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The role of the tangent bundle for symmetry operations and modulated structures

Philippe Kocian, Kurt Schenk and Gervais Chapuis*

Laboratoire de Cristallographie, IPSB – FSB, École Polytechnique Fédérale de Lausanne, Le Cubotron, Dorigny, CH-1015 Lausanne, Switzerland. Correspondence e-mail: gervais.chapuis@epfl.ch

An equivalence relation on the tangent bundle of a manifold is defined in order to extend a structure (modulated or not) onto it. This extension affords a representation of a structure in any tangent space and that in another tangent space can easily be derived. Euclidean symmetry operations associated with the tangent bundle are generalized and their usefulness for the determination of the intrinsic translation part in helicoidal axes and glide planes is illustrated. Finally, a novel representation of space groups is shown to be independent of any origin point.

1. Introduction

The choice of an origin point is a ubiquitous problem in crystallography, especially in the case of space-group operations. Commonly, symmetry elements do not all intersect in one point and no privileged point imposes itself as an origin. In fact, rules for selecting the origin must be provided (Wondratschek, 2002). Some privileged points corresponding to high symmetries arise from a set of rules laid down by Paul Niggli (1919), or also from an analysis of the normalizers of the space group under consideration (Burzlaff & Zimmermann, 1980). In any case, there will be some symmetry elements not containing this point; and if the corresponding symmetry operation does not possess any fixed point, the translation part does not correspond to the intrinsic translation vector, which is somewhat uncomfortable.

In general, the translation part associated with the representation of a Euclidean symmetry operation does not provide information about the intrinsic translation of the operation. Indeed, it is difficult to say whether the translation part of a symmetry operation corresponds to the intrinsic translation or to a specific choice of the origin, or both. It is only when the origin point lies on the symmetry element of an operation that the relevant information about the translation can be deduced: if the translation vector is the zero vector, then the symmetry operation contains a fixed point; if it is not the zero vector, it corresponds to the intrinsic translation vector of the operation, which is then a helicoidal axis or a glide plane.

Earlier we have introduced (Kocian *et al.*, 2009) the concept of representation of a structure (modulated or not) in the tangent space of a manifold. The importance of this representation for symmetry operations was illustrated. Indeed, such an operation is represented by a linear map between two tangent spaces. As the tangent point (the 'origin' point of the tangent space considered) may be arbitrarily chosen, it appears legitimate to look for a possibility to easily switch from one tangent space to another.

So, a formalism for the description of structures and symmetry operations, independent of the concept of origin point, is required. It is true that, once a coordinate system is selected, there is only one origin in the sense that there is only one point the coordinates of which are zero. However, thanks to the concept of tangent space, one may have an infinity of 'origin points'. Each of these simply corresponds to the zero vector, the basis point of which is the tangent point under consideration. Thus, an infinity of tangent-space representations of a crystal structure exists which may be regrouped in a structure in the tangent bundle of the considered manifold, the dimension of which is twice that of the structure in the manifold. Such a higher-dimensional structure may easily be obtained by introducing an equivalence relation on the tangent bundle thanks to which the representation of a structure in any tangent space is easily obtained. Corollarily, a formalism in which symmetry operations no longer depend on the choice of the origin point is afforded.

2. Fundamental equivalence relation on the tangent bundle of a manifold

The need for defining an equivalence relation on the tangent bundle arose from the study of the manifold- and tangent-space representation of a lattice in Euclidean space. Let us recall that any two points q and p in the Euclidean space may be linked by a geodesic c (straight line), linearly parameterized (*i.e.* with a constant velocity) between 0 and 1, such that $c(0) = q$ and $c(1) = p$. As shown earlier (Kocian *et al.*, 2009), the point p corresponds in fact to the tip of the tangent vector v of c at q. Let us focus on the point p: its position is independent of the starting point q and the curve linking q to p. Any curve parameterized linearly between 0 and 1, the starting point of which is any point q and the end point is p, is such that the tip of its tangent vector v at the starting point corresponds to p. We may then say that a couple $(q;\ v)$ is equivalent to another one $(q';\ v')$ if and only if $c_v(1) = c_{v'}(1)$, where c_v and $c_{v'}$ are the curves (linearly parameterized between 0 and 1), the starting points of which are q and q', respectively, and the tangent vectors of which are v and v', respectively, at their starting point. Note that a couple $(q;\ v)$ is in essence an element of the tangent bundle, as it is composed of a point q (belonging to the manifold under consideration) and a tangent vector v at q (belonging to the tangent space at q of the manifold).

