)}, n_{\sigma(3)})\,, \tag{1.16}$$

for all $(n_0, n_1, n_2, n_3) \in \mathbb{S}$, whence $\psi_\beta \circ \psi_\alpha^{-1} = \Lambda$ and $\psi_{\alpha_\sigma} \circ \psi_\alpha^{-1} = \Lambda_\sigma$. Thus, Λ_σ represents the change of coordinates when we pass from a reference frame to another one having the same origin, and Λ is the change of coordinates when we pass from a reference frame to another one having as origin one of the nearest neighbour points of the origin of the first reference frame.

Obviously, we can pass from a reference frame to any other one by performing successive such transformations, and the set of the changes of coordinates corresponding to all these transformations coincides with the group $\mathbb{G}'$ in the case of $\mathscr{R}$ and with the group $\mathbb{G}$ in the case of $\mathscr{P}$.

Let $\gamma, \gamma' \in \mathscr{F}$ and B, B$' \in \mathscr{P}$. Since $\Psi_\gamma \circ \Psi_{\gamma'}^{-1} \in \mathbb{G}$ and the distance $d : \mathbb{P} \times \mathbb{P} \to \mathbb{R}$ is $\mathbb{G}$-invariant, we get

$$d(\Psi_{\gamma'}(\mathrm{B}), \Psi_{\gamma'}(\mathrm{B}')) = d((\Psi_\gamma \circ \Psi_{\gamma'}^{-1})(\Psi_{\gamma'}(\mathrm{B})), (\Psi_\gamma \circ \Psi_{\gamma'}^{-1})(\Psi_{\gamma'}(\mathrm{B}')))$$
$$= d(\Psi_\gamma(\mathrm{B}), \Psi_\gamma(\mathrm{B}')) .$$

This shows that we can define

$$d: \mathscr{P} \times \mathscr{P} \to \mathbb{R}, d(\mathrm{B}, \mathrm{B}') = d(\Psi_\gamma(\mathrm{B}), \Psi_\gamma(\mathrm{B}')) , \tag{1.17}$$

independently of the reference frame γ we choose. The mapping d is the usual distance on $\mathscr{P}$.

In a similar way, we can define the intrinsic distance on the diamond structure,

$$\delta: \mathscr{R} \times \mathscr{R} \to \mathbb{N}, \delta(\mathrm{B}, \mathrm{B}') = (\psi_\gamma(\mathrm{B}), \psi_\gamma(\mathrm{B}')) , \tag{1.18}$$

and the mapping

$$N: \mathscr{R} \times \mathscr{R} \to \mathbb{N}, N(\mathrm{B}, \mathrm{B}') = N(\psi_\gamma(\mathrm{B}), \psi_\gamma(\mathrm{B}')) \tag{1.19}$$

independently of the reference frame γ we use.

The symmetry group of the diamond structure (denoted by O_h^7 in Crystal Physics) is defined as the group of all isometries of $\mathscr{P}$ that leave $\mathscr{R}$ invariant [13,14]. Let $\gamma \in \mathscr{F}$ be a fixed element of $\mathscr{F}$. Evidently, $\Psi_\gamma^{-1} \circ \Lambda \circ \Psi_\gamma$ and $\Psi_\gamma^{-1} \circ \Lambda_\sigma \circ \Psi_\gamma$ are isometries of $\mathscr{P}$ and hence they belong to O_h^7 for any $\sigma \in \Sigma_4$. From the definition of $\mathbb{G}$ it follows that $\Psi_\gamma^{-1} \circ g \circ \Psi_\gamma \in \mathrm{O}_\mathrm{h}^7$ for any $g \in \mathbb{G}$. Since $\mathbb{G}$ contains the transformations of coordinates corresponding to all changes of reference frames, one can see that $\mathrm{O}_\mathrm{h}^7 = \{ \Psi_\gamma^{-1} \circ g \circ \Psi_\gamma | g \in \mathbb{G}\}$.

The mapping $\mathbb{G} \to \mathrm{O}_\mathrm{h}^7$, $g \to \Psi_\gamma^{-1} \circ g \circ \Psi_\gamma$ is a group isomorphism and the symbol O_h^7 will also be used instead of $\mathbb{G}$ and $\mathbb{G}'$. Thus, we have defined a linear representation of O_h^7 in the space $\mathbb{P}$ and a representation of O_h^7 as group of permutations [15] in the space $\mathbb{S}$.

We combine some of the results we have just proved in

Theorem 1.

(a) $\mathrm{O}_\mathrm{h}^7 = \{g_1 \circ g_2 \circ g_3 \circ \cdots \circ g_n | n \in \mathbb{N}, g_1, \ldots, g_n \in \{\Lambda\} \cup \{\Lambda_\sigma | \sigma \in \Sigma_4\}\}$.

(b) A mathematical object is O_h^7*-invariant if and only if it is invariant under the*

transformations Λ *and* Λ_σ *for all* $\sigma\in\Sigma_4$.

(c) Each reference frame $\gamma\in\mathcal{F}$ *defines a bijection* $\Psi_\gamma:\mathcal{P}\to\mathbb{P}$ *and a bijection* $\psi_\gamma:\mathcal{R}\to\mathbb{S}$.

(d) For any γ, $\gamma'\in\mathcal{F}$ *the bijections* $\Psi_\gamma\circ\Psi_{\gamma'}^{-1}:\mathbb{P}\to\mathbb{P}$ *and* $\psi_\gamma\circ\psi_{\gamma'}^{-1}:\mathbb{S}\to\mathbb{S}$ *belong to* O_h^7.

(e) For any $\gamma\in\mathcal{F}$ *and for any* $g\in\mathrm{O}_\mathrm{h}^7$, *there exists* $\gamma'\in\mathcal{F}$ *such that* $g\circ\Psi_\gamma=\Psi_{\gamma'}$ *and* $g\circ\psi_\gamma=\psi_{\gamma'}$.

2. Γ-topological manifolds

Let E be a set and Sub E be the family of all subsets of E. For any $\mathcal{E}\subset\mathrm{Sub}\,E$ we denote by $\bigcup_{D\in\mathcal{E}}D$ ($\bigcap_{D\in\mathcal{E}}D$) the union (intersection) of the sets belonging to the family $\mathcal{E}$.

