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Elements of discrete differential calculus with applications to crystal physics

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Abstract

Some elements of discrete differential calculus with possible applications to the description of the physical phenomena occurring in crystals having two atoms per unit cell are developed in a natural way by using a convenient mathematical model for these crystals.

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0. Introduction

The description of physical phenomena based on the notion of real number and passage to the limit takes into consideration unphysical details (for example, one uses the properties of functions depending on the difference of values of a function taken at points situated at 10^{-1000} m distance) and ignores the discrete structure of matter. The possibilities of these mathematical objects in matter modelling are based on their formal properties, and attempts exist [1–8] to replace them by using mathematical objects having similar properties defined by using discrete spaces.

This method becomes adequate when the discrete spaces we use can be associated in a natural way with physical system.

The space of equilibrium positions of atoms in a crystal is a naturally defined discrete space, and we think that it offers a possibility to develop discrete differential calculus useful

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in the description of physical properties of crystals. In particular, the existing variants [6,8] of discrete differential calculus on $\mathbb{Z}^3$ may be useful in the description of the physical phenomena occurring in crystals having one atom per unit cell.

In this article we develop some elements of discrete differential calculus applicable to crystals having two atoms per unit cell.

1. A mathematical model for crystals having two atoms per unit cell

Let $\mathcal{E}_3$ be the set of all the points of the physical space identified by using the bijection

$$\mathcal{E}_3 \longrightarrow \mathbb{E}_3 \; : \; P \mapsto \mathbf{OP}$$

with the Euclidean space $\mathbb{E}_3 = \{\mathbf{OP} | P \in \mathcal{E}_3\}$ of all the vectors having as origin a fixed point $O \in \mathcal{E}_3$.

Let $\mathbf{e}_0, \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3 \in \mathbb{E}_3$ be four non-coplanar vectors. Using the vectors $\mathbf{e}_0, \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ and the vectors $\bar{\mathbf{e}}_0 = -\mathbf{e}_0, \bar{\mathbf{e}}_1 = -\mathbf{e}_1, \bar{\mathbf{e}}_2 = -\mathbf{e}_2, \bar{\mathbf{e}}_3 = -\mathbf{e}_3$ we will generate a discrete set $\mathcal{M}$ which can be used as a model for crystals having two atoms per unit cell. The point O belongs to $\mathcal{M}$. Starting from the point O considered as initial point we construct the representatives $\mathbf{OA}_0, \mathbf{OA}_1, \mathbf{OA}_2, \mathbf{OA}_3$ of the vectors $\mathbf{e}_0, \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$. The terminal points of these segments A_0, A_1, A_2, A_3 belong to $\mathcal{M}$, and by choosing each of them as initial point we construct representatives of the vectors $\bar{\mathbf{e}}_0, \bar{\mathbf{e}}_1, \bar{\mathbf{e}}_2, \bar{\mathbf{e}}_3$. The terminal points of the last constructed segments belong to $\mathcal{M}$, and by choosing each of them as initial point we construct representatives of the vectors $\mathbf{e}_0, \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$, and so on (we construct alternatively representatives of $\mathbf{e}_0, \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ and representatives of $\bar{\mathbf{e}}_0, \bar{\mathbf{e}}_1, \bar{\mathbf{e}}_2, \bar{\mathbf{e}}_3$ by choosing as initial point each of the last obtained points). Each point P belonging to the set $\mathcal{M}$ thus obtained can be described by using a sequence

$$\mathbf{e}_{i_1} \bar{\mathbf{e}}_{i_2} \mathbf{e}_{i_3} \bar{\mathbf{e}}_{i_4} \cdots \mathbf{e}'_{i_k}, \tag{1}$$

where $i_1, i_2, \ldots, i_k \in \{0, 1, 2, 3\}$, $\mathbf{e}'_{i_k} = \mathbf{e}_{i_k}$ for k odd, $\mathbf{e}_{i_k} = \bar{\mathbf{e}}_{i_k}$ for k even, and

$$\mathbf{OP} = \mathbf{e}_{i_1} + \bar{\mathbf{e}}_{i_2} + \mathbf{e}_{i_3} + \bar{\mathbf{e}}_{i_4} + \cdots + \mathbf{e}'_{i_k}. \tag{2}$$