2.1. Equivalence relation

Let us now generalize these concepts to any manifold M, parameterized by a one-to-one map $H : \mathbb{R}^n \to \mathbb{R}^n$ (M is then mostly $\mathbb{R}^n$, it is just endowed with a curved coordinate system). Let $H(q_1)$ and $H(p)$ be two points in M, with coordinates $H(u_{q_1})$ and $H(u_p)$ respectively [note that $u = (u^1;\ \ldots;\ u^n)$ are the natural coordinates in $\mathbb{R}^n$]. They may be linked by the curve parameterized between 0 and 1:

$$\begin{aligned} c_{v_1} : [0;\ 1] &\to M \\ t &\mapsto c_{v_1}(t) = H\big(u_{q_1} + (u_p - u_{q_1})t\big), \end{aligned}$$

the tangent vector of which at $H(q_1)$ is

$$\left.\frac{\mathrm{d}c_{v_1}(t)}{\mathrm{d}t}\right|_{t=0} = \dot{c}_{v_1}(0) = \mathrm{d}H_{q_1}(u_p - u_{q_1}) \doteqdot v_1;$$

in components:

$$v_1^{\,i} = \sum_{j=1}^{n} \left.\frac{\partial h^i(u)}{\partial u^j}\right|_{q_1} (u_p^{\,j} - u_{q_1}^{\,j}),$$

where $H = (h^1;\ \ldots;\ h^n)$ and $\mathrm{d}H$ is the differential map of H. Let us select another point $H(q_2)$, with coordinates $H(u_{q_2})$. It may be linked by the curve, also parameterized between 0 and 1:

$$\begin{aligned} c_{v_2} : [0;\ 1] &\to M \\ t &\mapsto c_{v_2}(t) = H\big(u_{q_2} + (u_p - u_{q_2})t\big), \end{aligned}$$

the tangent vector of which at $H(q_2)$ is

$$\left.\frac{\mathrm{d}c_{v_2}(t)}{\mathrm{d}t}\right|_{t=0} = \dot{c}_{v_2}(0) = \mathrm{d}H_{q_2}(u_p - u_{q_2}) \doteqdot v_2;$$

in components:

$$v_2^{\,i} = \sum_{j=1}^{n} \left.\frac{\partial h^i(u)}{\partial u^j}\right|_{q_2} (u_p^{\,j} - u_{q_2}^{\,j}).$$

Note that both curves c_{v_1} and c_{v_2} have the same end point $H(u_p)$.

Let us consider particularly the points $H(q_1)$ and $H(q_2)$ in M, and the vectors $v_1 \in \mathrm{T}_{H(q_1)}M$ and $v_2 \in \mathrm{T}_{H(q_2)}M$. A relation $\sim$ on the tangent bundle can be defined as follows:

$$\begin{aligned} &\big(H(u_{q_1});\ v_1\big) \sim \big(H(u_{q_2});\ v_2\big) \\ &\Leftrightarrow c_{v_1}(1) = H(u_p) = c_{v_2}(1), \end{aligned}$$

where $H(u_{q_1})$ and $H(u_{q_2})$ are the coordinates of $H(q_1)$ and $H(q_2)$, respectively.

The relation $\sim$ is an equivalence relation on the tangent bundle of M (which in fact corresponds to the tangent bundle of $\mathbb{R}^n$).

Indeed, it is immediately seen that $\sim$ is reflexive and symmetric. The transitivity is shown by considering three couples $\big(H(u_{q_1});\ v_1\big)$, $\big(H(u_{q_2});\ v_2\big)$ and $\big(H(u_{q_3});\ v_3\big)$ (where the foot of v_1, v_2, v_3 lies, respectively, in q_1, q_2, q_3), such that $\big(H(u_{q_1});\ v_1\big) \sim \big(H(u_{q_2});\ v_2\big)$ and $\big(H(u_{q_2});\ v_2\big) \sim \big(H(u_{q_3});\ v_3\big)$. Then, $c_{v_1}(1) = c_{v_2}(1) = c_{v_3}(1)$, where c_{v_α}, $1 \le \alpha \le 3$, are curves the expression of which in coordinates is

$$\begin{aligned} c_{v_\alpha} : [0;\ 1] &\to M \\ t &\mapsto c_{v_\alpha}(t) = H\big(u_{q_\alpha} + (u_p - u_{q_\alpha})\,t\big), \end{aligned}$$

Thus, $c_{v_1}(1) = c_{v_3}(1)$ and $\big(H(u_{q_1});\ v_1\big) \sim \big(H(u_{q_3});\ v_3\big)$.