A family $\mathcal{T}\subset\mathrm{Sub}\,E$ is called a topology on E if $\Phi\in\mathcal{T}$, $E\in\mathcal{T}$, $\bigcup_{D\in\mathcal{E}}D\in\mathcal{T}$ for all $\mathcal{E}\subset\mathcal{T}$ and $\bigcap_{D\in\mathcal{E}}D\in\mathcal{T}$ for all finite $\mathcal{E}\subset\mathcal{T}$. A topological space $(E,\mathcal{T})$, or simply E, is a set E together with a given topology $\mathcal{T}$ on E.

The family Sub E is a topology on E and $(E, \mathrm{Sub}\,E)$ is called a discrete topological space. The sets $\mathbb{S}$, $\mathcal{R}$ and O_h^7 will be regarded as discrete topological spaces.

Let $d:E\times E\to\mathbb{R}$ be a distance on the set E and $B(a,r)=\{x\in E\,|\,d(x,a)<r\}$ for any $a\in E$ and $r>0$. The family of all subsets $D\subset E$ such that for any $a\in D$ there exists $r>0$ satisfying $B(a,r)\subset D$ is a topology on E. The spaces $\mathbb{P}$ and $\mathbb{R}^n$ ($n\in\mathbb{N}\setminus\{0\}$) will be considered as topological spaces with the topology associated to the usual distance.

If $E_1\subset E$ is a subset of the topological space $(E,\mathcal{T})$ then $\mathcal{T}|_{E_1}=\{D\cap E_1\,|\,D\in\mathcal{T}\}$ is a topology on E_1. The space $(E_1,\mathcal{T}|_{E_1})$ is called a topological subspace of $(E,\mathcal{T})$. One can see that $\mathbb{S}$ can be regarded as a topological subspace of $\mathbb{P}$.

Let $(E,\mathcal{T})$, $(F,\mathcal{D})$ be two topological spaces. The family of all the sets $D\subset E\times F$ such that for any $(a,b)\in D$ there exists $U\in\mathcal{T}$, $V\in\mathcal{D}$ satisfying $(a,b)\in U\times V\subset D$ is a topology $\mathcal{T}\times\mathcal{D}$ on $E\times F$. The space $(E\times F,\mathcal{T}\times\mathcal{D})$ is called the product of the topological spaces $(E,\mathcal{T})$ and $(F,\mathcal{D})$. Evidently, the product of two discrete topological spaces is a discrete topological space, and particularly $\mathbb{S}\times\mathbb{S}$, $\mathrm{O}_\mathrm{h}^7\times\mathrm{O}_\mathrm{h}^7$ and $\mathrm{O}_\mathrm{h}^7\times\mathbb{S}$ are discrete topological spaces.

Let $(E,\mathcal{T})$, $(F,\mathcal{D})$ be two topological spaces. A mapping $f:E\to F$ is said to be a continuous mapping if $f^{-1}(V)=\{x\in E\,|\,f(x)\in V\}\in\mathcal{T}$ for all $V\in\mathcal{D}$. Obviously, if E is a discrete topological space then any mapping $f:E\to F$ is a continuous mapping. The continuous mapping $f:E\to F$ is called a homeomorphism if f is a bijection and $f^{-1}:F\to E$ is also a continuous mapping. The mappings $\eta:\mathbb{P}\to\mathbb{R}^3$, $\Psi_\gamma:\mathcal{P}\to\mathbb{P}$, $\psi_\gamma:\mathcal{R}\to\mathbb{S}$ defined in section 1 are homeomorphisms.

A topological group is a triple $(G,\cdot,\mathcal{G})$, denoted simply by G, such that $(G,\cdot)$ is a group, $(G,\mathcal{G})$ is a topological space and $G\times G\to G$, $(x,y)\mapsto x\cdot y^{-1}$ is a continuous mapping, where y^{-1} is the inverse of y.

The set $\mathrm{GL}(n, \mathbb{R})$ of all real $n \times n$ non-singular matrices $a = (a^i_j)$ (the matrix whose ith row and jth column entry is a^i_j), considered together with the multiplication given by

$$(a \cdot b)^i_j = \sum_{k=1}^{n} a^i_k b^k_j \tag{2.1}$$

for $a = (a^i_j)$ and $b = (b^i_j)$, is a group. The identification $(a^i_j) \to (a^1_1, a^1_2, ..., a^1_n, a^2_1, ..., a^2_n, a^3_1, ..., a^n_n)$ of $\mathrm{GL}(n, \mathbb{R})$ with a subset of $\mathbb{R}^{n^2}$ defines the structure of a topological space on $\mathrm{GL}(n, \mathbb{R})$. One sees also that $(a, b) \mapsto a \cdot b^{-1}$ is a continuous mapping and hence $\mathrm{GL}(n, \mathbb{R})$ is a topological group.

Let $I^1_1 = I^2_2 = I^3_3 = -I^4_4 = 1$, $I^i_j = 0$ for $i, j \in \{1, 2, 3, 4\}$ with $i \neq j$ and let $I = (I^i_j)$. For each matrix a we denote by $\tilde{a}$ its transpose $(\tilde{a})^i_j = a^j_i$. The set L of all the matrices $g \in \mathrm{GL}(4, \mathbb{R})$ satisfying the condition $g \cdot I \cdot \tilde{g} = I$ is a topological subgroup of $\mathrm{GL}(4, \mathbb{R})$. It is called the Lorentz group.

The group O^7_h together with the structure of a discrete topological space is a topological group.

Let E be a topological space, G a topological group and let e be the unit element of G. We say that the group G acts continuously on E if there is given a continuous mapping $G \times E \to E$, $(a, x) \mapsto a \cdot x$, such that $a(b \cdot x) = (a \cdot b)x$, $e \cdot x = x$ for all $a, b \in G$ and $x \in E$. The mapping $L \times \mathbb{R}^4 \to \mathbb{R}^4$, $((a^i_j), (x^i)) \mapsto (\sum_{k=1}^4 a^i_k x^k)$ defines an action of the Lorentz group L on the space $\mathbb{R}^4$ and the mappings $\mathrm{O}^7_\mathrm{h} \times \mathbb{S} \to \mathbb{S}$, $(g, n) \mapsto g(n)$, $\mathrm{O}^7_\mathrm{h} \times \mathbb{P} \to \mathbb{P}$, $(g, x) \mapsto g(x)$ considered in section 1 define actions of O^7_h on the spaces $\mathbb{S}$ and $\mathbb{P}$, respectively.