Denoting $\mathbf{w}_1 = \mathbf{e}_1 - \mathbf{e}_0$, $\mathbf{w}_2 = \mathbf{e}_2 - \mathbf{e}_0$, $\mathbf{w}_3 = \mathbf{e}_3 - \mathbf{e}_0$, one can see that

$$\mathcal{M} = \mathcal{M}_0 \cup \mathcal{M}_1,$$

where

$$\mathcal{M}_0 = \{\alpha \mathbf{w}_1 + \beta \mathbf{w}_2 + \gamma \mathbf{w}_3 \,|\, \alpha, \beta, \gamma \in \mathbb{Z}\},$$
$$\mathcal{M}_1 = \mathbf{e}_0 + \mathcal{M}_0 = \{\mathbf{e}_0 + \alpha \mathbf{w}_1 + \beta \mathbf{w}_2 + \gamma \mathbf{w}_3 \,|\, \alpha, \beta, \gamma \in \mathbb{Z}\}$$

are two Bravais lattices. When $\mathbf{e}_0$ is contained in the interior of the parallelepiped determined by $\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3$, the set $\mathcal{M}$ can be regarded as a model for a crystal having two atoms per unit cell. Particularly, in the case when $A_0A_1A_2A_3$ is a regular tetrahedron having the point O as

centre, we obtain a model for diamond type crystals (silicon, germanium, carbon-diamond, etc.) and zincblende type crystals [9–11].

Let $E(3) = O(3) \times \mathbb{R}^3 = \{\{\Lambda|\mathbf{v}\} \mid \Lambda \in O(3), \mathbf{v} \in \mathbb{R}^3\}$ be the group of all the isometries

$$\{\Lambda|\mathbf{v}\} : \mathbb{E}_3 \longrightarrow \mathbb{E}_3 : \mathbf{w} \mapsto \Lambda\mathbf{w} + \mathbf{v} \tag{3}$$

of the space $\mathbb{E}_3$,

$$\varepsilon : \mathbb{E}_3 \longrightarrow \mathbb{E}_3, \quad \varepsilon\mathbf{v} = \mathbf{v}, \qquad i : \mathbb{E}_3 \longrightarrow \mathbb{E}_3, \quad i\mathbf{v} = -\mathbf{v}$$

and let

$$G = \{g \in E(3) \mid g(\mathcal{M}) = \mathcal{M}\}$$

be the symmetry group of $\mathcal{M}$. One can remark that $\{i|\mathbf{e}_0\} \in G$, and

$$T = \{\{\varepsilon|\mathbf{w}\} \mid \mathbf{w} \in \mathcal{M}_0\} \subset G$$

is the subgroup of G containing all the translations which leave $\mathcal{M}$ invariant. Let Σ_4 be the group of all the permutations $\sigma : \{0, 1, 2, 3\} \longrightarrow \{0, 1, 2, 3\}$, and let

$$G_0 = \{\Lambda \in O(3) \mid \Lambda(\{A_0, A_1, A_2, A_3\}) = \{A_0, A_1, A_2, A_3\}\}.$$

Evidently, for each $\Lambda \in G_0$ there exists $\sigma_\Lambda \in \Sigma_4$ such that $\Lambda(A_j) = A_{\sigma_\Lambda(j)}$ for any $j \in \{0, 1, 2, 3\}$. The group G can be described in terms of T

$$G = \bigcup_{\Lambda \in G_0} T \circ \{\Lambda|\mathbf{0}\} \cup \bigcup_{\Lambda \in G_0} T \circ \{i \circ \Lambda|\mathbf{e}_0\}. \tag{4}$$

Let

$$\mathbb{M} = \{n = (n_0, n_1, n_2, n_3) \in \mathbb{Z}^4 \mid n_0 + n_1 + n_2 + n_3 \in \{0; 1\}\}. \tag{5}$$

By associating to each sequence $\mathbf{e}_{i_1}\bar{\mathbf{e}}_{i_2}\mathbf{e}_{i_3}\bar{\mathbf{e}}_{i_4}\cdots\mathbf{e}'_{i_k}$ the element $(n_0, n_1, n_2, n_3) \in \mathbb{M}$, where n_i is the number of appearances of $\mathbf{e}_i$ inside it minus the number of appearances of $\bar{\mathbf{e}}_i$, we obtain a mapping $h : \mathcal{M} \longrightarrow \mathbb{M}$. In the case

$$\left.\begin{array}{r}(n_0, n_1, n_2, n_3) \in \mathbb{M} \\ n_0\mathbf{e}_0 + n_1\mathbf{e}_1 + n_2\mathbf{e}_2 + n_3\mathbf{e}_3 = 0\end{array}\right\} \implies n_0 = n_1 = n_2 = n_3 = 0 \tag{6}$$

the only considered sequel, h is a bijection and the numerical space $\mathbb{M}$ can be used as a mathematical model for the discrete space $\mathcal{M}$.