2.2. Equivalence class

Once an equivalence relation is defined, one may regroup all equivalent elements in one set, called an equivalence class. Let us do this for the equivalence relation $\sim$ defined above. Consider the point $H(u_p) \in M$ that may be written as $\big(H(u_p);\ 0\big)$, a point of the tangent bundle $\mathrm{T}M$, by way of the natural immersion map $\iota : M \to \mathrm{T}M$. Then the curve

$$\begin{aligned} c : [0;\ 1] &\to M \\ t &\mapsto c_v(t) = H\big(u_p + (1 - t)\,w\big) \end{aligned}$$

links any point $c(0) = H(u_p + w)$ to $H(u_p)$. As w is any element of $\mathbb{R}^n$ and as H is one-to-one, then $c(0)$ can also be any point in $\mathbb{R}^n$. The tangent vector of this curve at $t = 0$ [*i.e.* at $H(u_p + w)$] is

$$\dot{c}(0) = -\mathrm{d}H_q(w) \doteqdot v,$$

where q is the point with coordinates $u_q = u_p + w$. In components:

$$v^i = \sum_{j=1}^{n} -\omega^i_j(u_p + w)\,w^j,$$

where $\omega^i_j(u_p + w) \doteqdot (\partial h^i/\partial u^j)(u_p + w)$ is the component $(i;\ j)$ of the matrix $\Omega(u_p + w)$ representing $\mathrm{d}H$. Thus, for the equivalence relation $\sim$, the equivalence class of $\big(H(u_p);\ 0\big)$ can be written as

$$\big[\big(H(u_p);\ 0\big)\big]_\sim \doteqdot \big(H(u_p + w);\ -\Omega(u_p + w)\,w\big),$$

where $w \in \mathbb{R}^n$ is a free n-dimensional parameter. In this class, there is also the element $\big(H(0);\ \Omega(0)\,u_p\big)$ (when $w = u_p$); thus, the same equivalence class may be described from this point:

$$\big[\big(H(u_p);\ 0\big)\big]_\sim = \big(H(\tilde{w});\ \Omega(\tilde{w})(u_p - \tilde{w})\big).$$

Note that the classes are disjoint if H is a diffeomorphism (*i.e.* when H is a one-to-one smooth map possessing a smooth inverse). Indeed, let us consider two points $\big(H(u_{p_1});\ 0\big)$ and $\big(H(u_{p_2});\ 0\big)$ of $\mathrm{T}M$. Their equivalence classes are, respectively,

$$\begin{aligned} &\big(H(u_{p_1} + w_1);\ -\Omega(u_{p_1} + w_1)\,w_1\big), \\ &\big(H(u_{p_2} + w_2);\ -\Omega(u_{p_2} + w_2)\,w_2\big), \end{aligned}$$

where $w_1, w_2 \in \mathbb{R}^n$ are two parameters. Consider the point $\big(H(u_q)\,;\; v_q\big)$ and suppose it belongs to both classes. This means that there exists $\tilde{w}_1, \tilde{w}_2 \in \mathbb{R}^n$ such that

$$\big(H(u_q);\; v_q\big) = \big(H(u_{p_1} + \tilde{w}_1);\; -\Omega(u_{p_1} + \tilde{w}_1)\,\tilde{w}_1\big),$$
$$\big(H(u_q);\; v_q\big) = \big(H(u_{p_2} + \tilde{w}_2);\; -\Omega(u_{p_2} + \tilde{w}_2)\,\tilde{w}_2\big).$$

Since H is one-to-one, $H(u_{p_1} + \tilde{w}_1) = H(u_q) = H(u_{p_2} + \tilde{w}_2)$ implies $u_{p_1} + \tilde{w}_1 = u_q = u_{p_2} + \tilde{w}_2$. Thus

$$\big(H(u_q);\; v_q\big) = \big(H(u_q);\; -\Omega(u_q)\,(u_q - u_{p_1})\big),$$
$$\big(H(u_q);\; v_q\big) = \big(H(u_q);\; -\Omega(u_q)\,(u_q - u_{p_2})\big).$$