Let $(F, \mathscr{D})$ be a topological space. A pseudogroup of homeomorphisms on F is a set Γ of homeomorphisms satisfying the following conditions [16,17]:

(a) each $f \in \Gamma$ is a homeomorphism of an open set of F onto an open set of F;

(b) for every $D \in \mathscr{D}$, the identity transformation of D is in Γ;

(c) if f is in Γ, then f^{-1} is in Γ;

(d) if $f \in \Gamma$ is a homeomorphism of U onto V and $f' \in \Gamma$ is a homeomorphism of U' onto V' and $V \cap U'$ is non-empty, then the homeomorphism $f' \circ f$ of $f^{-1}(V \cap U')$ onto $f'(V \cap U')$ is in Γ.

A pseudogroup Γ of homeomorphisms of F is said to be transitive if for every x, $y \in F$, there exists $f \in \Gamma$ such that $f(x) = y$.

Let $G \times F \to F$, $(a, x) \mapsto a \cdot x$ be an action of the group G on the topological space $(F, \mathscr{D})$ and let $L_a : F \to F$ be the mapping $L_a(x) = a \cdot x$ for any $a \in G$. The set $\{L_a|_D : D \to L_a(D) \mid a \in G, D \in \mathscr{D}\}$ of all the restrictions of the mappings L_a, $a \in G$ to the open sets $D \in \mathscr{D}$ is a pseudogroup of homeomorphisms of F. The symbol G will also be used to denote this pseudogroup. Particularly, we can consider the Lorentz pseudogroup of homeomorphisms L on the space $\mathbb{R}^4$ and the pseudogroup of homeomorphisms O^7_h on the spaces $\mathbb{P}$ and $\mathbb{S}$.

A topological space $(F, \mathscr{D})$ will be called a numerical space if either $F \subset \mathbb{C}^n$ or

$F \subset \mathrm{Sub}\,\mathbb{C}^n$, for a certain $n \in \mathbb{N}$. Evidently, $\mathbb{S}$, $\mathbb{P}$, $\mathbb{R}^n$, $\mathbb{C}^n$ are numerical spaces.

Let $(F, \mathscr{D})$ be a numerical space and let Γ be a pseudogroup of homeomorphisms on F. A Γ-atlas of a topological space $(M, \mathscr{T})$ is a family of pairs (U_i, φ_i), called charts, such that [17–19]

(a) each U_i is an open set of M and $\bigcup_i U_i = M$;

(b) each φ_i is a homeomorphism of U_i onto an open set of F;

(c) whenever $U_i \cap U_j$ is non-empty, the mapping $\varphi_j \circ \varphi_i^{-1}$ of $\varphi_i(U_i \cap U_j)$ onto $\varphi_j(U_i \cap U_j)$ is an element of Γ.

A Γ-atlas of M is said to be maximal if it is not contained in any other Γ-atlas of M. Every Γ-atlas is contained in a unique maximal Γ-atlas. A Γ-structure on M is a maximal Γ-atlas of M. A Γ-topological manifold is a Hausdorff space M (that is, a topological space M such that for any $x, y \in M$, $x \neq y$, there are two open sets D_1 and D_2 such that $x \in D_1$, $y \in D_2$, $D_1 \cap D_2 = \emptyset$) together with a fixed maximal Γ-structure. To give it we can indicate a corresponding Γ-atlas.

In the case $F = \mathbb{P}$ or $F = \mathbb{R}^n$, a pseudogroup of homeomorphisms Γ on F is said to be a pseudogroup of diffeomorphisms of class C^r $(r \in \mathbb{N})$, if each $f \in \Gamma$ is a differentiable mapping of class C^r. In this case, a Γ-topological manifold is said to be a Γ-differentiable manifold. Let $r \in \mathbb{N}$, $\gamma \in \mathscr{F}$ be a fixed element, $\Psi_\gamma: \mathscr{P} \to \mathbb{P}$ be the corresponding bijection (see section 1) and let Γ_1 be the set of all local C^r-diffeomorphisms of $\mathbb{P}$. The Γ_1-atlas whose unique chart is $(\mathscr{P}, \Psi_\gamma)$ determines on $\mathscr{P}$ the structure of a Γ_1-differentiable manifold for all $r \in \mathbb{N}$.

Let $\tilde{\mathscr{R}} \subset \mathscr{R}$ be a subset of $\mathscr{R}$ considered as a discrete topological space and let $\tilde{\psi}_\gamma: \tilde{\mathscr{R}} \to \psi_\gamma(\tilde{\mathscr{R}})$ be the restriction of the bijection $\psi_\gamma: \mathscr{R} \to \mathbb{S}$ corresponding to a fixed reference frame $\gamma \in \mathscr{F}$. The O_h^7-atlas $\{(\tilde{\mathscr{R}}, \tilde{\psi}_\gamma)\}$ determines on $\tilde{\mathscr{R}}$ the structure of an O_h^7-topological manifold, and it can model, for example, a "finite" crystal having the structure of diamond.

Sometimes it is more adequate to use a "preferential" Γ-atlas to define the structure of a Γ-topological manifold instead of a maximal Γ-atlas. Let F be a numerical space, $G \times F \to F$ be an action of a group G on F, M be a topological space and let $\varphi: M \to F$ be a homeomorphism. Then $\mathscr{A}_G = \{(M, \varphi_g) \mid g \in G\}$, where $\varphi_g: M \to F$, $\varphi_g(x) = g \cdot \varphi(x)$, is a "preferential" atlas, which can be used to bring on M the G-invariant structure of F.

In Special Relativity one considers space–time as a set $\mathscr{L}$ of all events. An inertial reference system establishes a bijection $\varphi: \mathscr{L} \to \mathbb{R}^4$ and one can see that the corresponding "preferential" L-atlas $\mathscr{A}_L$ coincides with the set of bijections corresponding to all inertial reference systems. The L-invariant mathematical objects we can consider on $\mathbb{R}^4$ can be brought on $\mathscr{L}$ by using this L-atlas and used in modelling physical phenomena. Similarly, theorem 1 from section 1 proves that the O_h^7-atlas $\mathscr{A}_{O_h^7}$ of $\mathscr{R}$ coincides with the set of the bijections corresponding to all reference frames. It allows us to bring on $\mathscr{R}$ the O_h^7-invariant mathematical objects we can consider on $\mathbb{S}$ and to use them in modelling physical phenomena. We have already used this atlas to define the mappings $\delta: \mathscr{R} \times \mathscr{R} \to \mathbb{N}$, $N: \mathscr{R} \times \mathscr{R} \to \mathbb{N}$

[see (1.18), (1.19)] and other examples will be given in the next section.

