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Diamond structure in a natural description

N Cotfas
Physics Department, University of Bucharest, Bucharest, PO Box 76-54, Romania

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Abstract. A natural way to describe the diamond structure using reference frames having four axes is presented. The symmetry group O_h^7 of the diamond structure has natural representations in the mathematical spaces that are used. Geometric quantities, operators and fields having physical meaning and an obvious O_h^7-invariant form are taken into consideration. Their expressions in the usual description are very intricate and difficult to use.

1. Introduction

Generally, systems having three axes of coordinates are used to describe the points of space. In the case of certain physical systems, some of these systems of coordinates are more adequate to use than others.

Within a crystal there are privileged points (the equilibrium positions of the atoms of the crystal) and for each of them there are priviledged directions (for example, the directions corresponding to the nearest atoms), and hence a system whose origin is the equilibrium position of an atom of the crystal and whose axes pass through the equilibrium positions of three nearest atoms is a privileged system of coordinates.

Such a system can be associated in a natural way to each atom in a crystal having the structure of a Bravais lattice, but in the case of a crystal having the diamond structure any atom has four nearest atoms and the problem to choose three axes from the four equivalent ones cannot be solved in a natural way. The single natural solution seems to be to keep all four axes.

We must also keep the systems corresponding to all atoms of the crystal (we cannot choose some of them in a natural way). The term 'reference frame' will be used for such a system having four axes. The purpose of this paper is to present a description for a crystal having the diamond structure by using the class of all reference frames.

A way to associate 'coordinates' to each point of space with respect to a fixed reference frame is presented. The geometric and physical quantities or properties of the crystal that can be formulated in terms of space positions correspond to mathematical objects in the space of the coordinates. We indicate such mathematical objects that can be associated to the crystal by using a reference frame in a way that does not depend on the chosen reference frame. In mathematical terms, the changes of coordinates corresponding to the changes of the reference frames form a group (we prove that it is isomorphic to the well known space group O_h^7), and a mathematial object that we can consider in the space of coordinates can have geometric or physical meaning only if it is invariant under this group of transformations.

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We shall prove that this description leads us to develop a mathematical formalism that allows us to consider mathematical objects having an obvious O_h^7 symmetry and which are useful in modelling some geometric and physical properties. Their expressions in the usual description are very intricate. In this description the case of the diamond structure becomes almost as simple as the case of a simple cubic lattice for certain problems.

The idea of using additional coordinates has been considered before, for example, by Janner and Janssen [1, 2] and Nebola *et al* [3, 4] in connection with the notion of superspace groups (higher-dimensional space groups). Janner and Janssen consider a periodically distorted crystal regarded as a perfect crystal with a deviation that itself has symmetry properties. In this case they show that a space group with dimension higher than 3 is obtained if Euclidean symmetries and the symmetries due to the deviation are considered together. Particular examples of four-dimensional superspace groups with applications were considered by Nebola *et al*.

The way we use the additional coordinate is very different. We use four axes but we use neither four-dimensional space groups nor representations of groups in four-dimensional spaces. We only consider the space group O_h^7, its corresponding point group, its subgroup of three-dimensional translations, and representations in three-dimensional spaces or representations as a group of permutations of a discrete set S (which is not a linear space). The set S (which is a subset of $\mathbb{R}^4$) is identified with a subset of a three-dimensional space P (isomorphic to $\mathbb{R}^3$) and it describes the points of the three-dimensional diamond structure. We do not use four-dimensional Bravais lattices. We use an additional axis but not an additional dimension. The fourth axis is only used to obtain an adequate description for the elements of a three-dimensional space (the space P) whose elements are subsets of the four-dimensional space $\mathbb{R}^4$ (in mathematical terms it is a factor space obtained by factoring $\mathbb{R}^4$ by one of its subspaces).

2. The mathematical spaces *P* and *S*

We shall use the notation $x \in M$ for 'the element x belongs to the set M' and $M_1 \subset M_2$ for 'M_1 is a subset of M_2'. If $f: M_1 \to M_2$ and $g: M_2 \to M_3$ are two mappings, then we denote by $g \circ f: M_1 \to M_3$ or only by $g \circ f$ the mapping $(g \circ f)(x) = g(f(x))$ for any $x \in M_1$. If $h: M_3 \to M_4$ is another mapping, then we remark that

$$(h \circ (g \circ f))(x) = h((g \circ f)(x)) = h(g(f(x))) = (h \circ g)(f(x)) = ((h \circ g) \circ f)(x)$$

that is, $h \circ (g \circ f) = (h \circ g) \circ f$ and we denote this mapping by $h \circ g \circ f$. For any bijective mapping $f: M_1 \to M_2$ we denote its inverse by $f^{-1}: M_2 \to M_1$, that is $f^{-1}(y) = x$, where $x \in M_1$ is the unique element having the property $f(x) = y$.

In the usual description of the space (with the aid of a system of three axes of coordinates) any point of space corresponds to an ordered set of three real numbers (x, y, z). If we denote by $\mathbb{R}$ the set of all real numbers, by $\mathbb{R}^3$ the set

$$\{(x, y, z) \mid x \in \mathbb{R}, y \in \mathbb{R}, z \in \mathbb{R}\}$$

of all ordered sets of three real numbers (x, y, z), and by $\mathcal{P}$ the set of all points of the physical space, then any reference system defines a bijection

$$\chi: \mathcal{P} \to \mathbb{R}^3 \qquad \chi(A) = (x, y, z)$$

which associates to each point $A \in \mathcal{P}$ its coordinates (x, y, z).

If we fix a point $\mathrm{O} \in \mathcal{P}$ then we can associate an oriented segment $\overrightarrow{\mathrm{OA}}$ to each point $\mathrm{A} \in \mathcal{P}$ in a bijective way. Thus, the set $\mathcal{P}$ of all points of the space can be identified with the space

$$\mathscr{E}_0 = \{\overrightarrow{\mathrm{OA}} \mid \mathrm{A} \in \mathcal{P}\}$$

of all oriented segments having O as origin. In the space $\mathscr{E}_0$ we have the usual addition $\overrightarrow{\mathrm{OA}} + \overrightarrow{\mathrm{OB}}$ of the oriented segments (the parallelogram rule), the multiplication by a real number $a \cdot \overrightarrow{\mathrm{OA}}$, and the scalar product $\overrightarrow{\mathrm{OA}} \cdot \overrightarrow{\mathrm{OB}} = \|\overrightarrow{\mathrm{OA}}\| \cdot \|\overrightarrow{\mathrm{OB}}\| \cdot \cos\theta$ (where $\|\overrightarrow{\mathrm{OA}}\|$ is the length of $\overrightarrow{\mathrm{OA}}$ and θ is the angle between $\overrightarrow{\mathrm{OA}}$ and $\overrightarrow{\mathrm{OB}}$). Their properties are well known (in mathematical terms, $\mathscr{E}_0$ is a Euclidean space). We remark that $\overrightarrow{\mathrm{OA}} \cdot \overrightarrow{\mathrm{OB}} = \overrightarrow{\mathrm{OB}} \cdot \overrightarrow{\mathrm{OA}}$ and $\|\overrightarrow{\mathrm{OA}}\|^2 = \overrightarrow{\mathrm{OA}} \cdot \overrightarrow{\mathrm{OA}}$. The usual distance between two points of the space $\mathrm{A}, \mathrm{B} \in \mathcal{P}$ denoted by $\|\overrightarrow{\mathrm{AB}}\|$ is given by $\|\overrightarrow{\mathrm{AB}}\| = \|\overrightarrow{\mathrm{OB}} - \overrightarrow{\mathrm{OA}}\|$.