Since H is a diffeomorphism, Ω is a field of square matrices of maximal rank. Thus Ω^{-1} exists and from the previous equalities we have $u_q - u_{p_1} = -\Omega(u_q)^{-1}\,v_q = u_q - u_{p_2}$, hence $u_{p_1} = u_{p_2}$ and $H(u_{p_1}) = H(u_{p_2})$. The two classes coincide.

Note that for crystallographic applications, H is a one-to-one map which is sometimes smooth only piecewise, and the inverse of which is also piecewise smooth. This does not cause any difficulties, because it can always be well approximated by a diffeomorphism (H is a wavefunction which can be developed in a Fourier series and approximated by a smooth map with a finite number of terms).

2.3. The Euclidean case

Let us consider the n-dimensional Euclidean manifold $\mathbb{R}^n$ endowed with the natural coordinate system $u = (u^1;\; \ldots;\; u^n)$. The equivalence relation on the tangent bundle defined above becomes very intuitive in this case. Indeed, recalling that in the Euclidean case the end point of a geodesic linking two points q and p, and linearly parameterized between 0 and 1, corresponds to the tip of the tangent vector of this geodesic at q (Kocian *et al.*, 2009), the relation

$$(u_{q_1};\; v_1) \sim (u_{q_2};\; v_2) \;\Leftrightarrow\; c_{v_1} = u_p = c_{v_2} \qquad (1a)$$

may be written as

$$(u_{q_1};\; v_1) \sim (u_{q_2};\; v_2) \;\Leftrightarrow\; u_{q_1} + v_1 = u_{q_2} + v_2. \qquad (1b)$$

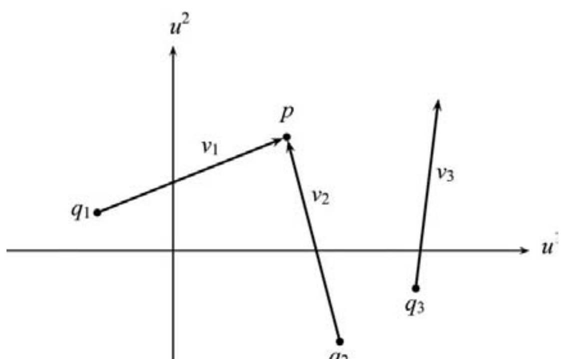

Figure 1
Illustration of the equivalence relation on the tangent bundle in the case of the two-dimensional Euclidean manifold. Two couples $(u_{q_1};\; v_1)$ and $(u_{q_2};\; v_2)$ are equivalent if and only if the tip of v_1 is at the same point as the tip of v_2. The couple $(u_{q_3};\; v_3)$ is not equivalent to the two previous couples because the tip of v_3 is not at p.

This means that two points q_1 and q_2, with coordinates u_{q_1} and u_{q_2}, are related if the tip of the vectors v_1 and v_2 with initial points q_1 and q_2, respectively, are at the same point (see Fig. 1). Recall that even if the end point p may be seen as the tip of a vector (v_1 or v_2 in our case), this vector is element of a tangent space and not of the manifold.

The equivalence class of a point $(u_p;\; 0)$ in the tangent bundle of the Euclidean manifold is given by

$$[(u_p;\; 0)]_\sim = (u_p + w;\; -w), \quad \text{where } w \in \mathbb{R}^n. \qquad (2)$$

Indeed, according to relation (1), any point q with coordinates $u_q = u_p + w$ and vector $-w$ are such that $u_q - w = u_p + w - w = u_p + 0$ $(= u_p)$. Expression (2) shows that the point p, the coordinates of which in the Euclidean space are u_p, is represented by the vector $-w = u_p - u_q$ in the tangent space at $u_q \doteq u_p + w$. The equivalence class of $(u_p;\; 0)$ is called the tangent-bundle representation of the point p.