We conclude this section by indicating a geometric interpretation for the mappings $\delta: \mathscr{R}\times\mathscr{R}\to\mathbb{N}$, $N: \mathscr{R}\times\mathscr{R}\to\mathbb{N}$. For any B, $B'\in\mathscr{R}$ the numbers $\delta(B, B')$ and $N(B, B')$ represent the minimum number of elementary segments (segments having two nearest neighbour structure points as endpoints) that one must traverse to reach point B′ on the diamond structure starting from B and the number of paths having this length that connect these two points, respectively. To prove this we use a convenient chart $(\mathscr{R}, \psi_\gamma)$ satisfying the condition $\psi_\gamma(B') = (0, 0, 0, 0)$, that is, a chart corresponding to a reference frame having B′ as origin. In this reference frame, to describe the point B we can use a sequence (1.11) having the property that for any $j\in\{0, 1, 2, 3\}$ at most one of e_j, $\bar{e}_j$ appears in it. Evidently, it has a minimum number of components $|n_0|+|n_1|+|n_2|+|n_3|=\delta(n, o)$, where $n=(n_0, n_1, n_2, n_3)=\psi_\gamma(B)$ and $o=(0, 0, 0, 0)=\psi_\gamma(B')$. The number of barred components in such a sequence is the sum m of the negative components of (n_0, n_1, n_2, n_3) taken with opposite sign and that of non-barred components is the sum p of the positive components of (n_0, n_1, n_2, n_3). We can pass from one such sequence to another by separate permutations of the barred components and of the non-barred components. But not all $(-m)!p!$ sequences thus obtained are distinct. For each sequence there are $|n_0|!\,|n_1|!\,|n_2|!\,|n_3|!$ permutations that leave it unchanged, and hence the number of minimal paths is

$$\frac{(-m)!p!}{|n_0|!\,|n_1|!\,|n_2|!\,|n_3|!}=N(n, o)\ .$$

The mappings $\delta: \mathscr{R}\times\mathscr{R}\to\mathbb{N}$ and $N: \mathscr{R}\times\mathscr{R}\to\mathbb{N}$ are difficult to describe classically. For example, the definition

$$\delta(n, n')=\sum_{j=0}^{3}|n_j-n'_j|$$

of δ in a chart occupies almost half a page if it is transposed in a classical description of the diamond structure [20].

These two mappings have physical meaning. In a crystal having the structure of diamond we can assume that two atoms B and B′ are bound to each other by means of other atoms along all minimal paths connecting them. The "intensity" of this bond depends on the numbers $\delta(B, B')$ and $N(B, B')$.

The problem of the O_h^7-invariance of δ and N, which is obvious in our description, becomes a difficult problem in the classical description.

3. Vector bundles and applications to Crystal Physics

Let W be a finite-dimensional vector space over the field $\mathbb{K}=\mathbb{R}$ or $\mathbb{C}$ and let $\pi: E\to M$ be a continuous mapping of the topological space E onto the topological space M. We denote by E_x the set $\pi^{-1}(x)$ and call it the fibre over the point x for all $x \in M$. A vector chart (U, φ, W) on E is a homeomorphism $\varphi: \pi^{-1}(U) \to U \times W$ such that U is an open subset of M and $\pi(\varphi^{-1}(x, h)) = x$ for all $(x, h) \in U \times W$.

For a given vector chart (U, φ, W) and for each $x \in U$ the mapping $\varphi|_{E_x}: E_x \to \{x\} \times W$ is a bijection. We denote by t_x the mapping $t_x: W \to E_x$ satisfying the relation $\varphi(t_x(h)) = (x, h)$ for all $h \in W$.

Two vector charts (U, φ, W), (U', φ', W) on E are called compatible if either $U \cap U' = \emptyset$ or $U \cap U' \neq \emptyset$ and $x \mapsto t_x'^{-1} \circ t_x$ is a continuous mapping of $U \cap U'$ into the group $\mathrm{GL}(W)$ of all linear isomorphisms of W. A vector atlas on E is a family $\{(U_j, \varphi_j, W)\}$ of mutually compatible vector charts such that $\bigcup_j U_j = M$. A triple (E, π, M) considered together with a fixed vector atlas $\{(U_j, \varphi_j, W)\}$ is said to be a vector bundle [18]. The elements E, π, M, W are called the total space, the projection, the base space and the fibre, respectively.

The bijections $t_x: W \to E_x$ corresponding to all the vector charts at x define the structure of a vector space on E_x.

The triple $(M \times W, \pi, W)$ considered together with the atlas $\{(M, \varphi, W)\}$ whose unique vector chart is (M, φ, W) and where $\pi(x, h) = x$, $\varphi: M \times W \to M \times W$, $\varphi(x, h) = (x, h)$, is a vector bundle. It is said to be a trivial vector bundle.

The bijection $\Psi_\gamma: \mathscr{P} \to \mathbb{P}$ corresponding to a fixed reference frame $\gamma \in \mathscr{F}$ (see section 1) defines the structure of a vector space on $\mathscr{P}$. The study of trivial vector bundles such as $(\mathscr{R} \times \mathbb{C}, \pi, \mathscr{R})$, $(\mathbb{S} \times \mathbb{C}, \pi, \mathbb{S})$, $(\mathscr{R} \times \mathscr{P}, \pi, \mathscr{R})$ and possible utilizations in Crystal Physics are the objectives of this last section.

A morphism of a vector bundle (E, π, M) to a vector bundle (E', π', M') is a pair of continuous mappings $F: E \to E'$, $f: M \to M'$ such that $f \circ \pi = \pi' \circ F$ and $F|_{E_x}: E_x \to E'_{f(x)}$ is a linear morphism for any $x \in M$. We say that (F, f) is an isomorphism if F and f are bijective and (F^{-1}, f^{-1}) is a morphism of (E', π', M') to (E, π, M). An isomorphism of (E, π, M) to itself is called an automorphism.