If we denote by i, j, k three elements of $\mathscr{E}_0$ which satisfy

$$\|i\| = \|j\| = \|k\| = 1 \qquad i \cdot j = j \cdot k = k \cdot i = 0 \tag{2.1}$$

then any element $\overrightarrow{\mathrm{OA}} \in \mathscr{E}_0$ can be written in a unique way in the form

$$\overrightarrow{\mathrm{OA}} = x \cdot i + y \cdot j + z \cdot k \tag{2.2}$$

where x, y, z are real numbers (in mathematical terms i, j, k is an orthonormal basis of the space $\mathscr{E}_0$). They determine a bijection

$$\varphi : \mathscr{E}_0 \to \mathbb{R}^3 \qquad \varphi(\overrightarrow{\mathrm{OA}}) = (x, y, z).$$

In addition, if $\varphi(\overrightarrow{\mathrm{OA}}_1) = (x_1, y_1, z_1)$, $\varphi(\overrightarrow{\mathrm{OA}}_2) = (x_2, y_2, z_2)$, then

$$\varphi(\overrightarrow{\mathrm{OA}}_1 + \overrightarrow{\mathrm{OA}}_2) = (x_1 + x_2, y_1 + y_2, z_1 + z_2)$$

$$= (x_1, y_1, z_1) + (x_2, y_2, z_2) = \varphi(\overrightarrow{\mathrm{OA}}_1) + \varphi(\overrightarrow{\mathrm{OA}}_2)$$

and

$$\varphi(a \cdot \overrightarrow{\mathrm{OA}}_1) = (ax_1, ay_1, az_1) = a \cdot (x_1, y_1, z_1) = a \cdot \varphi(\overrightarrow{\mathrm{OA}}_1)$$

(that is, φ is a linear isomorphism) and also

$$\overrightarrow{\mathrm{OA}}_1 \cdot \overrightarrow{\mathrm{OA}}_2 = x_1 \cdot x_2 + y_1 \cdot y_2 + z_1 \cdot z_2 \tag{2.3}$$

$$\|\overrightarrow{\mathrm{A}_1\mathrm{A}_2}\| = [(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2]^{1/2}. \tag{2.4}$$

We consider the oriented segments (see figure 1)

$$\begin{aligned} e_0 &= -i - j - k \qquad & e_2 &= i - j + k \\ e_1 &= -i + j + k \qquad & e_3 &= i + j - k \end{aligned} \tag{2.5}$$

and we denote by A_0, A_1, A_2, A_3 the corresponding points, that is, $e_0 = \overrightarrow{\mathrm{OA}}_0$, $e_1 = \overrightarrow{\mathrm{OA}}_1$, $e_2 = \overrightarrow{\mathrm{OA}}_2$, $e_3 = \overrightarrow{\mathrm{OA}}_3$. We remark that $\|\overrightarrow{\mathrm{A}_0\mathrm{A}_1}\| = \|\overrightarrow{\mathrm{A}_0\mathrm{A}_2}\| = \|\overrightarrow{\mathrm{A}_0\mathrm{A}_3}\| = \|\overrightarrow{\mathrm{A}_1\mathrm{A}_2}\| = \|\overrightarrow{\mathrm{A}_1\mathrm{A}_3}\| = \|\overrightarrow{\mathrm{A}_2\mathrm{A}_3}\|$ and $\|\overrightarrow{\mathrm{OA}}_0\| = \|\overrightarrow{\mathrm{OA}}_1\| = \|\overrightarrow{\mathrm{OA}}_2\| = \|\overrightarrow{\mathrm{OA}}_3\|$, that is $\mathrm{A}_0\mathrm{A}_1\mathrm{A}_2\mathrm{A}_3$ is a regular tetrahedron and O is its centre.

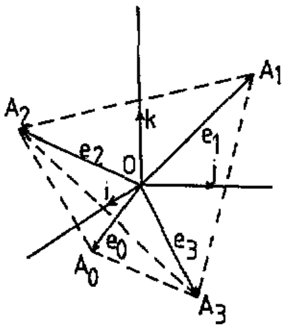

Figure 1. The system of oriented segments e_0, e_1, e_2, e_3 is used to obtain a new description for the points of space.

For any $x_0, x_1, x_2, x_3 \in \mathbb{R}$ we have $x_0e_0 + x_1e_1 + x_2e_2 + x_3e_3 \in \mathscr{E}_0$, and if we want to determine its coordinates with respect to the basis i, j, k we write

$$x_0 \cdot e_0 + x_1 \cdot e_1 + x_2 \cdot e_2 + x_3 \cdot e_3 = x \cdot i + y \cdot j + z \cdot k$$

and use (2.5). We get

$$\begin{aligned} x &= -x_0 - x_1 + x_2 + x_3 \\ y &= -x_0 + x_1 - x_2 + x_3 \\ z &= -x_0 + x_1 + x_2 - x_3. \end{aligned} \tag{2.6}$$

Conversely, each element $x \cdot i + y \cdot j + z \cdot k \in \mathscr{E}_0$ can be written as a linear combination of e_0, e_1, e_2, e_3 by using the system of equation (2.6). This can be done in an infinite number of ways

$$x \cdot i + y \cdot j + z \cdot k = \lambda e_0 + [(y+z)/2 + \lambda]e_1 + [(x+z)/2 + \lambda]e_2 + [(x+y)/2 + \lambda]e_3 \tag{2.7}$$

where $\lambda \in \mathbb{R}$. Generally,

$$x_0e_0 + x_1e_1 + x_2e_2 + x_3e_3 = x_0'e_0 + x_1'e_1 + x_2'e_2 + x_3'e_3$$

if and only if there is $\lambda \in \mathbb{R}$ such that

$$x_0' = x_0 + \lambda \qquad x_1' = x_1 + \lambda \qquad x_2' = x_2 + \lambda \qquad x_3' = x_3 + \lambda.$$

Thus, each element $\overrightarrow{OA} \in \mathscr{E}_0$ corresponds to a set

$$\{(x_0 + \lambda, x_1 + \lambda, x_2 + \lambda, x_3 + \lambda) \mid \lambda \in \mathbb{R}\}.$$

Such a set is well determined by one of its elements and we denote by $[x_0, x_1, x_2, x_3]$ the set having (x_0, x_1, x_2, x_3) as one of its elements

$$[x_0, x_1, x_2, x_3] = \{(x_0 + \lambda, x_1 + \lambda, x_2 + \lambda, x_3 + \lambda) \mid \lambda \in \mathbb{R}\}.$$

Let P be the set whose elements are all these sets

$$P = \{[x_0, x_1, x_2, x_3] \mid (x_0, x_1, x_2, x_3) \in \mathbb{R}^4\}.$$

The space P has the structure of a vector space given by

$$\begin{aligned} &[x_0, x_1, x_2, x_3] + [y_0, y_1, y_2, y_3] = [x_0 + y_0, x_1 + y_1, x_2 + y_2, x_3 + y_3] \\ &a \cdot [x_0, x_1, x_2, x_3] = [ax_0, ax_1, ax_2, ax_3]. \end{aligned} \tag{2.8}$$

These operations are well defined since if we add an arbitrary representative

$(x_0+\lambda_1,\ x_1+\lambda_1,\ x_2+\lambda_1,\ x_3+\lambda_1)$ of $[x_0, x_1, x_2, x_3]$ and an arbitrary representative $(y_0+\lambda_2, y_1+\lambda_2, y_2+\lambda_2, y_3+\lambda_2)$ of $[y_0, y_1, y_2, y_3]$ we get a representative

$$(x_0+y_0+\lambda_1+\lambda_2, x_1+y_1+\lambda_1+\lambda_2, x_2+y_2+\lambda_1+\lambda_2, x_3+y_3+\lambda_1+\lambda_2)$$

of $[x_0+y_0, x_1+y_1, x_2+y_2, x_3+y_3]$, and if we multiply a real number a to a representative $(x_0+\lambda,\ x_1+\lambda,\ x_2+\lambda,\ x_3+\lambda)$ of $[x_0,\ x_1,\ x_2,\ x_3]$ we get a representative $(ax_0+a\lambda, ax_1+a\lambda, ax_2+a\lambda, ax_3+a\lambda)$ of $[ax_0, ax_1, ax_2, ax_3]$.

In mathematical terms, P is the factor space $\mathbb{R}^4/\{(\lambda,\lambda,\lambda,\lambda)\,|\,\lambda\in\mathbb{R}\}$ of $\mathbb{R}^4$ corresponding to its vector subspace $\{(\lambda,\lambda,\lambda,\lambda)\,|\,\lambda\in\mathbb{R}\}$.

The system e_0, e_1, e_2, e_3 defines a bijection

$$\psi:\mathscr{E}_0\to P \qquad \psi(\overrightarrow{\mathrm{OA}})=[x_0, x_1, x_2, x_3]$$

where $\overrightarrow{\mathrm{OA}}=x_0e_0+x_1e_1+x_2e_2+x_3e_3$. In addition, we remark that if $\psi(\overrightarrow{\mathrm{OA}})=[x_0, x_1, x_2, x_3]$ and $\psi(\overrightarrow{\mathrm{OB}})=[y_0, y_1, y_2, y_3]$ then

$$\begin{aligned}\psi(\overrightarrow{\mathrm{OA}}+\overrightarrow{\mathrm{OB}})&=[x_0+y_0, x_1+y_1, x_2+y_2, x_3+y_3]\\&=[x_0, x_1, x_2, x_3]+[y_0, y_1, y_2, y_3]=\psi(\overrightarrow{\mathrm{OA}})+\psi(\overrightarrow{\mathrm{OB}})\end{aligned}$$

and

$$\psi(a\cdot\overrightarrow{\mathrm{OA}})=[ax_0, ax_1, ax_2, ax_3]=a\cdot[x_0, x_1, x_2, x_3]=a\cdot\psi(\overrightarrow{\mathrm{OA}})$$

that is, ψ is a linear isomorphism.