Two sequences (1) are said to be equivalent if one of them can be obtained from the other one by using operations such as

$$\cdots\mathbf{e}_i\bar{\mathbf{e}}_j\mathbf{e}_k\cdots \longrightarrow \cdots\mathbf{e}_k\bar{\mathbf{e}}_j\mathbf{e}_i\cdots$$

(permutation of two neighbouring non-barred components),

$$\cdots\bar{\mathbf{e}}_i\mathbf{e}_j\bar{\mathbf{e}}_k\cdots \longrightarrow \cdots\bar{\mathbf{e}}_k\mathbf{e}_j\bar{\mathbf{e}}_i\cdots$$

(permutation of two neighbouring barred components),

$$\cdots \mathbf{e}_i \bar{\mathbf{e}}_j \mathbf{e}_j \bar{\mathbf{e}}_k \cdots \longrightarrow \cdots \mathbf{e}_i \bar{\mathbf{e}}_k \cdots \text{ or } \cdots \bar{\mathbf{e}}_i \mathbf{e}_j \bar{\mathbf{e}}_j \mathbf{e}_k \cdots \longrightarrow \cdots \bar{\mathbf{e}}_i \mathbf{e}_k \cdots$$

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

$$\cdots \mathbf{e}_i \bar{\mathbf{e}}_k \cdots \longrightarrow \cdots \mathbf{e}_i \bar{\mathbf{e}}_j \mathbf{e}_j \bar{\mathbf{e}}_k \cdots \text{ or } \cdots \bar{\mathbf{e}}_i \mathbf{e}_k \cdots \longrightarrow \cdots \bar{\mathbf{e}}_i \mathbf{e}_j \bar{\mathbf{e}}_j \mathbf{e}_k \cdots$$

(insertion of a sequence of the form $\bar{\mathbf{e}}_j \mathbf{e}_j$ or $\mathbf{e}_j \bar{\mathbf{e}}_j$). This is an equivalence relation, and we can divide the space $\mathcal{F}$ of all sequences (1) into equivalence classes. One can remark that two sequences (1) describe the same point of $\mathcal{M}$ if and only if they are equivalent, and the set $\mathcal{M}$ can be identified with the set of all equivalence classes thus obtained

$$\mathcal{M} = \mathcal{F} / \sim .$$

The function

$$\delta : \mathbb{M} \times \mathbb{M} \longrightarrow \mathbb{N}, \quad \delta(n, n') = \sum_{i=0}^{3} |n_i - n'_i|, \tag{7}$$

is a G-invariant distance on $\mathbb{M}$. The point $n' \in \mathbb{M}$ is said to be a δ-neighbour of order k of the point $n \in \mathbb{M}$ if $\delta(n, n') = k$. Particularly, the points

$$\begin{aligned} n^0 &= (n_0 + \chi(n), n_1, n_2, n_3), & n^1 &= (n_0, n_1 + \chi(n), n_2, n_3), \\ n^2 &= (n_0, n_1, n_2 + \chi(n), n_3), & n^3 &= (n_0, n_1, n_2, n_3 + \chi(n)), \end{aligned} \tag{8}$$

where

$$\chi(n) = (-1)^{n_0+n_1+n_2+n_3}$$

are the first δ-neighbours of $n = (n_0, n_1, n_2, n_3)$, and

$$n^{jk} = (n^j)^k,$$

where $j, k \in \{0, 1, 2, 3\}$, $j \neq k$, are the second δ-neighbours of n. One can remark that $n^{jj} = n$ for any $n \in \mathbb{M}$, $j \in \{0, 1, 2, 3\}$, and

$$h(\mathcal{M}_0) = \{n \in \mathbb{M} \mid \chi(n) = 1\}, \qquad h(\mathcal{M}_1) = \{n \in \mathbb{M} \mid \chi(n) = -1\}.$$

In the case of many crystals having two atoms per unit cell, the chemical bonds correspond to the pairs of atoms (n, n') satisfying the condition $\delta(n, n') = 1$, and this justifies the importance of the distance δ.

The description of $\mathcal{M}$ as set of equivalence classes of formal sequences $\mathcal{M} = \mathcal{F} / \sim$ allows us to determine the number of δ-neighbours of order k of a point n, that is, the cardinal

$$Card\{ n' \mid \delta(n, n') = k\}.$$

Each element of $\mathcal{F} / \sim$, that is, each class of equivalent sequences contains either a sequence

$$\mathbf{e}_{i_1} \bar{\mathbf{e}}_{i_2} \mathbf{e}_{i_3} \bar{\mathbf{e}}_{i_4} \cdots \mathbf{e}_{i_{2j-1}} \bar{\mathbf{e}}_{i_{2j}}$$

such that

$$i_1 \le i_3 \le \cdots \le i_{2j-1}, \qquad i_2 \le i_4 \le \cdots \le i_{2j},$$
$$\{i_1, i_3, \ldots, i_{2j-1}\} \cap \{i_2, i_4, \ldots, i_{2j}\} = \emptyset$$

or a sequence

$$\mathbf{e}_{i_1}\overline{\mathbf{e}}_{i_2}\mathbf{e}_{i_3}\overline{\mathbf{e}}_{i_4}\cdots\overline{\mathbf{e}}_{i_{2j}}\mathbf{e}_{i_{2j+1}}$$

such that

$$i_1 \le i_3 \le \cdots \le i_{2j+1}, \quad i_2 \le i_4 \le \cdots \le i_{2j},$$
$$\{i_1, i_3, \ldots, i_{2j+1}\} \cap \{i_2, i_4, \ldots, i_{2j}\} = \emptyset.$$