Let $\gamma \in \mathscr{F}$ be a reference frame and let $F_\gamma: \mathscr{R} \times \mathbb{C} \to \mathbb{S} \times \mathbb{C}$ be the mapping $F_\gamma(\mathrm{B}, h) = (\psi_\gamma(\mathrm{B}), h)$. The pair of mappings (F_γ, ψ_γ) is an isomorphism of $(\mathscr{R} \times \mathbb{C}, \pi, \mathscr{R})$ to $(\mathbb{S} \times \mathbb{C}, \pi, \mathbb{S})$. For each $g: \mathbb{S} \to \mathbb{S}$ belonging to O_h^7 and $F_g: \mathbb{S} \times \mathbb{C} \to \mathbb{S} \times \mathbb{C}$, $F_g(n, h) = (g(n), h)$, the pair (F_g, g) is an automorphism of $(\mathbb{S} \times \mathbb{C}, \pi, \mathbb{S})$. Thus, each reference frame defines an isomorphism of $(\mathscr{R} \times \mathbb{C}, \pi, \mathscr{R})$ to $(\mathbb{S} \times \mathbb{C}, \pi, \mathbb{S})$ and the O_h^7-invariant mathematical objects we can consider on $(\mathbb{S} \times \mathbb{C}, \pi, \mathbb{S})$ can be brought on $(\mathscr{R} \times \mathbb{C}, \pi, \mathscr{R})$.

Let (E, π, M) be a vector bundle. A cross-section of (E, π, M) is a continuous mapping $s: M \to E$ such that $(\pi \circ s)(x) = x$ for all $x \in M$. We denote by $\mathscr{S}(E, \pi, M)$ the set of all sections of (E, π, M). The set $\mathscr{S}(E, \pi, M)$ has the structure of a vector space over the field $\mathbb{K}$ with respect to the laws of composition $(s_1 + s_2)(x) = s_1(x) + s_2(x)$ and $(\alpha \cdot s)(x) = \alpha \cdot s(x)$.

For a trivial vector bundle $(M \times W, \pi, M)$ any cross-section s is of the form $s(x) = (x, h(x))$ and it can be identified with the mapping $h: M \to W$, $x \mapsto h(x)$. Let $l^2(\mathscr{R})$ $[l^2(\mathbb{S})]$ be the set of all the sections $s(\mathrm{B}) = (\mathrm{B}, h(\mathrm{B}))$ $[s(n) = (n,$

$h(n))$] belonging to $\mathscr{S}(\mathscr{R}\times\mathbb{C}, \pi, \mathscr{R})$ [$\mathscr{S}(\mathbb{S}\times\mathbb{C}, \pi, \mathbb{S})$] which have the property that the family $(|h(\mathrm{B})|^2)_{\mathrm{B}\in\mathscr{R}}$ [$(|h(n)|^2)_{n\in\mathbb{S}}$] is absolutely summable [21]. We use the symbol $\sum_{\mathrm{B}\in\mathscr{R}}|h(\mathrm{B})|^2$ [$\sum_{n\in\mathbb{S}}|h(n)|^2$] to denote the corresponding sum. One can prove that $l^2(\mathscr{R})$ [$l^2(\mathbb{S})$] has the structure of a Hilbert space with respect to the scalar product $\langle h_1, h_2\rangle=\sum_{\mathrm{B}\in\mathscr{R}}h_1(\mathrm{B})\cdot\overline{h_2(\mathrm{B})}$ [$\langle h_1, h_2\rangle=\sum_{n\in\mathbb{S}}h_1(n)\cdot\overline{h_2(n)}$].

To give a physical interpretation for $l^2(\mathscr{R})$, we consider the case of an electron in a crystal with the diamond structure. We assume that the only possible positions of the electron are in the proximity of an atom of the crystal. Let $|\mathrm{B}\rangle$ be the wavefunction corresponding to the following case: the electron is in the proximity of the atom $\mathrm{B}\in\mathscr{R}$ [22]. The general wavefunction is a superposition $\sum_{\mathrm{B}\in\mathscr{R}}h(\mathrm{B})\cdot|\mathrm{B}\rangle$ and it is square integrable if and only if $h\in l^2(\mathscr{R})$.

We obtain a unitary linear representation [23] of O_h^7 in $l^2(\mathbb{S})$ by associating to each $g:\mathbb{S}\to\mathbb{S}$, $g\in\mathrm{O}_\mathrm{h}^7$, the transformation

$$T_g:l^2(\mathbb{S})\to l^2(\mathbb{S})\ ,\ (T_g(h))(n)=h(g^{-1}(n))\ . \tag{3.1}$$

Indeed,

$$\begin{aligned}[T_{g_1}(T_{g_2}(h))](n)&=(T_{g_2}(h))(g_1^{-1}(n))=h[g_2^{-1}(g_1^{-1}(n))]\\&=h[(g_1g_2)^{-1}(n)]=[T_{g_1\circ g_2}(h)](n)\end{aligned}$$

for any $n\in\mathbb{S}$ and

$$\begin{aligned}\langle T_g(h_1), T_g(h_2)\rangle&=\sum_{n\in\mathbb{S}}[T_g(h_1)](n)\cdot\overline{[T_g(h_2)](n)}\\&=\sum_{n\in\mathbb{S}}h_1(g^{-1}(n))\overline{h_2(g^{-1}(n))}\\&=\sum_{n\in\mathbb{S}}h_1(n)\overline{h_2(n)}=\langle h_1, h_2\rangle\end{aligned}$$

for any $g\in\mathrm{O}_\mathrm{h}^7$, $h_1, h_2\in l^2(\mathbb{S})$.