The correspondence $\eta:P\to\mathbb{R}^3$ between the two descriptions

$$\begin{tikzcd} & \mathscr{E}_0 \arrow[dl, "\psi"'] \arrow[dr, "\varphi"] & \\ P \arrow[rr, "\eta"] & & \mathbb{R}^3 \end{tikzcd}$$

is $\eta=\varphi\circ\psi^{-1}$ given by (2.6), where

$$\eta([x_0, x_1, x_2, x_3])=(-x_0-x_1+x_2+x_3,\ -x_0+x_1-x_2+x_3,\ -x_0+x_1+x_2-x_3). \tag{2.9}$$

Its inverse, given by (2.7), is $\eta^{-1}:\mathbb{R}^3\to P$, where

$$\eta^{-1}(x, y, z)=[0, (y+z)/2, (x+z)/2, (x+y)/2] \tag{2.10}$$

(we have used the representative corresponding to $\lambda=0$). The mapping η is a linear isomorphism. It allows us to bring the mathematical structures we usually consider on $\mathbb{R}^3$ to P. For $\psi(\overrightarrow{\mathrm{OA}})=[x_0, x_1, x_2, x_3]$ and $\psi(\overrightarrow{\mathrm{OB}})=[y_0, y_1, y_2, y_3]$ the expression of the scalar product $\overrightarrow{\mathrm{OA}}\cdot\overrightarrow{\mathrm{OB}}$ in terms of P can be obtained from (2.3) by using η; thus

$$\begin{aligned}\overrightarrow{\mathrm{OA}}\cdot\overrightarrow{\mathrm{OB}}&=3(x_0y_0+x_1y_1+x_2y_2+x_3y_3)-(x_0y_1+x_0y_2+x_0y_3+x_1y_0\\&\qquad+x_1y_2+x_1y_3+x_2y_0+x_2y_1+x_2y_3+x_3y_0+x_3y_1+x_3y_2)\\&=3\sum_{i=0}^{3}x_iy_i-\sum_{i\neq j}x_iy_j.\end{aligned}$$

We also denote

$$\langle [x_0, x_1, x_2, x_3], [y_0, y_1, y_2, y_3] \rangle = 3 \sum_{i=0}^{3} x_i y_i - \sum_{i \neq j} x_i y_j. \tag{2.11}$$

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

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \eta^{-1}\left(\frac{\mathrm{d}}{\mathrm{d}t}(\eta \circ f)\right). \tag{2.12}$$

To each mapping $g: \mathbb{R}^3 \to \mathbb{R}^3$ we associate the mapping $\eta^{-1} \circ g \circ \eta: P \to P$, i.e.

$$\begin{array}{ccc} P & \xrightarrow{\eta^{-1} \circ g \circ \eta} & P \\ \downarrow \eta & & \downarrow \eta \\ \mathbb{R}^3 & \xrightarrow{g} & \mathbb{R}^3 \end{array}$$

In particular, from the representation [5] of the complete tetrahedral group T_d as linear isomorphisms of $\mathbb{R}^3$:

$$\begin{array}{ll}
\varepsilon(x, y, z) = (x, y, z) & \rho_{yz}(x, y, z) = (x, -z, -y) \\
\delta_{2x}(x, y, z) = (x, -y, -z) & \rho_{y\bar{z}}(x, y, z) = (x, z, y) \\
\delta_{2y}(x, y, z) = (-x, y, -z) & \rho_{zx}(x, y, z) = (-z, y, -x) \\
\delta_{2z}(x, y, z) = (-x, -y, z) & \rho_{z\bar{x}}(x, y, z) = (z, y, x) \\
\sigma_{4x}(x, y, z) = (-x, z, -y) & \delta_{3xyz}(x, y, z) = (z, x, y) \\
\sigma_{4x}^{-1}(x, y, z) = (-x, -z, y) & \delta_{3xyz}^{-1}(x, y, z) = (y, z, x) \\
\sigma_{4y}(x, y, z) = (-z, -y, x) & \delta_{3xy\bar{z}}(x, y, z) = (-z, -x, y) \\
\sigma_{4y}^{-1}(x, y, z) = (z, -y, -x) & \delta_{3xy\bar{z}}^{-1}(x, y, z) = (-y, z, -x) \\
\sigma_{4z}(x, y, z) = (y, -x, -z) & \delta_{3\bar{x}y\bar{z}}(x, y, z) = (z, -x, -y) \\
\sigma_{4z}^{-1}(x, y, z) = (-y, x, -z) & \delta_{3\bar{x}y\bar{z}}^{-1}(x, y, z) = (-y, -z, x) \\
\rho_{xy}(x, y, z) = (-y, -x, z) & \delta_{3\bar{x}\bar{y}z}(x, y, z) = (-z, x, -y) \\
\rho_{x\bar{y}}(x, y, z) = (y, x, z) & \delta_{3\bar{x}\bar{y}z}^{-1}(x, y, z) = (y, -z, -x)
\end{array} \tag{2.13}$$

we can obtain a representation of T_d as linear isomorphisms of P (we denote by the same symbol the corresponding isomorphisms):

$$\begin{array}{ll}
\varepsilon[x_0, x_1, x_2, x_3] = [x_0, x_1, x_2, x_3] & \rho_{yz}[x_0, x_1, x_2, x_3] = [x_1, x_0, x_2, x_3] \\
\delta_{2x}[x_0, x_1, x_2, x_3] = [x_1, x_0, x_3, x_2] & \rho_{y\bar{z}}[x_0, x_1, x_2, x_3] = [x_0, x_1, x_3, x_2] \\
\delta_{2y}[x_0, x_1, x_2, x_3] = [x_2, x_3, x_0, x_1] & \rho_{zx}[x_0, x_1, x_2, x_3] = [x_2, x_1, x_0, x_3] \\
\delta_{2z}[x_0, x_1, x_2, x_3] = [x_3, x_2, x_1, x_0] & \rho_{z\bar{x}}[x_0, x_1, x_2, x_3] = [x_0, x_3, x_2, x_1] \\
\sigma_{4x}[x_0, x_1, x_2, x_3] = [x_3, x_2, x_0, x_1] & \delta_{3xyz}[x_0, x_1, x_2, x_3] = [x_0, x_3, x_1, x_2] \\
\sigma_{4x}^{-1}[x_0, x_1, x_2, x_3] = [x_2, x_3, x_1, x_0] & \delta_{3xyz}^{-1}[x_0, x_1, x_2, x_3] = [x_0, x_2, x_3, x_1] \\
\sigma_{4y}[x_0, x_1, x_2, x_3] = [x_1, x_2, x_3, x_0] & \delta_{3xy\bar{z}}[x_0, x_1, x_2, x_3] = [x_2, x_1, x_3, x_0]
\end{array} \tag{2.14}$$

$$\sigma_{4y}^{-1}[x_0, x_1, x_2, x_3] = [x_3, x_0, x_1, x_2] \qquad \delta_{3x\bar{y}\bar{z}}^{-1}[x_0, x_1, x_2, x_3] = [x_3, x_1, x_0, x_2]$$
$$\sigma_{4z}[x_0, x_1, x_2, x_3] = [x_2, x_0, x_3, x_1] \qquad \delta_{3\bar{x}y\bar{z}}[x_0, x_1, x_2, x_3] = [x_3, x_0, x_2, x_1]$$
$$\sigma_{4z}^{-1}[x_0, x_1, x_2, x_3] = [x_1, x_3, x_0, x_2] \qquad \delta_{3\bar{x}y\bar{z}}^{-1}[x_0, x_1, x_2, x_3] = [x_1, x_3, x_2, x_0]$$
$$\rho_{xy}[x_0, x_1, x_2, x_3] = [x_3, x_1, x_2, x_0] \qquad \delta_{3\bar{x}\bar{y}z}[x_0, x_1, x_2, x_3] = [x_1, x_2, x_0, x_3]$$
$$\rho_{x\bar{y}}[x_0, x_1, x_2, x_3] = [x_0, x_2, x_1, x_3] \qquad \delta_{3\bar{x}\bar{y}z}^{-1}[x_0, x_1, x_2, x_3] = [x_2, x_0, x_1, x_3].$$

We can consider

$$\mathrm{T_d} = \{\Lambda_\sigma : P \to P, \Lambda_\sigma[x_0, x_1, x_2, x_3] = [x_{\sigma(0)}, x_{\sigma(1)}, x_{\sigma(2)}, x_{\sigma(3)}] \,|\, \sigma \in \Sigma_4\}$$

where

$$\Sigma_4 = \{\sigma : \{0, 1, 2, 3\} \to \{0, 1, 2, 3\} \,|\, \sigma \text{ is a bijective mapping}\}$$

is the group of all permutations of the set $\{0, 1, 2, 3\}$. Thus, we have a linear representation of $\mathrm{T_d}$ in P.