Evidently, such a representative is unique, and it will be called the canonical representative. To determine $Card\{n' \mid \delta(0, n') = k\}$ we use the following result:

Lemma. *Let $j \in \mathbb{N}$, and let $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ be three formal symbols.*
(a) *There exist exactly $j + 1$ sequences*

$$\mathbf{a}_{i_1}\mathbf{a}_{i_2}\mathbf{a}_{i_3}\cdots\mathbf{a}_{i_j}$$

such that

$$i_1, i_2, \ldots, i_j \in \{1, 2\}, \quad i_1 \le i_2 \le \cdots \le i_j$$

and $j - 1$ of them contain both $\mathbf{a}_1$ and $\mathbf{a}_2$.
(b) *There exist exactly $\frac{1}{2}(j + 1)(j + 2)$ sequences*

$$\mathbf{a}_{i_1}\mathbf{a}_{i_2}\mathbf{a}_{i_3}\cdots\mathbf{a}_{i_j}$$

such that

$$i_1, i_2, \ldots, i_j \in \{1, 2, 3\}, \quad i_1 \le i_2 \le \cdots \le i_j$$

and $\frac{1}{2}(j + 1)(j + 2) - 3j$ of them contains all the three symbols.

Proof.
(a) The conditions are satisfied by the sequences

$$\mathbf{a}_2\mathbf{a}_2\mathbf{a}_2\cdots\mathbf{a}_2, \quad \mathbf{a}_1\mathbf{a}_2\mathbf{a}_2\cdots\mathbf{a}_2, \quad \mathbf{a}_1\mathbf{a}_1\mathbf{a}_2\cdots\mathbf{a}_2, \quad \cdots \quad \mathbf{a}_1\mathbf{a}_1\mathbf{a}_1\cdots\mathbf{a}_1.$$

(b) For each $l \in \{0, 1, 2, \ldots, j\}$ there exist exactly $j - l + 1$ sequences containing l times the symbol $\mathbf{a}_1$. Evidently, there exist three sequences containing only one symbol, and $3(j - 1)$ sequences containing two symbols. □

Theorem. *For any $n \in \mathbb{M}$ and $k \in \mathbb{N}$.*

$$Card\{\, n' \mid \delta(n, n') = k \,\} = \begin{cases} 10\,j^2 + 2 & \text{if } k = 2j, \\ 10\,j^2 + 10\,j + 4 & \text{if } k = 2j + 1. \end{cases} \tag{9}$$

Proof. Evidently,

$$Card\{n' \mid \delta(n, n') = k\} = Card\{n' \mid \delta(0, n') = k\},$$

where $0 = (0, 0, 0, 0) \in \mathbb{M}$. In the case $\delta(0, n') = 2j$ the canonical sequence describing the point n' contains j barred symbols and j non-barred symbols. There exists $2(j+1)(j+2)$ sequences having the non-barred positions occupied by the same symbol, $6(j-1)(j+1)$ sequences having the non-barred positions occupied by exactly two symbols, and there exist $4[\frac{1}{2}(j+1)(j+2) - 3j]$ sequences having the non-barred positions occupied by exactly three symbols.Thus,

$$\begin{aligned} &Card\{ n' \mid \delta(0, n') = 2j\} \\ &\quad = 2(j+1)(j+2) + 6(j-1)(j+1) + 4[\tfrac{1}{2}(j+1)(j+2) - 3j] \\ &\quad = 10\, j^2 + 2. \end{aligned}$$

In a similar way, one obtains

$$\begin{aligned} Card\{n' \mid \delta(0, n') = 2j+1\} &= 2(j+1)(j+2) + 6j(j+1) \\ &\quad + 4[\tfrac{1}{2}(j+2)(j+3) - 3(j+1)] \\ &= 10\, j^2 + 10\, j + 4. \qquad \square \end{aligned}$$

A mapping $c : \{0, 1, 2, \ldots, k\} \longrightarrow \mathbb{M} : j \mapsto c_j$ is said to be a path on $\mathbb{M}$ if $\delta(c_j, c_{j+1}) \leq 1$ for any $j \in \{0, 1, 2, \ldots, k-1\}$. In the case $c_0 = c_k$ the path c is called a closed path. A path c such that $\delta(c_j, c_{j+1}) = 1$, for any $j \in \{0, 1, 2, \ldots, k-1\}$, will be called a non-singular path.