As an example, let us find the tangent-bundle representation of a periodic lattice in the n-dimensional Euclidean space

$$\Lambda = \{B\lambda \mid \lambda \in \mathbb{Z}^n\},$$

where $B \in \mathrm{GL}_n(\mathbb{R})$ (*i.e.* B is an invertible $n \times n$ matrix). Each point $B\lambda \in \Lambda$ may be seen as an element of the tangent bundle $\mathbb{R}^n \times \mathbb{R}^n = \mathbb{R}^{2n}$ of the Euclidean manifold $\mathbb{R}^n$, and written as the couple $(B\lambda;\; 0)$. The equivalence class (the tangent-bundle representation) of each point is then

$$[(B\lambda;\; 0)]_\sim = (B\lambda + w_\lambda;\; -w_\lambda), \text{ where } w_\lambda \in \mathbb{R}^n.$$

Thus, we obtain a kind of lattice in the tangent bundle, the dimension of which is twice that of Λ. It may be written as

$$\Xi = \{(B\lambda + w_\lambda;\; -w_\lambda) \mid \lambda \in \mathbb{Z}^n,\; w_\lambda \in \mathbb{R}^n\}.$$

If for each $\lambda \in \mathbb{Z}^n$ we choose $w_\lambda = -B\lambda$, we obtain representatives of each class $[(B\lambda\,;\; 0)]_\sim$ that all belong to the tangent space at the origin:

$$(0\,;\; B\lambda), \quad \lambda \in \mathbb{Z}^n;$$

Thus, we obtain the representation of the lattice Λ in the tangent space at the origin. More generally, if we choose $w_\lambda = u_q - B\lambda$, where u_q are the coordinates of a point q, all representatives of each equivalence class belong to the same tangent space at q:

$$(u_q;\; -u_q + B\lambda), \quad \lambda \in \mathbb{Z}^n,$$

we obtain the representation of Λ in the tangent space at the chosen point q. Fig. 2 shows the situation in the case of a one-dimensional periodic lattice. Equivalence classes of each node are straight lines of slope -1 passing through the corresponding point.

2.4. The modulated case

Let us consider a manifold M, which is mostly $\mathbb{R}^n$, but endowed with a curved coordinate system. M is then parameterized by a one-to-one map $H : \mathbb{R}^n \to \mathbb{R}^n$, which is, for crystallographic applications, a periodic wavefunction of the position, $u \longmapsto H(u) = H(k \cdot u)$. In many concrete cases, H is smooth piecewise only. But thanks to Fourier's development, one can always find an appropriate smooth approximation that is a diffeomorphism, such that the concepts introduced above can be used.

In the Euclidean case, two couples $(u_{q_1};\ v_1)$ and $(u_{q_2};\ v_2)$ are equivalent if and only if the tip of v_1 corresponds to that of v_2. This equivalence is due to the fact that the tip of a vector corresponds to the end point of a curve linearly parameterized between 0 and 1, the starting point of which corresponds to the foot of the vector. In the modulated case, this no longer holds because the end point of a curve (in the modulated space) parameterized between 0 and 1 does, in general, not correspond to the tip of its tangent vector at the initial point (see Fig. 3). Thus, the equivalence relation defined on the tangent bundle is perhaps less intuitive in the modulated case (compared to the Euclidean one), even if the principle is exactly the same.

As seen previously, the equivalence class of a point $\big(H(u_p)\,;\ 0\big)$ in the tangent bundle of the manifold (parameterized by H) is given by

$$\big[\big(H(u_p);\ 0\big)\big]_\sim = \big(H(u_p + w);\ -\Omega(u_p + w)\, w\big), \quad w \in \mathbb{R}^n,$$

where Ω is the matrix representation of $\mathrm{d}H$. From this expression, we see that the point $H(p)$, the coordinates of which in the manifold are $H(u_p)$, is represented, in the tangent space at $H(u_q) \doteqdot H(u_p + w)$, by the vector $-\Omega(u_p + w)\, w = \Omega(u_q)\,(u_p - u_q)$. As in the Euclidean case, the equivalence class of $\big(H(u_p)\,;\ 0\big)$ is called the tangent-bundle representation of the point $H(p)$.