In addition, we remark that any element of $\mathrm{T_d}$ can be obtained by composing the elements $\Lambda_1 = \delta_{3\bar{x}yz}^{-1}$, $\Lambda_2 = \rho_{y\bar{z}}$, $\Lambda_3 = \rho_{yz}$, that is

$$\mathrm{T_d} = \{\Lambda_{i_1} \circ \Lambda_{i_2} \circ \ldots \circ \Lambda_{i_n} \,|\, n \in \mathbb{N}, i_1, i_2, \ldots, i_n \in \{1, 2, 3\}\}$$

where

$$\begin{aligned} \Lambda_1[x_0, x_1, x_2, x_3] &= [x_0, x_2, x_3, x_1] \\ \Lambda_2[x_0, x_1, x_2, x_3] &= [x_0, x_1, x_3, x_2] \\ \Lambda_3[x_0, x_1, x_2, x_3] &= [x_1, x_0, x_2, x_3] \end{aligned} \tag{2.15}$$

and $\mathbb{N} = \{0, 1, 2, 3, 4, \ldots\}$.

We denote by

$$\mathbb{Z} = \{\ldots, -4, -3, -2, -1, 0, 1, 2, 3, 4, \ldots\}$$

the set of all integer numbers and by $\{0;1\}$ the set having two elements: 0 and 1. We consider the set

$$S = \{(n_0, n_1, n_2, n_3) \in \mathbb{Z}^4 \,|\, n_0 + n_1 + n_2 + n_3 \in \{0;1\}\} \tag{2.16}$$

whose elements are all the ordered sets containing four integer numbers with the property that $n_0 + n_1 + n_2 + n_3$ is either 0 or 1. To each element $(n_0, n_1, n_2, n_3) \in S$ we associate the element

$$[n_0, n_1, n_2, n_3] = \{(n_0 + \lambda, n_1 + \lambda, n_2 + \lambda, n_3 + \lambda) \,|\, \lambda \in \mathbb{R}\} \in P.$$

We remark that if $(n_0, n_1, n_2, n_3) \in S$ then (n_0, n_1, n_2, n_3) is the unique element of S which belongs to $[n_0, n_1, n_2, n_3]$. Indeed, from $(n_0 + \lambda, n_1 + \lambda, n_2 + \lambda, n_3 + \lambda) \in S$ we get $\lambda \in \mathbb{Z}$ and $n_0 + \lambda + n_1 + \lambda + n_2 + \lambda + n_3 + \lambda \in \{0; 1\}$. Since $n_0 + n_1 + n_2 + n_3 \in \{0; 1\}$ it follows that $\lambda = 0$.

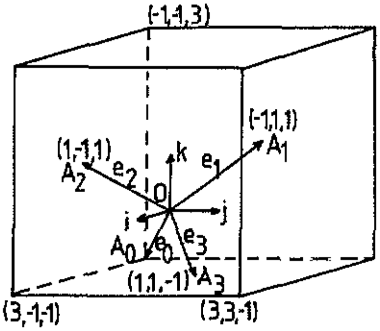

Figure 2. The orthonormal basis i, j, k is used to describe the face-centred cubic lattice.

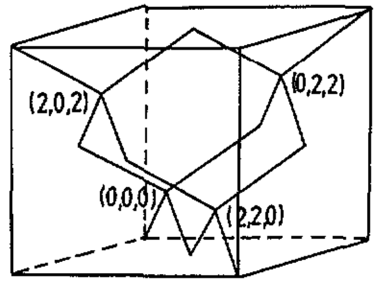

Figure 3. The diamond structure can be obtained from a face-centred cubic lattice by adding new points.

Thus, the set S can be identified with the subset

$$\{[n_0, n_1, n_2, n_3] \mid (n_0, n_1, n_2, n_3) \in S\} \subset P \tag{2.17}$$

of P. For any $(n_0, n_1, n_2, n_3) \in S$ we have

$$\Lambda_\sigma(n_0, n_1, n_2, n_3) = (n_{\sigma(0)}, n_{\sigma(1)}, n_{\sigma(2)}, n_{\sigma(3)}) \in S$$

that is, the set S is an invariant subset of P with respect to the representation of $\mathrm{T_d}$ in P. The restriction $\Lambda_{\sigma|S}$ of Λ_σ to $S \subset P$ represents a bijection from S to S.

The complete tetrahedral group $\mathrm{T_d}$ is isomorphic to the group of transformations

$$\{\Lambda_\sigma : S \to S, \Lambda_\sigma(n_0, n_1, n_2, n_3) = (n_{\sigma(0)}, n_{\sigma(1)}, n_{\sigma(2)}, n_{\sigma(3)}) \mid \sigma \in \Sigma_4\}$$

(it will also be denoted by $\mathrm{T_d}$).

In mathematical terms, we have defined a faithful representation by permutations [6] of $\mathrm{T_d}$ in the set S.

3. The space group $\mathrm{O_h^7}$

We consider a face-centred cubic lattice and we use the orthonormal basis i, j, k shown in figure 2 to describe it (that is, the isomorphism $\varphi : \mathscr{E}_0 \to \mathbb{R}^3$). The diamond structure can be obtained [5, 7, 8] by adding a basis in the Wigner–Seitz cell consisting of two identical atoms: one at point $(-1, -1, -1)$ and one at point $(0, 0, 0)$ in the case of the Wigner–Seitz cell centred at point $(-1, -1, -1)$. Thus, the new structure points $(0, 0, 0)$, $(0, 2, 2)$, $(2, 0, 2)$ and $(2, 2, 0)$ are added within the considered cube (figure 3).

We denote by $\mathscr{R}$ the set of all points of the diamond structure; obviously $\mathscr{R} \subset \mathscr{P}$. A mapping $\nu : \mathscr{P} \to \mathscr{P}$ is called an isometry if $\|\overrightarrow{\mathrm{AB}}\| = \|\overrightarrow{\nu(\mathrm{A})\nu(\mathrm{B})}\|$ for any $\mathrm{A}, \mathrm{B} \in \mathscr{P}$. We say that $\mathscr{R}$ is invariant under the isometry $\nu : \mathscr{P} \to \mathscr{P}$ if $\nu(\mathrm{A}) \in \mathscr{R}$ for any $\mathrm{A} \in \mathscr{R}$. We shall describe the symmetry group of the diamond structure which consists of all the isometries of $\mathscr{P}$ that leave $\mathscr{R}$ invariant.

We denote $\tau=(-1,-1,-1)$, $t_1=(0,2,2)$, $t_2=(2,0,2)$, $t_3=(2,2,0)$,

$$\varepsilon=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}\qquad i=\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&-1\end{pmatrix}.$$

For any matrix

$$\alpha=\begin{pmatrix}\alpha_{11}&\alpha_{12}&\alpha_{13}\\\alpha_{21}&\alpha_{22}&\alpha_{23}\\\alpha_{31}&\alpha_{32}&\alpha_{33}\end{pmatrix}$$

whose elements are real numbers and for any $a=(a_1,a_2,a_3)\in\mathbb{R}^3$ we denote by $\{\alpha|a\}$ the mapping $\{\alpha|a\}:\mathbb{R}^3\to\mathbb{R}^3$, $\{\alpha|a\}(x,y,z)=(\alpha_{11}x+\alpha_{12}y+\alpha_{13}z+a_1,\alpha_{21}x+\alpha_{22}y+\alpha_{23}z+a_2,\alpha_{31}x+\alpha_{32}y+\alpha_{33}z+a_3)$. We remark that the transformations (2.13) are of this kind.