Evidently, a non-singular path $c : \{0, 1, 2, \ldots, k\} \longrightarrow \mathbb{M} : j \mapsto c_j$ such that $c_0 = 0$ can be described by using a sequence

$$\mathbf{e}_{i_1} \bar{\mathbf{e}}_{i_2} \mathbf{e}_{i_3} \bar{\mathbf{e}}_{i_4} \cdots \mathbf{e}'_{i_k} \in \mathcal{F}.$$

We consider the set

$$\mathbb{P} = \left\{ (n^+, n^-) = (n_0^+, n_1^+, n_2^+, n_3^+, n_0^-, n_1^-, n_2^-, n_3^-) \in \mathbb{N}^8 \;\middle|\; \sum_{j=0}^{3} n_j^+ - \sum_{j=0}^{3} n_j^- \in \{0, 1\} \right\}$$

and the mapping

$$\Omega : \mathcal{F} \longrightarrow \mathbb{P}, \quad \Omega(\mathbf{e}_{i_1} \bar{\mathbf{e}}_{i_2} \mathbf{e}_{i_3} \bar{\mathbf{e}}_{i_4} \cdots \mathbf{e}'_{i_k}) = (n^+, n^-),$$

where n_j^+ is the number of appearances of $\mathbf{e}_j$, and n_j^- is the number of appearances of $\bar{\mathbf{e}}_j$ in the considered formal sequence.

For any $(n^+, n^-) \in \mathbb{P}$, the set $\Omega^{-1}\{(n^+, n^-)\} \subset \mathcal{F}$ contains

$$N(n^+, n^-) = \frac{\left(\sum_{j=0}^{3} n_j^+\right)! \left(\sum_{j=0}^{3} n_j^-\right)!}{\prod_{j=0}^{3} n_j^+ !\, n_j^- !} \tag{10}$$

formal sequences describing non-singular paths $c:\{0,1,2,\ldots,l\}\longrightarrow\mathbb{M}: j\mapsto c_j$ satisfying the conditions

$$l=\sum_{j=0}^{3}n_j^+ +\sum_{j=0}^{3}n_j^-,$$

$$c_0=0,\qquad c_l=n^+-n^-=(n_0^+-n_0^-,n_1^+-n_1^-,n_2^+-n_2^-,n_3^+-n_3^-).$$

In the case $l<k$, starting from each non-singular path $c:\{0,1,2,\ldots,l\}\longrightarrow\mathbb{M}: j\mapsto c_j$ we obtain the singular paths

$$c_\eta:\{0,1,2,\ldots,k\}\longrightarrow\mathbb{M},\quad c_\eta(j)=c_{\eta(j)}$$

by using all the increasing surjections $\eta:\{0,1,2,\ldots,k\}\longrightarrow\{0,1,2,\ldots,l\}$. The number of these singular paths corresponds to the number of combinations with repetition of $l+1$ things $k-l$ at a time, and it is $k!/[l!(k-l)!]$.

Thus, the number of paths (singular and non-singular) $c:\{0,1,2,\ldots,k\}\longrightarrow\mathbb{M}: j\mapsto c_j$ connecting the points 0 and n is given by the formula

$$N_k(0,n)=\sum_{l\le k}\sum_{(n^+,n^-)\in\mathbb{P}_{n,l}}\frac{k!}{l!(k-l)!}N(n^+,n^-), \tag{11}$$

where

$$\mathbb{P}_{n,l}=\left\{(n^+,n^-)\in\mathbb{P}\,|\,n^+-n^-=n,\sum_{j=0}^{3}n_j^+ +\sum_{j=0}^{3}n_j^-=l\right\}. \tag{12}$$

2. Elements of discrete differential calculus and applications

Following certain ideas of the discrete differential calculus [1–8] and the analogy with the methods of differential geometry [12] we define some elements of a discrete differential calculus on the space $\mathbb{M}$ with possible applications to crystal physics. We will use the notations and terminology from differential geometry in order to indicate the correspondence with the continuous case.