We consider the operator

$$A:l^2(\mathbb{S})\to l^2(\mathbb{S})\ ,\ (Ah)(n)=\sum_{n'\in\mathbb{S}}v(\delta(n, n'))\cdot h(n') \tag{3.2}$$

for any mapping $v:\mathbb{N}\to\mathbb{R}$ such that the sum exists and $Ah\in l^2(\mathbb{S})$ for any $h\in l^2(\mathbb{S})$. The four nearest neighbour points of the point $n=(n_0, n_1, n_2, n_3)\in\mathbb{S}$ are

$$\begin{aligned}&n^0=(n_0+\epsilon(n), n_1, n_2, n_3)\ ,\qquad n^1=(n_0, n_1+\epsilon(n), n_2, n_3)\ ,\\&n^2=(n_0, n_1, n_2+\epsilon(n), n_3)\ ,\qquad n^3=(n_0, n_1, n_2, n_3+\epsilon(n))\ ,\end{aligned} \tag{3.3}$$

where $\epsilon(n)=(-1)^{n_0+n_1+n_2+n_3}$. Let $u:\mathbb{N}\to\mathbb{R}$ be the mapping $u(0)=-4$, $u(1)=1$, $u(j)=0$ for $j>1$ and let

$$\Delta_d:l^2(\mathbb{S})\to l^2(\mathbb{S})\ ,$$

$$(\Delta_d h)(n) = -4h(n) + \sum_{n' \in \mathbb{S}, \delta(n,n')=1} h(n') = \sum_{j=0}^{3} h(n^j) - 4h(n) \tag{3.4}$$

be the corresponding operator.

Theorem 2.
(a) The operators A defined by (3.2) are O_h^7-invariant operators, that is, $A = T_g^{-1} \circ A \circ T_g$ for any $g \in \mathrm{O}_\mathrm{h}^7$.
(b) If $k = [k_0, k_1, k_2, k_3] \in \mathbb{P}$ satisfies

$$\sin(-k_0 - k_1 + k_2 + k_3)\sin(-k_0 + k_1 - k_2 + k_3)\sin(-k_0 + k_1 + k_2 - k_3) = 0\,,$$

then the mapping $h_k : \mathbb{S} \to \mathbb{C}$, $h_k(n) = \exp(\mathrm{i}\langle k, n\rangle)$ is an eigenfunction [it belongs to an extension of the space $l^2(\mathbb{S})$] of the operator Δ_d corresponding to the eigenvalue

$$E_k = 4[-1 + \cos(-k_0 - k_1 + k_2 + k_3) \times \cos(-k_0 + k_1 - k_2 + k_3)\cos(-k_0 + k_1 + k_2 - k_3)]\,.$$

Indeed,

$$\begin{aligned}[(A \circ T_g)(h)](n) &= [A(T_g(h))](n) \\ &= \sum_{n' \in \mathbb{S}} v[\delta(n, n')] \cdot [T_g(h)](n') \\ &= \sum_{n' \in \mathbb{S}} v[\delta(n, n')] \cdot h(g^{-1}(n')) \\ &= \sum_{n' \in \mathbb{S}} v[\delta(g^{-1}(n), g^{-1}(n'))] \cdot h(g^{-1}(n')) \\ &= \sum_{n' \in \mathbb{S}} v[\delta(g^{-1}(n), n')] \cdot h(n') \\ &= (Ah)(g^{-1}(n)) = [T_g(Ah)](n) = [(T_g \circ A)(h)](n)\end{aligned}$$

for any $g \in \mathrm{O}_\mathrm{h}^7$, $h \in l^2(\mathbb{S})$ and $n \in \mathbb{S}$. The second part of the theorem can be easily proved by direct computation [20,24]. □

In the case of a parallelepipedic (Bravais) lattice one considers [25] the space of Jacobi matrices $l^2(\mathbb{Z}^3)$ and the operator (called the discrete Laplacian)

$$\begin{aligned}&\Delta_d : l^2(\mathbb{Z}^3) \to l^2(\mathbb{Z}^3)\,, \\ &(\Delta_d h)(m) = \sum_{\substack{m' \in \mathbb{Z}^3 \\ |m' - m|_+ = 1}} [h(m') - h(m)] \\ &\qquad = \sum_{\substack{m' \in \mathbb{Z}^3 \\ |m' - m|_+ = 1}} h(m') - 6h(m)\,,\end{aligned} \tag{3.5}$$

where $|m'-m|_+ = \sum_{j=1}^{3} |m'_j - m_j|$. The operators (3.4) and (3.5) have similar expressions and properties. They are useful in the construction of the Hamiltonian when we want to describe the motion of an electron inside a crystal with the diamond structure and the structure of a Bravais lattice, respectively.

Let $\mathbb{P}_0$ be the vector subspace

$$\{(X_0, X_1, X_2, X_3) \in \mathbb{R}^4 | X_0 + X_1 + X_2 + X_3 = 0\}$$

of $\mathbb{R}^4$ and let $\mu : \mathbb{P} \to \mathbb{P}_0$ be the linear isomorphism

$$\mu[x_0, x_1, x_2, x_3] = 3^{-1/2}(3x_0 - x_1 - x_2 - x_3, 3x_1 - x_2 - x_3 - x_0, \\ 3x_2 - x_3 - x_0 - x_1, 3x_3 - x_0 - x_1 - x_2) . \quad (3.6)$$

One can see that for any reference frame $\gamma \in \mathscr{F}$, the bijection $\chi_\gamma = \mu \circ \Psi_\gamma : \mathscr{P} \to \mathbb{P}_0$ associates to each point $\mathrm{B} \in \mathscr{P}$ its orthogonal projections on the four axes of the reference frame γ.

Each atom of the crystal oscillates with respect to its equilibrium position and in interaction with its four nearest neighbour atoms. An important problem in Crystal Physics is the description of the small vibrations of the atoms of the crystal. To suggest a possible utilization of the trivial vector bundle $(\mathscr{R} \times \mathscr{P}, \pi, \mathscr{R})$ in this problem, we shall consider the small oscillations of the atoms of the crystal under some theoretical assumptions about the interaction of the atoms.

Let $\gamma = (\mathrm{A}, \mathrm{A}_0, \mathrm{A}_1, \mathrm{A}_2, \mathrm{A}_3) \in \mathscr{F}$ be a fixed reference frame (an "initial" reference frame) and let e_0, e_1, e_2, e_3 be the vectors corresponding to the directed line segments $\overrightarrow{\mathrm{AA}}_0, \overrightarrow{\mathrm{AA}}_1, \overrightarrow{\mathrm{AA}}_2, \overrightarrow{\mathrm{AA}}_3$. To any other point $\mathrm{B} \in \mathscr{R}$ taken as origin, we associate the reference frame γ_B whose j-axis is parallel to e_j for any $j \in \{0, 1, 2, 3\}$.