The group of transformations

$$T=\{\{\varepsilon|n_1t_1+n_2t_2+n_3t_3\}|n_1\in\mathbb{Z},n_2\in\mathbb{Z},n_3\in\mathbb{Z}\}$$

is the group of all the translations that leave invariant the diamond structure [5]. In addition, the diamond structure is also left invariant [5] under the transformations $\{\alpha|0\}\in\mathrm{T_d}$ and under the transformation $\{i|\tau\}$.

Any isometry of $\mathcal{P}$ which leaves invariant the diamond structure can be obtained by composing these transformations [5].

If we denote

$$\{\alpha|a\}\circ T=\{\{\alpha|a\}\circ\{\varepsilon|n_1t_1+n_2t_2+n_3t_3\}|n_1\in\mathbb{Z},n_2\in\mathbb{Z},n_3\in\mathbb{Z}\}$$

(the set of all the transformations that can be obtained by composing $\{\alpha|a\}$ and a transformation belonging to T), then $\mathrm{O_h^7}$ is the union [5]:

$$\mathrm{O_h^7}=\bigcup_{\{\alpha|0\}\in\mathrm{T_d}}\{\alpha|0\}\circ T\cup\bigcup_{\{\alpha|0\}\in\mathrm{T_d}}\{i\circ\alpha|\tau\}\circ T \tag{3.1}$$

of all the sets $\{\alpha|0\}\circ T$ and $\{i\circ\alpha|\tau\}\circ T$, where $\{i\circ\alpha|\tau\}=\{i|\tau\}\circ\{\alpha|0\}$ and $\{\alpha|0\}\in\mathrm{T_d}$.

We shall use the isomorphism η to obtain a representation of $\mathrm{O_h^7}$ in P. The transformations

$$\begin{aligned}
&\{\varepsilon|t_1\}:\mathbb{R}^3\to\mathbb{R}^3 &&\{\varepsilon|t_1\}(x,y,z)=(x,y+2,z+2)\\
&\{\varepsilon|t_2\}:\mathbb{R}^3\to\mathbb{R}^3 &&\{\varepsilon|t_2\}(x,y,z)=(x+2,y,z+2)\\
&\{\varepsilon|t_3\}:\mathbb{R}^3\to\mathbb{R}^3 &&\{\varepsilon|t_3\}(x,y,z)=(x+2,y+2,z)\\
&\{i|\tau\}:\mathbb{R}^3\to\mathbb{R}^3 &&\{i|\tau\}(x,y,z)=(-x-1,-y-1,-z-1)
\end{aligned} \tag{3.2}$$

correspond to the transformations (we denote them by the same symbols)

$\{\varepsilon|t_1\}:P\to P$

$\{\varepsilon|t_1\}[x_0,x_1,x_2,x_3]=[0,-x_0+x_1+2,-x_0+x_2+1,-x_0+x_3+1]=[x_0-1,x_1+1,x_2,x_3]$

$\{\varepsilon|t_2\}:P\to P$

$$\{\varepsilon|t_2\}[x_0,x_1,x_2,x_3]=[0,-x_0+x_1+1,-x_0+x_2+2,-x_0+x_3+1]=[x_0-1,x_1,x_2+1,x_3] \tag{3.3}$$

$$\{\varepsilon|t_3\}:P\rightarrow P$$

$$\{\varepsilon|t_3\}[x_0,x_1,x_2,x_3]=[0,-x_0+x_1+1,-x_0+x_2+1,-x_0+x_3+2]=[x_0-1,x_1,x_2,x_3+1]$$

$$\{i|\tau\}:P\rightarrow P$$

$$\{i|\tau\}[x_0,x_1,x_2,x_3]=[0,x_0-x_1-1,x_0-x_2-1,x_0-x_3-1]=[-x_0+1,-x_1,-x_2,-x_3].$$

We denote the transformation $\{i|\tau\}:P\rightarrow P$ by Λ_0 and we remark that

$$\begin{aligned}
\{\varepsilon|t_1\}&=\Lambda_3\circ\Lambda_0\circ\Lambda_3\circ\Lambda_0\\
\{\varepsilon|t_2\}&=\Lambda_1\circ\Lambda_1\circ\Lambda_3\circ\Lambda_0\circ\Lambda_3\circ\Lambda_1\circ\Lambda_0\\
\{\varepsilon|t_3\}&=\Lambda_1\circ\Lambda_3\circ\Lambda_0\circ\Lambda_3\circ\Lambda_1\circ\Lambda_1\circ\Lambda_0
\end{aligned} \tag{3.4}$$

and hence

$$\mathrm{O}_{\mathrm{h}}^7=\{\Lambda_{i_1}\circ\Lambda_{i_2}\circ\ldots\circ\Lambda_{i_n}|n\in\mathbb{N},i_1,i_2,\ldots,i_n\in\{0,1,2,3\}\}.$$

In particular, $\mathrm{O}_{\mathrm{h}}^7$ is isomorphic to the subgroup of the group of all bijective transformations of S generated by the transformations $\Lambda_0,\Lambda_1,\Lambda_2,\Lambda_3:S\rightarrow S$,

$$\begin{aligned}
\Lambda_0(n_0,n_1,n_2,n_3)&=(-n_0+1,-n_1,-n_2,-n_3)\\
\Lambda_1(n_0,n_1,n_2,n_3)&=(n_0,n_2,n_3,n_1)\\
\Lambda_2(n_0,n_1,n_2,n_3)&=(n_0,n_1,n_3,n_2)\\
\Lambda_3(n_0,n_1,n_2,n_3)&=(n_1,n_0,n_2,n_3).
\end{aligned} \tag{3.5}$$

A mathematical object is $\mathrm{O}_{\mathrm{h}}^7$-invariant if and only if it is invariant under the transformations Λ_0, Λ_1, Λ_2 and Λ_3.

4. Intrinsic distance and minimal paths on the diamond structure

Let $\mathbb{N}=\{0,1,2,3,\ldots\}$ be the set of all natural numbers. We denote $k!=1\times2\times3\times\ldots\times k$ for any $k\in\mathbb{N}$, $k\geqslant2$, and $0!=1$, $1!=1$. The mappings

$$d:S\times S\rightarrow\mathbb{N}$$

$$d(n,n')=\sum_{i=0}^{3}|n_i-n_i'|=|n_0-n_0'|+|n_1-n_1'|+|n_2-n_2'|+|n_3-n_3'| \tag{4.1}$$

$$N:S\times S\rightarrow\mathbb{N}$$

$$N(n,n')=\frac{\left[\sum\limits_{n_i'>n_i}(n_i'-n_i)\right]!\cdot\left[\sum\limits_{n_i'<n_i}(n_i-n_i')\right]!}{(|n_0-n_0'|!)(|n_1-n_1'|!)(|n_2-n_2'|!)(|n_3-n_3'|!)} \tag{4.2}$$

where $n=(n_0,n_1,n_2,n_3)\in S$ and $n'=(n_0',n_1',n_2',n_3')\in S$, are $\mathrm{O}_{\mathrm{h}}^7$-invariant mappings, that is, $d(g(n),g(n'))=d(n,n')$, $N(g(n),g(n'))=N(n,n')$ for any $g:S\rightarrow S$ belonging to $\mathrm{O}_{\mathrm{h}}^7$. Indeed, for any $j\in\{0,1,2,3\}$ we have $d(\Lambda_j(n),\Lambda_j(n'))=d(n,n')$ and $N(\Lambda_j(n),\Lambda_j(n'))=N(n,n')$.

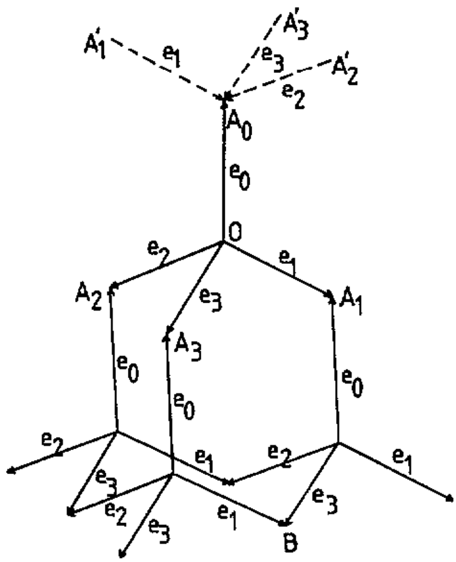

Figure 4. The diamond structure can be generated by starting from the point O and constructing alternately representatives of e_0, e_1, e_2, e_3 and $\bar{e}_0$, $\bar{e}_1$, $\bar{e}_2$, $\bar{e}_3$ having as origins each of the last obtained points.