May the tangent-bundle representation of the modulated lattice $\tilde{\Lambda}$ serve as example:

$$\tilde{\Lambda} = \{H(B\lambda) \mid \lambda \in \mathbb{Z}^n\},$$

where $B \in \mathrm{GL}_n(\mathbb{R})$ and $H : \mathbb{R}^n \to \mathbb{R}^n$ is the one-to-one map defining the modulation. Each point $H(B\lambda)$ of $\tilde{\Lambda}$ may be written as an element $(H(B\lambda);\ 0)$ of the tangent bundle of the manifold. Its tangent-space representation (equivalence class) is then

$$[(H(B\lambda);\ 0)]_\sim = (H(B\lambda + w_\lambda);\ -\Omega(B\lambda + w_\lambda)\, w_\lambda),$$

where $w_\lambda \in \mathbb{R}^n$. Thus, the set of elements

$$\tilde{\Xi} = \big\{\big(H(B\lambda + w_\lambda)\,;\ -\Omega(B\lambda + w_\lambda)\, w_\lambda\big) \mid \lambda \in \mathbb{Z}^n,\ w_\lambda \in \mathbb{R}^n\big\}$$

forms a kind of lattice in the tangent bundle. For each $\lambda \in \mathbb{Z}^n$, choosing $w_\lambda = u_q - B\lambda$, the representatives of each class, all belonging to the same tangent space at $H(q)$, are

$$\big(H(u_q)\,;\ \Omega(u_q)\,(-u_q + B\lambda)\big), \quad \lambda \in \mathbb{Z}^n.$$

This is the representation of $\tilde{\Lambda}$ in the tangent space at the chosen point $H(q)$. Typically, if $u_q = u_o = 0$, we find

$$\big\{(H(0)\,;\ \Omega(0)B\lambda) \mid \lambda \in \mathbb{Z}^n\big\},$$

for the representation of $\tilde{\Lambda}$ in the tangent space at the origin.

Fig. 4 shows the situation in the case of a one-dimensional modulated lattice, where the modulation is given by

$$u \longmapsto H(u) \doteqdot u + A\sin(ku),$$

$A, k \in \mathbb{R}$. The equivalence class of any node $a\lambda$, where $a \in \mathbb{R}_+$ and $w \in \mathbb{R}$, is

$$\Big(a\lambda + w + A\sin\big(k(a\lambda + w)\big);\ -w\big[1 + kA\cos\big(k(a\lambda + w)\big)\big]\Big).$$

Note that the term $1 + kA\cos(k(a\lambda + w))$ is the 1×1 matrix corresponding to the derivative of the map H at $u = a\lambda + w$. From this expression, we see that the representation of $\tilde{\Lambda}$ in any tangent space (any 'vertical' cut) forms a periodic lattice, in the sense that it is a $\mathbb{Z}$-module. This result, already presented in our previous work (Kocian *et al.*, 2009), is a consequence of the linearity of the derivative map and of the fact that tangent spaces are vector spaces. Fig. 5 illustrates the importance of the condition that H be one-to-one; as soon as this condition is not satisfied, each 'equivalence class' crosses

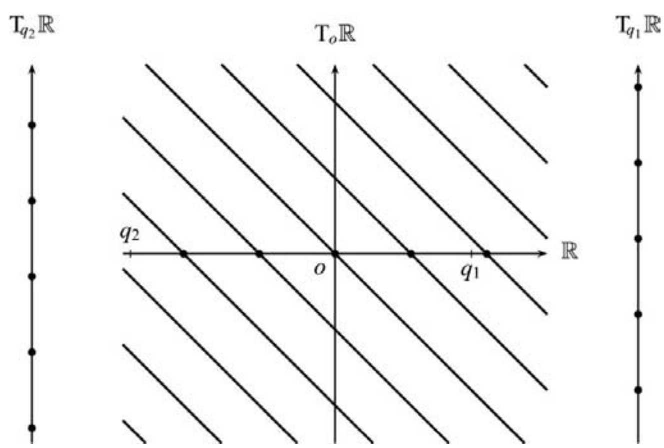

Figure 2
Representation of a one-dimensional periodic lattice in the tangent bundle $T\mathbb{R}$ of the one-dimensional Euclidean manifold. $T\mathbb{R}$ can be seen as the Cartesian product of $\mathbb{R}$ and $\mathbb{R}$, that is $\mathbb{R}^2$ (to each point of $\mathbb{R}$ is associated a one-dimensional tangent space $\mathbb{R}$). Thus, a vertical cut through any point q corresponds to the representation of the lattice in the tangent space at q; this is shown on the left- and right-hand parts of the figure.