The pair of mappings (F_γ, ψ_γ), where $F_\gamma : \mathscr{R} \times \mathscr{P} \to \mathbb{S} \times \mathbb{P}_0$, $F_\gamma(\mathrm{B}, \mathrm{D}) = (\psi_\gamma(\mathrm{B}), \chi_{\gamma_\mathrm{B}}(\mathrm{D}))$, is an isomorphism of the trivial vector bundle $(\mathscr{R} \times \mathscr{P}, \pi, \mathscr{R})$ to the trivial vector bundle $(\mathbb{S} \times \mathbb{P}_0, \pi, \mathbb{S})$.

Let $\gamma, \gamma' \in \mathscr{F}$ be two arbitrary reference frames. One can see that there exist $g : \mathbb{S} \to \mathbb{S}$, $g \in \mathrm{O}_\mathrm{h}^7$ and $\sigma \in \Sigma_4$ such that $\psi_{\gamma'} \circ \psi_\gamma^{-1} = g$ and

$$F_g = F_{\gamma'} \circ F_\gamma^{-1} : \mathbb{S} \times \mathbb{P}_0 \to \mathbb{S} \times \mathbb{P}_0 ,$$

$$F_g((n_0, n_1, n_2, n_3); (X_0, X_1, X_2, X_3)) \\ = (g(n_0, n_1, n_2, n_3), (X_{\sigma(0)}, X_{\sigma(1)}, X_{\sigma(2)}, X_{\sigma(3)})) .$$

Particularly, for $g = \Lambda$ and $g = \Lambda_\sigma$ we have

$$F_\Lambda((n_0, n_1, n_2, n_3), (X_0, X_1, X_2, X_3)) \\ = ((-n_0 + 1, -n_1, -n_2, -n_3), (X_0, X_1, X_2, X_3)) , \quad (3.7)$$

$$F_{\Lambda_\sigma}((n_0, n_1, n_2, n_3), (X_0, X_1, X_2, X_3)) \\ = ((n_{\sigma(0)}, n_{\sigma(1)}, n_{\sigma(2)}, n_{\sigma(3)}), (X_{\sigma(0)}, X_{\sigma(1)}, X_{\sigma(2)}, X_{\sigma(3)})) . \quad (3.8)$$

The pairs (F_g, g) are automorphisms of $(\mathbb{S}\times\mathbb{P}_0, \pi, \mathbb{S})$ and any mathematical object invariant under these automorphisms (that is, O_h^7-invariant) can be brought on the trivial vector bundle $(\mathscr{R}\times\mathscr{P}, \pi, \mathscr{R})$ by using the isomorphisms (F_γ, ψ_γ), where $\gamma\in\mathscr{F}$.

We use a cross-section $s:\mathbb{S}\to\mathbb{S}\times\mathbb{P}_0$, $s(n)=(n, X(n))$, or simply

$$X:\mathbb{S}\to\mathbb{P}_0,\ n\mapsto X(n)=(X_0^n, X_1^n, X_2^n, X_3^n)$$

to describe the positions of the atoms of the crystal with respect to their equilibrium positions. A mapping

$$X:\mathbb{R}\times\mathbb{S}\to\mathbb{P}_0,\ X(t,n)=(X_0^n(t), X_1^n(t), X_2^n(t), X_3^n(t))$$

will be used to describe the time evolutions of the atoms of the crystal with respect to their equilibrium positions.

We assume that the projection on the j-axis of the force that acts on atom n depends on the position of atom n with respect to its equilibrium position and also of the positions of its four nearest neighbour atoms n^j, $j\in\{0, 1, 2, 3\}$, with respect to their equilibrium positions. In addition, we assume that it is a linear dependence. Then we get the system of equations

$$m\frac{\mathrm{d}^2}{\mathrm{d}t^2}X_j^n(t)=\sum_{l=0}^{3}\beta_{jl}X_l^n(t)+\sum_{q=0}^{3}\sum_{l=0}^{3}\beta_{jl}^q X_l^{n^q}(t)\ , \quad n\in\mathbb{S}, j\in\{0, 1, 2, 3\}\ , \tag{3.9}$$

where m is the mass of an atom of the crystal, β_{jl}, β_{jl}^q are constants and n^q, $q\in\{0, 1, 2, 3\}$, are the four nearest neighbour atoms of atom n [see (3.3)]. The condition $X_0^n(t)+X_1^n(t)+X_2^n(t)+X_3^n(t)=0$ and the local symmetry show that some of the constants β_{jl}, β_{jl}^q are equal and they can be expressed by using three independent constants β, β', β'':

$$\beta_{jl}=\begin{cases}\beta & \text{for } j=l\ ,\\ -\frac{1}{3}\beta & \text{for } j\neq l\ ,\end{cases}$$
$$\beta_{jl}^q=\begin{cases}\beta' & \text{for } j=l=q\ ,\\ -\frac{1}{3}\beta' & \text{for } q=j\neq l \text{ or } j\neq l=q\ ,\\ \beta'' & \text{for } j=l\neq q\ ,\\ \frac{1}{6}\beta'-\frac{1}{2}\beta'' & \text{for } j\neq l\neq q\neq j\ .\end{cases} \tag{3.10}$$

Theorem 3. *The system of equations (3.9) with β_{jl}, β_{jl}^q given by (3.10) is O_h^7-invariant.*

Proof. The invariance under the transformation Λ is obvious [see (3.7)]. Since $\beta_{jl}=\beta_{\sigma(j)\sigma(l)}$ and $\beta_{jl}^q=\beta_{\sigma(j)\sigma(l)}^{\sigma(q)}$, it follows that the equation

$$m\frac{\mathrm{d}^2}{\mathrm{d}t^2}X_{\sigma(j)}^{\Lambda\sigma(n)}=\sum_{l=0}^{3}\beta_{jl}X_{\sigma(l)}^{\Lambda\sigma(n)}+\sum_{q=0}^{3}\sum_{l=0}^{3}\beta_{jl}^q X_{\sigma(l)}^{(\Lambda\sigma(n))^{\sigma(q)}}$$

belongs to the system (3.9) and hence is invariant under the transformation Λ_σ for any $\sigma \in \Sigma_4$ [see (3.8)].