To find the geometric meaning of the mappings d and N we shall prove that there is a family of natural bijections $\psi_i:\mathcal{R}\to S$ such that $\psi_i\circ\psi_j^{-1}:S\to S$ belongs to O_h^7 for any ψ_i and ψ_j. Let i, j, k be a fixed orthonormal basis, e_0, e_1, e_2, e_3 the vectors defined according to (2.5) and $\bar{e}_0=-e_0$, $\bar{e}_1=-e_1$, $\bar{e}_2=-e_2$, $\bar{e}_3=-e_3$.

The diamond structure can be generated as follows (figure 4). We construct representatives of the vectors e_0, e_1, e_2, e_3 having the point O as origin; then by choosing each of the endpoints thus obtained as origins we construct representatives of the vectors $\bar{e}_0$, $\bar{e}_1$, $\bar{e}_2$, $\bar{e}_3$. We continue by constructing representatives of the vectors e_0, e_1, e_2, e_3 having as origins the endpoints of each of the last obtained segments, then similarly for $\bar{e}_0$, $\bar{e}_1$, $\bar{e}_2$, $\bar{e}_3$, and so on. The points that can be obtained in this way (some of them coincide) form the diamond structure (the set $\mathcal{R}$).

Each point belonging to $\mathcal{R}$ can be described by a finite sequence

$$e_{i_1}\bar{e}_{i_2}e_{i_3}\bar{e}_{i_4}\ldots e'_{i_k} \tag{4.3}$$

where $i_j\in\{0,1,2,3\}$, $e'_{i_k}=e_{i_k}$ for k odd and $e'_{i_k}=\bar{e}_{i_k}$ for k even (the 'bar symbols' and the 'non-bar symbols' alternate inside them and each of them starts by a 'non-bar symbol'). Two such sequences describe the same point if and only if one of them can be obtained from the other one by using operations such as:

$$\ldots e_i\bar{e}_je_k\ldots\to\ldots e_k\bar{e}_je_i\ldots$$

(permutation of two neighbouring 'non-bar' components),

$$\ldots\bar{e}_ie_j\bar{e}_k\ldots\to\ldots\bar{e}_ke_j\bar{e}_i\ldots$$

(permutation of two neighbouring 'bar' components),

$$\ldots e_i\bar{e}_j e_j\bar{e}_k \ldots \to \ldots e_i\bar{e}_k \ldots$$

or

$$\ldots \bar{e}_i e_j\bar{e}_j e_k \ldots \to \ldots \bar{e}_i e_k \ldots$$

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

$$\ldots e_i\bar{e}_k \ldots \to \ldots e_i\bar{e}_j e_j\bar{e}_k \ldots$$

or

$$\ldots \bar{e}_i e_k \ldots \to \ldots \bar{e}_i e_j\bar{e}_j e_k \ldots$$

(insertion of a sequence of the form $\bar{e}_je_j$ or $e_j\bar{e}_j$). For example, $e_3\bar{e}_0e_1$, $e_1\bar{e}_0e_3$, $e_3\bar{e}_0e_2\bar{e}_2e_1$, $e_2\bar{e}_0e_3\bar{e}_2e_1$, etc, describe the point B (see figure 4).

We can divide the set of all sequences (4.3) into classes by putting together in the same class all the sequences that describe the same point. The set $\mathfrak{R}$ can be identified as the set of all these classes.

We associate to each sequence (4.3) 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 $i \in \{0, 1, 2, 3\}$. For example, $(-1, 1, 0, 1)$ corresponds to each of the sequences which describe the point B.

We remark that we associate the same element to all the sequences which describe the same point and the associated elements (n_0, n_1, n_2, n_3) belong to S. Thus, we have defined a bijection

$$\psi:\mathfrak{R} \to S. \tag{4.4}$$

This bijection depends on the choice of the point $\mathrm{O} \in \mathfrak{R}$ and the indexation by 0, 1, 2, 3 of its four nearest points. We obtain in a similar way a bijection for any element $(\mathrm{D}, \mathrm{D}_0, \mathrm{D}_1, \mathrm{D}_2, \mathrm{D}_3) \in \mathfrak{R}^5$ such that $\mathrm{D}_0, \mathrm{D}_1, \mathrm{D}_2, \mathrm{D}_3$ are the four nearest points of D by setting $e_i = \overrightarrow{\mathrm{DD}_i}$ for any $i \in \{0, 1, 2, 3\}$.

In particular, if we pass from the bijection corresponding to $(\mathrm{O}, \mathrm{A}_0, \mathrm{A}_1, \mathrm{A}_2, \mathrm{A}_3)$ to one corresponding to $(\mathrm{O}, \mathrm{A}_0, \mathrm{A}_2, \mathrm{A}_3, \mathrm{A}_1)$, $(\mathrm{O}, \mathrm{A}_0, \mathrm{A}_1, \mathrm{A}_3, \mathrm{A}_2)$, $(\mathrm{O}, \mathrm{A}_1, \mathrm{A}_0, \mathrm{A}_2, \mathrm{A}_3)$ or $(\mathrm{A}_0, \mathrm{O}, \mathrm{A}'_1, \mathrm{A}'_2, \mathrm{A}'_3)$ (see figure 4) then the coordinates of an arbitrary point change according to the transformations $\Lambda_1, \Lambda_2, \Lambda_3, \Lambda_0$ given by (3.5), respectively. In addition, we can pass to any other choice by composing these transformations.

In mathematical terms, the set of all the bijections $\psi:\mathfrak{R} \to S$ defined above can be considered as an atlas of global maps for $\mathfrak{R}$ whose changes of map belong to the representation of O_h^7 in S. It allows us to add to the set $\mathfrak{R}$ the O_h^7-invariant structure of S by using such a map, independent of the chosen map.

Let $\psi_1:\mathfrak{R} \to S$ and $\psi_2:\mathfrak{R} \to S$ be two maps. We define two mappings

$$d:\mathfrak{R} \times \mathfrak{R} \to \mathbb{N} \qquad d(\mathrm{A}, \mathrm{A}') = d(\psi_1(\mathrm{A}), \psi_1(\mathrm{A}')) \tag{4.5}$$

$$N:\mathfrak{R} \times \mathfrak{R} \to \mathbb{N} \qquad N(\mathrm{A}, \mathrm{A}') = N(\psi_1(\mathrm{A}), \psi_1(\mathrm{A}')). \tag{4.6}$$

Since $\psi_2 \circ \psi_1^{-1}:S \to S$ belongs to O_h^7 and d, N are O_h^7-invariant, it follows that

$$\begin{aligned} d(\psi_1(\mathrm{A}), \psi_1(\mathrm{A}')) &= d((\psi_2 \circ \psi_1^{-1})(\psi_1(\mathrm{A})), (\psi_2 \circ \psi_1^{-1})(\psi_1(\mathrm{A}'))) \\ &= d(\psi_2(\mathrm{A}), \psi_2(\mathrm{A}')) \end{aligned}$$

and similarly for N. This means that the definitions of $d, N:\mathfrak{R} \times \mathfrak{R} \to \mathbb{N}$ are independent of the chosen description ψ_1.

We shall prove that the numbers $d(\mathrm{A}, \mathrm{A}')$ and $N(\mathrm{A}, \mathrm{A}')$ represent the minimum number of elementary segments (segments having two nearest structure points as endpoints) that one must traverse to reach the point A′ on the diamond structure starting from A (we call it the intrinsic distance between A and A′) and respectively the number of paths having this length that connect these two points. Since d and N are O_h^7-invariant we can use the particular description in which $\psi(\mathrm{A}') = (0, 0, 0, 0)$. To describe the point A we can use a sequence (4.3) having the property that for any $i \in \{0, 1, 2, 3\}$ at most one of e_i, $\bar{e}_i$ appears inside it. Evidently, it contains $|n_0| + |n_1| + |n_2| + |n_3| = d(n, \mathrm{o})$ components, where $n = (n_0, n_1, n_2, n_3) = \psi(\mathrm{A})$ and $\mathrm{o} = (0, 0, 0, 0) = \psi(\mathrm{A}')$.