The definition of the tangent space of a differentiable manifold at a fixed point x as the space of vectors tangent to the curves passing through x suggests us to associate the space

$$T_n\mathbb{M}=\{(n,n),(n,n^0),(n,n^1),(n,n^2),(n,n^3)\}$$

to each point $n\in\mathbb{M}$. Let $\mathcal{F}(\mathbb{M})$ be the algebra of all the functions $f:\mathbb{M}\longrightarrow\mathbb{C}$. As in the case of differential geometry, we identify the elements (n,n), (n,n^0), (n,n^1), (n,n^2), (n,n^3) called tangent vectors, respectively, with the operators

$$0_n,(\partial/\partial x^0)_n,(\partial/\partial x^1)_n,(\partial/\partial x^2)_n,(\partial/\partial x^3)_n:\mathcal{F}(\mathbb{M})\longrightarrow\mathbb{C},$$

where

$$0_nf=0,\qquad(\partial/\partial x^j)_nf=\tau_j^{-1}(f(n^j)-f(n)) \tag{13}$$

and $\tau_j \neq 0$ are real constants. For any $f,\ g \in \mathcal{F}(\mathbb{M}),\ \alpha,\ \beta \in \mathbb{C}$, one obtains

$$(\partial/\partial x^j)_n(\alpha f + \beta g) = \alpha(\partial/\partial x^j)_n f + \beta(\partial/\partial x^j)_n g \tag{14}$$

but

$$(\partial/\partial x^j)_n(fg) = f(n^j)(\partial/\partial x^j)_n g + (\partial/\partial x^j)_n f\ g(n). \tag{15}$$

If $F : \mathbb{M} \longrightarrow \mathbb{M}$ is a mapping such that

$$\delta(F(n), F(n')) \leq \delta(n, n')$$

for any $n,\ n' \in \mathbb{M}$, then we can define the mappings

$$F_* : T\mathbb{M} \longrightarrow T\mathbb{M}, \quad F_*(n, n') = (F(n), F(n')),$$

$$F_* : \mathcal{X}(\mathbb{M}) \longrightarrow \mathcal{X}(\mathbb{M}) : X \mapsto F_*X, \quad (F_*X)_{F(n)} = F_* X_n,$$

where

$$T\mathbb{M} = \bigcup_{n\in\mathbb{M}} T_n\mathbb{M}$$

and

$$\mathcal{X}(\mathbb{M}) = \{X : \mathbb{M} \longrightarrow T\mathbb{M} : n \mapsto X_n \mid X_n \in T_n\mathbb{M}\}$$

is the space of all vector fields. Each vector field $X \in \mathcal{X}(\mathbb{M})$ defines an application

$$X : \mathcal{F}(\mathbb{M}) \longrightarrow \mathcal{F}(\mathbb{M}) : f \mapsto Xf, \qquad (Xf)(n) = X_n f. \tag{16}$$

The path $c : \{0, 1, 2, \ldots, k\} \longrightarrow \mathbb{M}$ is said to be a solution of the equation defined by the vector field $X \in \mathcal{X}(\mathbb{M})$ if

$$X_{c_j} = (c_j, c_{j+1})$$

for any $j \in \{0, 1, 2, \ldots, k-1\}$.

Following the analogy with the differential geometry, we define the vector space

$$T_n^*\mathbb{M} = \{\varphi : T_n\mathbb{M} \longrightarrow \mathbb{C} \mid \varphi(n, n) = 0\},$$

its canonical basis

$$(\mathrm{d}x^j)_n : T_n\mathbb{M} \longrightarrow \mathbb{C}, \quad \langle(\mathrm{d}x^j)_n, (\partial/\partial x^k)_n\rangle = \delta_{jk} \tag{17}$$

and the space of 1-forms

$$\mathcal{D}^1(\mathbb{M}) = \{\omega : \mathbb{M} \longrightarrow T^*\mathbb{M} : n \mapsto \omega_n \mid \omega_n \in T_n^*\mathbb{M}\},$$

where

$$T^*\mathbb{M} = \bigcup_{n\in\mathbb{M}} T_n^*\mathbb{M}.$$

The mapping

$$\mathcal{F}(\mathbb{M}) \times \mathcal{D}^1(\mathbb{M}) \longrightarrow \mathcal{D}^1(\mathbb{M}) : (f, \omega) \mapsto f\omega, \quad (f\omega)_n = f(n)\omega_n \tag{18}$$

defines a structure of $\mathcal{F}(\mathbb{M})$-module on $\mathcal{D}^1(\mathbb{M})$.

Each 1-form $\omega \in \mathcal{D}^1(\mathbb{M})$ can be written in the form

$$\omega = \sum_{j=0}^{3} \omega_j \, \mathrm{d}x^j,$$

where $\omega_j \in \mathcal{F}(\mathbb{M})$ are the functions

$$\omega_j : \mathbb{M} \longrightarrow \mathbb{C}, \quad \omega_j(n) = \langle \omega_n, \, (\partial/\partial x^j)_n \rangle,$$

and it defines an application

$$\omega : \mathcal{X}(\mathbb{M}) \longrightarrow \mathcal{F}(\mathbb{M}) : X \mapsto \omega(X), \quad (\omega(X))(n) = \langle \omega_n, X_n \rangle. \tag{19}$$

For any function $f \in \mathcal{F}(\mathbb{M})$, the 1-form

$$\mathrm{d}f : \mathbb{M} \longrightarrow T^*\mathbb{M} : \; n \mapsto (\mathrm{d}f)_n, \quad \langle (\mathrm{d}f)_n, (\partial/\partial x^j)_n \rangle = (\partial/\partial x^j)_n f \tag{20}$$

corresponds to the total differential of f. One can remark that $\mathrm{d}f = 0$ if and only if f is a constant function.