We shall determine particular solutions of (3.9) of the form

$$X_j^n(t) = \exp[\mathrm{i}(\langle k, n\rangle - \omega t)]\, Y_j(k)\,, \quad k \in \mathbb{P}, \omega \in \mathbb{R}\,. \tag{3.11}$$

We get

$$-m\omega^2 Y_j(k) = \sum_{l=0}^{3} \beta_{jl} Y_l(k) + \sum_{l=0}^{3} \left\{ \sum_{q=0}^{3} \beta_{jl}^q \exp\left[\mathrm{i}\epsilon(n)\left(3k_q - \sum_{p\neq q} k_p\right)\right]\right\} Y_l(k)\,,$$

and hence

$$-m\omega^2 Y_j(k) = \sum_{l=0}^{3} \left[\beta_{jl} + \sum_{q=0}^{3} \beta_{jl}^q \cos\left(3k_q - \sum_{p\neq q} k_p\right)\right] Y_l(k)\,, \tag{3.12}$$

$$0 = \sum_{l=0}^{3} \left[\sum_{q=0}^{3} \beta_{jl}^q \sin\left(3k_q - \sum_{p\neq q} k_p\right)\right] Y_l(k)\,. \tag{3.13}$$

We consider only the case

$$\sum_{q=0}^{3} \beta_{jl}^q \sin\left(3k_q - \sum_{p\neq q} k_p\right) = 0\,. \tag{3.14}$$

For $\beta' \neq \beta''$ we get

$$K_q = 3k_q - \sum_{p\neq q} k_p \in \{a\pi | a \in \mathbb{Z}\}\,, \tag{3.15}$$

whence

$$\epsilon_q = \cos K_q \in \{1, -1\}\,.$$

Since $K_0 + K_1 + K_2 + K_3 = 0$, it follows that the only possible values of $\epsilon = (\epsilon_0, \epsilon_1, \epsilon_2, \epsilon_3)$ are $(1, 1, 1, 1)$, $(-1, -1, -1, -1)$, $(-1, -1, 1, 1)$, $(-1, 1, -1, 1)$, $(-1, 1, 1, -1)$, $(1, -1, -1, 1)$, $(1, -1, 1, -1)$ and $(1, 1, -1, -1)$. Denoting $\lambda = -m\omega^2$, eqs. (3.12) become

$$\sum_{l=0}^{3} \left(\beta_{jl} + \sum_{q=0}^{3} \beta_{jl}^q \epsilon_q \right) Y_l(k) = \lambda Y_j(k)\,, \quad j \in \{0, 1, 2, 3\}\,. \tag{3.16}$$

Only three of these equations are independent. Replacing $Y_0(k)$ by $-Y_1(k) - Y_2(k) - Y_3(k)$ and denoting

$$B_{jl} = (\beta_{jl} - \beta_{j0}) + \sum_{q=0}^{3} (\beta_{jl}^q - \beta_{j0}^q)\epsilon_q\,, \tag{3.17}$$

we get the system of linear equations

$$\begin{pmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \\ B_{31} & B_{32} & B_{33} \end{pmatrix} \begin{pmatrix} Y_1(k) \\ Y_2(k) \\ Y_3(k) \end{pmatrix} = \lambda \begin{pmatrix} Y_1(k) \\ Y_2(k) \\ Y_3(k) \end{pmatrix} .$$

It can be written as $(B-\lambda I)Y(k)=0$ in obvious notation.

In the case $\epsilon=(1,1,1,1)$ we have

$$B-\lambda I=\begin{pmatrix} \frac{4}{3}\beta+\frac{4}{3}\beta'+4\beta''-\lambda & 0 & 0 \\ 0 & \frac{4}{3}\beta+\frac{4}{3}\beta'+4\beta''-\lambda & 0 \\ 0 & 0 & \frac{4}{3}\beta+\frac{4}{3}\beta'+4\beta''-\lambda \end{pmatrix},$$

and the system (3.18) has non-trivial solutions only for

$$\lambda_1=\tfrac{4}{3}\beta+\tfrac{4}{3}\beta'+4\beta'' .$$

For this value of λ any $Y(k)\in\mathbb{P}_0$ is a solution of eqs. (3.16).

The case $\epsilon=(-1,-1,-1,-1)$ is similar to the previous one and we get

$$\lambda_2=\tfrac{4}{3}\beta-\tfrac{4}{3}\beta'-4\beta'' .$$

In the case $\epsilon=(-1,-1,1,1)$ we get

$$B-\lambda I=\begin{pmatrix} \frac{4}{3}\beta-2\beta'+2\beta''-\lambda & -\beta'+\beta'' & -\beta'+\beta'' \\ 0 & \frac{4}{3}\beta+\beta'-\beta''-\lambda & -\beta'+\beta'' \\ 0 & -\beta'+\beta'' & \frac{4}{3}\beta+\beta'-\beta''-\lambda \end{pmatrix}.$$

We obtain the non-trivial solutions

$$Y(k)=\begin{pmatrix} -1 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad Y'(k)=\begin{pmatrix} 0 \\ 0 \\ 1 \\ -1 \end{pmatrix}, \quad Y''(k)=\begin{pmatrix} -1 \\ -1 \\ 1 \\ 1 \end{pmatrix},$$

for $\lambda_3=\frac{4}{3}\beta-2\beta'+2\beta''$, $\lambda_4=\frac{4}{3}\beta+2\beta'-2\beta''$, $\lambda_5=\frac{4}{3}\beta$, respectively.

In each of the remaining cases one obtains also the values λ_3, λ_4, λ_5 and solutions that differ from $Y(k)$, $Y'(k)$, $Y''(k)$ by a permutation of the components.

One can express ω in terms of the constants β, β', β'' by using the relation $\lambda=-m\omega^2$ and can determine the corresponding values of k by using the relation $\epsilon_q=\cos K_q$ and (3.15).

4. Concluding remarks

We have presented the first elements of a natural mathematical description for crystals having the diamond structure and suggestions about the description of the physical phenomena occurring in such crystals. A less abstract presentation and connections with the usual description can be found in ref. [20].

We have considered only the simple case of an "infinite" crystal without defects or impurities and we have used only atlases of global charts and trivial vector bundles. The case of a real crystal (that is, a finite crystal with defects and impurities) seems to be able to be studied by using atlases of "local" charts and locally trivial vector bundles.

The expressions of our O_h^7-invariant mathematical objects in a usual description of these crystals are very intricate and difficult to use. They have an obvious invariant form in our description but their O_h^7-invariance is difficult to prove by using the corresponding expressions in a usual description.

The mathematical spaces we use are also interesting from a mathematical point of view.

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