The number m of 'bar' components in such a sequence is the sum of the negative components of (n_0, n_1, n_2, n_3) taken to opposite sign and that of 'non-bar' 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 'bar' components and of the 'non-bar' components. But not all $(-m)! \cdot p!$ sequences thus obtained are distinct. For each sequence there are $|n_0|! \cdot |n_1|! \cdot |n_2|! \cdot |n_3|!$ permutations that leave it unchanged.

The mappings $d: \mathfrak{R} \times \mathfrak{R} \to \mathbb{N}$ and $N: \mathfrak{R} \times \mathfrak{R} \to \mathbb{N}$ are difficult to describe classically.

The point $(x, y, z) \in \mathbb{Z}^3$ is a point of the diamond structure if and only if there exists $\lambda \in \mathbb{R}$ such that

$$(\lambda, (y + z)/2 + \lambda, (x + z)/2 + \lambda, (x + y)/2 + \lambda) \in \mathbb{Z}^4 \tag{4.7}$$

and

$$\lambda + (y + z)/2 + \lambda + (x + z)/2 + \lambda + (x + y)/2 + \lambda \in \{0; 1\}. \tag{4.8}$$

It follows that $\lambda \in \mathbb{Z}$ and x, y, z are either all even or all odd. In the case x, y, z even, (4.8) becomes $x + y + z + 4\lambda = 0$ and hence (x, y, z) corresponds to

$$((-x - y - z)/4, (-x + y + z)/4, (x - y + z)/4, (x + y - z)/4) \in S.$$

In the case x, y, z odd we get $x + y + z + 4\lambda = 1$ and hence (x, y, z) corresponds to

$$((-x - y - z + 1)/4, (-x + y + z + 1)/4, (x - y + z + 1)/4, (x + y - z + 1)/4) \in S.$$

The intrinsic distance

$$d: \mathfrak{R} \times \mathfrak{R} \to \mathbb{N} \qquad d(\mathrm{A}, \mathrm{A}') = \sum_{i=0}^{3} |n_i - n_i'|$$

where $(n_0, n_1, n_2, n_3) = \psi(\mathrm{A})$ and $(n_0', n_1', n_2', n_3') = \psi(\mathrm{A}')$, has the following expression in the classical description

$$\begin{aligned} d((x, y, z), (x', y', z')) = \tfrac{1}{4}(&|-x - y - z + x' + y' + z'| + |-x + y + z + x' - y' - z'| \\ &+ |x - y + z - x' + y' - z'| + |x + y - z - x' - y' + z'|) \end{aligned} \tag{4.9a}$$

for x, x' both even and x, x' both odd

$$\begin{aligned} d((x, y, z), (x', y', z')) = \tfrac{1}{4}(&|-x - y - z + x' + y' + z' - 1| \\ &+ |-x + y + z + x' - y' - z' - 1| + |x - y + z - x' + y' - z' - 1| \\ &+ |x + y - z - x' - y' + z' - 1|) \end{aligned} \tag{4.9b}$$

for x even and x' odd

$$d((x,y,z),(x',y',z')) = \tfrac{1}{4}(|-x-y-z+1+x'+y'+z'| + |-x+y+z+1+x'-y'-z'| + |x-y+z+1-x'+y'-z'| + |x+y-z+1-x'-y'+z'|) \tag{4.9c}$$

for x odd and x' even.

In a crystal having the structure of diamond we can assume that two atoms A and A′ 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 $d(\mathrm{A}, \mathrm{A}')$ and $N(\mathrm{A}, \mathrm{A}')$.

In a fixed description $\psi : \mathfrak{R} \to S$, the points corresponding to

$$S_1 = \{(n_0, n_1, n_2, n_3) \in S \mid n_0 + n_1 + n_2 + n_3 = 1\}$$

form a face-centred cubic lattice. The corresponding intrinsic distance is

$$d_1 : S_1 \times S_1 \to \mathbb{N} \qquad d_1(n, n') = \tfrac{1}{2}\sum_{i=0}^{3} |n_i - n_i'|$$

and the number of minimal paths is given by the same formula as in the case of the diamond structure.

5. A class of O_h^7-invariant operators

We denote by $\mathbb{C}$ the field of complex numbers and for any $z = x + \mathrm{i}y \in \mathbb{C}$ we denote by $\bar{z} = x - \mathrm{i}y$ its conjugate and by $|z| = (z\bar{z})^{1/2}$ its absolute value. Let $z_0, z_1, z_2, z_3, \ldots$ be a sequence of complex numbers. The series $\Sigma_{j=0}^{\infty} z_j$ is called absolutely convergent if the series $\Sigma_{j=0}^{\infty} |z_j|$ is convergent. Let $\pi : \mathbb{N} \to \mathbb{N}$ be a bijective mapping. It is known [9] that if the series $\Sigma_{j=0}^{\infty} z_j$ is absolutely convergent then the series $\Sigma_{j=0}^{\infty} z_{\pi(j)}$ is also absolutely convergent and they have the same sum.

Let $\pi_1 : \mathbb{N} \to S$, $\pi_2 : \mathbb{N} \to S$ be two bijective mappings. We can obtain such a bijection, for example, by associating 0 to $(0,0,0,0) \in S$, 1, 2, 3, 4 to the four elements $n \in S$ which satisfy the condition $d(n, o) = 1$, the numbers $5, 6, \ldots, 16$ to the twelve elements $n \in S$ which satisfy the condition $d(n, o) = 2$, etc. Let $u : S \to \mathbb{C}$ be a mapping. If $\Sigma_{j=0}^{\infty} u(\pi_1(j))$ is absolutely convergent then we say [9] that $\Sigma_{n\in S} u(n)$ is absolutely summable and its sum is

$$\sum_{n\in S} u(n) = \sum_{j=0}^{\infty} u(\pi_1(j)). \tag{5.1}$$

Since $\pi_1^{-1} \circ \pi_2 : \mathbb{N} \to \mathbb{N}$ is a bijection and $\Sigma_{j=0}^{\infty} u(\pi_1(j))$ is absolutely convergent it follows that $\Sigma_{j=0}^{\infty} u\big(\pi_1((\pi_1^{-1} \circ \pi_2)(j))\big)$, that is $\Sigma_{j=0}^{\infty} u(\pi_2(j))$, is absolutely convergent and

$$\sum_{j=0}^{\infty} u(\pi_1(j)) = \sum_{j=0}^{\infty} u(\pi_2(j)).$$

Thus, the definition of $\Sigma_{n\in S} u(n)$ does not depend on the bijection $\pi_1 : \mathbb{N} \to S$ we use to define it.

We consider the space

$$l^2(S) = \left\{ u : S \to \mathbb{C} \,\middle|\, \sum_{n\in S} |u(n)|^2 \text{ is absolutely summable} \right\} \tag{5.2}$$

of all the mappings $u : S \to \mathbb{C}$ having the property that $\Sigma_{n\in S} |u(n)|^2$ is absolutely summable. The space $l^2(S)$ has the structure of a Hilbert space [10] given by

$$\begin{aligned} &u_1 + u_2 : S \to \mathbb{C} \qquad (u_1 + u_2)(n) = u_1(n) + u_2(n) \\ &a \cdot u : S \to \mathbb{C} \qquad (a \cdot u)(n) = a(u(n)) \\ &\langle u_1, u_2 \rangle = \sum_{n\in S} u_1(n) \cdot \overline{u_2(n)}. \end{aligned} \tag{5.3}$$

We obtain a unitary linear representation [11] of O_h^7 in $l^2(S)$ by associating to each $g : S \to S$, $g \in O_h^7$, the transformation

$$T_g : l^2(S) \to l^2(S) \qquad (T_g(u))(n) = u((g^{-1})(n)). \tag{5.4}$$

Indeed,

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

for any $n \in S$ and

$$\begin{aligned} \langle T_g(u_1), T_g(u_2) \rangle &= \sum_{n\in S} [T_g(u_1)](n) \cdot \overline{[T_g(u_2)](n)} \\ &= \sum_{n\in S} u_1[(g^{-1})(n)] \cdot \overline{u_2[(g^{-1})(n)]} \\ &= \sum_{n\in S} u_1(n) \cdot \overline{u_2(n)} = \langle u_1, u_2 \rangle \end{aligned}$$

for any $g \in O_h^7$, $u_1, u_2 \in l^2(S)$.

To give a physical interpretation, we consider the case of an electron lying inside of a crystal having the structure of diamond. We assume that the only possible positions of the electron are in the proximity of an atom of the crystal. Let $|n\rangle$ be the wavefunction corresponding to the following case: the electron is in the proximity of the atom $n \in S$. The general wavefunction is a superposition

$$\sum_{n\in S} u(n) \cdot |n\rangle$$

and it is square-integrable if and only if $u \in l^2(S)$.