The 1-form $\omega \in \mathcal{D}^1(\mathbb{M})$ is said to be exact if there exists $f \in \mathcal{F}(\mathbb{M})$ such that $\omega = \mathrm{d}f$.

For $\omega \in \mathcal{D}^1(\mathbb{M})$ and a path $c : \{0, 1, 2, \ldots, k\} \longrightarrow \mathbb{M}$, the number

$$\int_c \omega = \sum_{j=0}^{k-1} \tau(c_j, c_{j+1}) \, \omega_{c_j}(c_j, c_{j+1}), \tag{21}$$

where

$$\tau : T\mathbb{M} \longrightarrow \mathbb{R}, \quad \tau(n, n) = 0, \quad \tau(n, n^j) = \tau_j,$$

represents the integral of ω along the path c. Particularly, for $f \in \mathcal{F}(\mathbb{M})$

$$\int_c \mathrm{d}f = f(c_k) - f(c_0) \tag{22}$$

and one can see that $\omega \in \mathcal{D}^1(\mathbb{M})$ is an exact form if and only if $\int_c \omega = 0$, for any closed path c. Indeed, in this case we can fix a point $n \in \mathbb{M}$, a constant $\kappa \in \mathbb{C}$, and we can consider the function

$$f : \mathbb{M} \longrightarrow \mathbb{C}, \qquad f(n') = \begin{cases} \kappa & \text{for } n' = n, \\ \displaystyle\int_{\tilde{c}} \omega + \kappa & \text{for } n' \neq n, \end{cases} \tag{23}$$

where $\tilde{c} : \{0, 1, 2, \ldots, k\} \longrightarrow \mathbb{M}$ is a path such that $\tilde{c}_0 = n$, $\tilde{c}_k = n'$.

Since, for any closed path $c : \{0, 1, 2\} \longrightarrow \mathbb{M}$, $c_0 = n'$, $c_1 = n'^j$, $c_2 = n'$, we get $\int_c \omega = 0$, that is,

$$\omega(n')(n', n'^j) + \omega(n'^j)(n'^j, n') = 0,$$

it follows that the definition of f does not depend on the path $\tilde{c}$ connecting n and n' we choose. The function f has the property $\omega = \mathrm{d}f$.

A crystal is a very complicated physical system, and the existing mathematical models are based on ample simplifying assumptions. When we analyse the evolution of an electron lying inside the crystal, we can assume that at each moment of time the electron may be located, with some probability, near any atom, and it moves through the crystal jumping from one atom to another. By using discrete time, we can consider that the classical trajectories of the electron correspond to the paths $c : \{0, 1, 2, \ldots, k\} \longrightarrow \mathbb{M}$, where $k \in \mathbb{N}$. Thus, we consider that the interval of time needed for an electron to pass from an atom to a neighbouring atom is the same in all the cases, and it is chosen as the elementary interval of time. During an elementary interval of time, an electron may remain in the vicinity of the same atom or to pass in the vicinity of a neighbouring atom.

In the case of a crystal placed in an uniform field, we assume that there exists a 1-form

$$S : \mathbb{M} \longrightarrow T^*\mathbb{M} : n \mapsto S_n, \quad S_n(n, n^j) = s_j,$$

such that the action along to a path $c : \{0, 1, 2, \ldots, k\} \longrightarrow \mathbb{M}$ to be $\int_c S$.

Particularly, in the case when c corresponds to a formal sequence belonging to $\Omega^{-1}\{(n^+, n^-)\}$, we get

$$\int_c S = \sum_{j=0}^{3} (n_j^+ + n_j^-)\tau_j s_j.$$

The usual formulation of quantum mechanics in terms of path integrals [13] suggests us to consider the function

$$K(n, k; 0, 0) = \sum_{c \in \mathcal{C}(n,k)} \exp\left[\frac{\mathrm{i}}{\hbar}\int_c S\right],$$

where $\mathcal{C}(n, k)$ is the set of all the paths (singular and non-singular) $c : \{0, 1, 2, \ldots, k\} \longrightarrow \mathbb{M}$ satisfying the conditions $c_0 = 0$ and $c_k = n$. We think that

$$\frac{|K(n, k; 0, 0)|^2}{|K(n', k; 0, 0)|^2}$$

may be a candidate for the description of the ratio between the probability to find the electron in the vicinity of n at time k and the probability to find the electron in the vicinity of n' at time k, when it is known that at time 0 it was in the vicinity of 0. By using the results presented in the previous section we get

$$K(n,k;0,0)$$
$$= \sum_{l\leq k} \sum_{(n^+,n^-)\in\mathbb{P}_{n,l}} \frac{k!}{l!(k-l)!} N(n^+,n^-) \exp\left[\frac{\mathrm{i}}{\hbar}\sum_{j=0}^{3}(n_j^+ + n_j^-)\tau_j s_j\right]. \tag{24}$$

The operators of the form

$$H : \mathcal{F}(\mathbb{M}) \longrightarrow \mathcal{F}(\mathbb{M}),$$
$$(Hf)(n) = \theta f(n) + \sum_{j=0}^{3} \theta_j f(n^j) + \sum_{j\neq k} \theta_{jk} f(n^{jk}). \tag{25}$$

where $\theta,\ \theta_j,\ \theta_{jk} \in \mathbb{R}$, belonging to the algebra generated by the operators

$$\partial/\partial x^j : \mathcal{F}(\mathbb{M}) \longrightarrow \mathcal{F}(\mathbb{M})$$

may be useful in crystal physics [9,10]. If $\theta_j = \theta_{\sigma_\Lambda(j)}$, $\theta_{jk} = \theta_{\sigma_\Lambda(j)\sigma_\Lambda(k)}$ for any $\Lambda \in G_0$, then the operator H is a G-invariant operator.

Using the identification $n = (n_0, n_1, n_2, n_3) = n_0\mathbf{e}_0 + n_1\mathbf{e}_1 + n_2\mathbf{e}_2 + n_3\mathbf{e}_3$, we can find eigenfunctions of H of the form

$$\psi : \mathbb{M} \longrightarrow \mathbb{C}, \qquad \psi(n) = \begin{cases} \alpha \exp(\mathrm{i}\langle \mathbf{k}, n\rangle) & \text{for } \chi(n) = 1, \\ \beta \exp(\mathrm{i}\langle \mathbf{k}, n\rangle) & \text{for } \chi(n) = -1, \end{cases} \tag{26}$$

where $\mathbf{k} \in \mathbb{E}_3$, and $\alpha,\ \beta \in \mathbb{C}$. Indeed, the relation

$$H\psi = \lambda\psi$$

is equivalent with the system of equations

$$\alpha\theta + \beta\sum_{j=0}^{3}\theta_j \exp(\mathrm{i}K_j) + \alpha\sum_{j\neq m}\theta_{jm}\exp(\mathrm{i}K_j - \mathrm{i}K_m) = \lambda\alpha, \tag{27}$$

$$\beta\theta + \alpha\sum_{j=0}^{3}\theta_j \exp(-\mathrm{i}K_j) + \beta\sum_{j\neq m}\theta_{jm}\exp(-\mathrm{i}K_j + \mathrm{i}K_m) = \lambda\beta, \tag{28}$$

where $K_j = \langle \mathbf{k}, \mathbf{e}_j\rangle$, and this system has solutions $(\alpha,\ \beta) \neq (0,0)$ if λ is a root of the equation

$$\begin{vmatrix} \theta + \sum_{j\neq m}\theta_{jm}\exp(\mathrm{i}K_j - \mathrm{i}K_m) - \lambda & \sum_{j=0}^{3}\theta_j \exp(\mathrm{i}K_j) \\ \sum_{j=0}^{3}\theta_j \exp(-\mathrm{i}K_j) & \theta + \sum_{j\neq m}\theta_{jm}\exp(-\mathrm{i}K_j + \mathrm{i}K_m) - \lambda \end{vmatrix} = 0. \tag{29}$$

The subspace

$$l^2(\mathbb{M}) = \left\{ f : \mathbb{M} \longrightarrow \mathbb{C} \,\middle|\, \sum_{n\in\mathbb{M}} |f(n)|^2 \text{ is convergent} \right\}$$

of $\mathcal{F}(\mathbb{M})$ has a natural structure of Hilbert space given by

$$\langle f_1, f_2 \rangle = \sum_{n \in \mathbb{M}} f_1(n) \overline{f_2(n)} \tag{30}$$

and may also be useful in a quantum description of the crystal properties [9,10].

Beside the fibre bundles $T\mathbb{M}$ and $T^*\mathbb{M}$ considered above, other fibre bundles having as basis the space $\mathbb{M}$ may be useful in the description of the physical phenomena occurring in crystals [11].

3. Concluding remarks

A discrete description is useful in modelling when it is based on some discrete spaces associated in a natural way to the physical system. Beside the universal discrete differential calculus [5–8], we think that it is very important to develop variants adequate to some particular physical systems. The crystals are among the systems where such a calculus can be developed in a natural way.

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