We consider the operator

$$A : l^2(S) \to l^2(S) \qquad (Au)(n) = \sum_{n'\in S} v(d(n, n')) \cdot u(n') \tag{5.5}$$

for any mapping $v : \mathbb{N} \to \mathbb{R}$ such that the sum exists and $Au \in l^2(S)$ for any $u \in l^2(S)$. The operators thus defined are O_h^7-invariant, that is, $A = T_g^{-1} \circ A \circ T_g$ for any $g \in O_h^7$. Indeed,

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

$$= \sum_{n' \in S} v[d(g^{-1}(n), n')] \cdot u(n') = (Au)[g^{-1}(n)]$$

$$= [T_g(Au)](n) = [(T_g \circ A)(u)](n)$$

for any $g \in O_h^7$, $u \in l^2(S)$ and $n \in S$.

The operator A corresponding to v is a Hermitian operator if and only if

$$\sum_{n \in S} \left(\sum_{n' \in S} v[d(n, n')] \cdot u_1(n') \cdot \overline{u_2(n)} \right)$$
$$= \sum_{n' \in S} \left(\sum_{n \in S} v(d(n, n')) u_1(n') \overline{u_2(n)} \right)$$

for any $u_1, u_2 \in l^2(S)$.

The four nearest points of the point $n = (n_0, n_1, n_2, n_3) \in S$ are (figure 5)

$$\begin{aligned} &n^0 = (n_0 + \varepsilon(n), n_1, n_2, n_3) \qquad && n^2 = (n_0, n_1, n_2 + \varepsilon(n), n_3) \\ &n^1 = (n_0, n_1 + \varepsilon(n), n_2, n_3) \qquad && n^3 = (n_0, n_1, n_2, n_3 + \varepsilon(n)) \end{aligned} \tag{5.6}$$

where

$$\varepsilon(n) = (-1)^{n_0 + n_1 + n_2 + n_3}. \tag{5.7}$$

Let $v : \mathbb{N} \to \mathbb{R}$ be the mapping $v(0) = -4$, $v(1) = 1$, $v(j) = 0$ for $j > 1$ and $\Delta_d : l^2(S) \to l^2(S)$,

$$(\Delta_d u)(n) = -4u(n) + \sum_{n', d(n,n')=1} u(n') = \sum_{j=0}^{3} u(n^j) - 4u(n) \tag{5.8}$$

the corresponding operator. If $k = [k_0, k_1, k_2, k_3] \in P$ satisfies

$$\sin(k_0 + k_1 - k_2 - k_3) \sin(k_0 - k_1 + k_2 - k_3) \sin(k_0 - k_1 - k_2 + k_3) = 0 \tag{5.9}$$

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

$$\begin{aligned} E_k = 4[-1 + &\cos(k_0 + k_1 - k_2 - k_3) \cos(k_0 - k_1 + k_2 - k_3) \\ &\times \cos(k_0 - k_1 - k_2 + k_3)]. \end{aligned} \tag{5.10}$$

Indeed,

$$\langle k, n \rangle = 3 \sum_{j=0}^{3} k_j \cdot n_j - \sum_{m \neq j} k_m \cdot n_j = \sum_{j=0}^{3} \left(3k_j - \sum_{m \neq j} k_m \right) \cdot n_j$$

and the equation $\Delta_d u_k = E_k \cdot u_k$ is equivalent to

$$\begin{aligned} \exp[\mathrm{i}\varepsilon(n)(3k_0 - k_1 - k_2 - k_3)] &+ \exp[\mathrm{i}\varepsilon(n)(-k_0 + 3k_1 - k_2 - k_3)] \\ &+ \exp[\mathrm{i}\varepsilon(n)(-k_0 - k_1 + 3k_2 - k_3)] \\ &+ \exp[\mathrm{i}\varepsilon(n)(-k_0 - k_1 - k_2 + 3k_3)] = E + 4. \end{aligned}$$

For $E_k \in \mathbb{R}$ we get

$$\begin{aligned} \cos(3k_0 - k_1 - k_2 - k_3) &+ \cos(-k_0 + 3k_1 - k_2 - k_3) \\ &+ \cos(-k_0 - k_1 + 3k_2 - k_3) + \cos(-k_0 - k_1 - k_2 + 3k_3) = E_k + 4 \end{aligned}$$

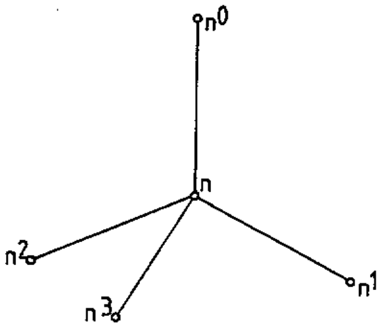

Figure 5. The four nearest points of the point n are n^0, n^1, n^2, n^3.

and

$$\sin(3k_0 - k_1 - k_2 - k_3) + \sin(-k_0 + 3k_1 - k_2 - k_3) + \sin(-k_0 - k_1 + 3k_2 - k_3) + \sin(-k_0 - k_1 - k_2 + 3k_3) = 0$$

which are equivalent to (5.10) and (5.9).

In the case of a Bravais lattice one considers [12] the space of Jacobi matrices $l^2(\mathbb{Z}^3)$, which is defined similarly to $l^2(S)$, and the operator $\Delta_d : l^2(\mathbb{Z}^3) \to l^2(\mathbb{Z}^3)$,

$$(\Delta_d u)(m) = \sum_{\substack{m' \in \mathbb{Z}^3, \\ |m'-m|_+ = 1}} [u(m') - u(m)] = -6u(m) + \sum_{\substack{m' \in \mathbb{Z}^3, \\ |m'-m|_+ = 1}} u(m')$$

where $|m' - m|_+ = \Sigma_{j=1}^3 |m'_j - m_j|$. It is called the discrete Laplacian. We remark that it corresponds to the operator (5.8) considered in the case of the diamond structure.

6. A class of O_h^7-invariant scalar fields

A mapping $f : P \to \mathbb{C}$ is $\mathrm{T_d}$-invariant if and only if $f[x_0, x_1, x_2, x_3] = f[x_{\sigma(0)}, x_{\sigma(1)}, x_{\sigma(2)}, x_{\sigma(3)}]$ for any $\sigma \in \Sigma_4$. If $f : P \to \mathbb{C}$ is $\mathrm{T_d}$-invariant and if $\Sigma_{n \in S} f(\varepsilon(n)(x - n))$ is absolutely summable for any $x \in P$ (this occurs, for example, if there is $r \in (0, \infty)$ such that $f[x_0, x_1, x_2, x_3] = 0$ for any $x = [x_0, x_1, x_2, x_3] \in P$, satisfying the condition $\langle x, x\rangle > r^2$), then the mapping $V : P \to \mathbb{C}$, $V(x) = \Sigma_{n \in S} f(\varepsilon(n)(x - n))$ is O_h^7-invariant. Indeed, for any $j \in \{1, 2, 3\}$ we get

$$\begin{aligned} V(\Lambda_j(x)) &= \sum_{n \in S} f\big(\varepsilon(n)(\Lambda_j(x) - n)\big) = \sum_{n \in S} f\big(\varepsilon(\Lambda_j(n))(\Lambda_j(x) - \Lambda_j(n))\big) \\ &= \sum_{n \in S} f\big(\Lambda_j(\varepsilon(n)(x - n))\big) = \sum_{n \in S} f\big(\varepsilon(n)(x - n)\big) = V(x). \end{aligned}$$

We have also

$$\begin{aligned} V(\Lambda_0(x)) &= \sum_{n \in S} f\big(\varepsilon(n)(\Lambda_0(x) - n)\big) \\ &= \sum_{n \in S} f\big(\varepsilon(\Lambda_0(n))(\Lambda_0(x) - \Lambda_0(n))\big) \\ &= \sum_{n \in S} f\big(-\varepsilon(n)(-x + n)\big) = V(x). \end{aligned}$$

7. Conclusions

A difficult problem may become a simpler one if an adequate description is used. The presented description seems to be useful in this sense. New O_h^7 spaces such as $S \times P$, $P \times P$, etc, and new O_h^7-invariant mathematical objects useful in modelling some physical aspects can be obtained by starting from the O_h^7 spaces and O_h^7-invariant objects considered above. Such developments are in progress and they will be the subject of another article.

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