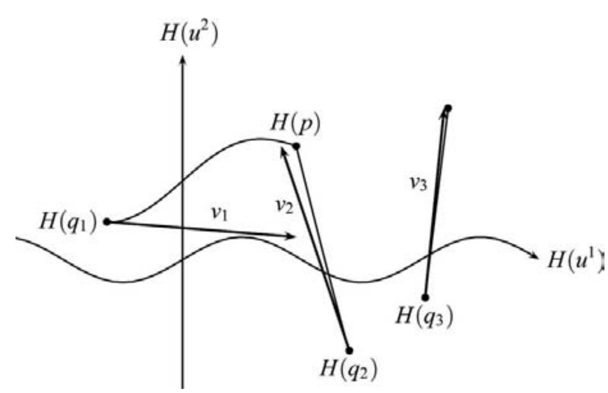

Figure 3
Illustration of the equivalence relation on the tangent bundle of a manifold in the modulated case (modulated manifold). Two couples $(H(u_{q_1});\ v_1)$ and $(H(u_{q_2});\ v_2)$ are equivalent if and only if the curves c_{v_1} and c_{v_2}, associated with the vectors v_1 and v_2, respectively, have the same end point $H(p)$. The couple $(H(u_{q_3});\ v_3)$ is not equivalent to the two previous ones, since the end point of the curve c_{v_3} associated with v_3 is different from $H(p)$.

itself and others. This is in fact completely normal, since M does not have the structure of a manifold any more.

Thanks to the $\sim$ equivalence relation on the tangent bundle of a manifold, we can obtain the representation of a lattice, therefore a crystal structure, in the tangent bundle of the manifold. With this higher-dimensional structure, one can easily find the representation of the crystal structure in any tangent space. Moreover, it provides a continuous way for passing from the manifold representation of a structure to any tangent-space representation.

3. Symmetry operations in the tangent bundle

As shown earlier (Kocian *et al.*, 2009), any symmetry operation ϕ has two representations: one in the manifold and one in the tangent space. In the first case, the operation is a map from the manifold to itself, carrying points into other points. In the second case, the operation is represented by a linear map carrying vectors of one tangent space into vectors of another one. Both representations contain the same information; the second one is practical because the operation corresponds to a linear map.

We have seen that the Euclidean manifold and any tangent space are geometrically equivalent. In particular the Euclidean manifold, endowed with the natural coordinate system, and its tangent space at the origin are indistinguishable. Indeed, it is only the concept of origin which distinguishes one from the other. The representation of any point, or set of points (*e.g.* a lattice or a crystal structure) in any tangent space (especially that at the origin) of the Euclidean manifold is completely equivalent to that in the manifold.

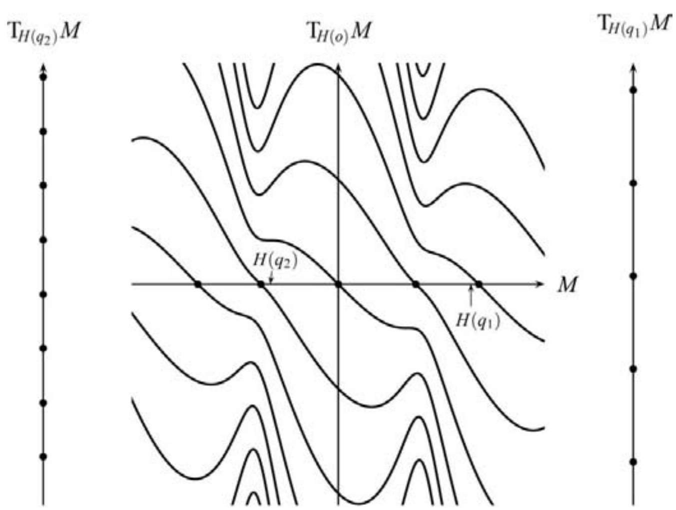

Figure 4
Representation of a one-dimensional sinusoidal modulated lattice in the tangent bundle TM of a (modulated) manifold. TM can also be seen as the Cartesian product of $\mathbb{R} \times \mathbb{R}$, where the first $\mathbb{R}$ corresponds to the manifold M (it is just parameterized by a map different from the identity) and the second to the tangent space at any point of M. A 'vertical' cut through any point $H(q)$ corresponds to the representation of the lattice in the tangent space at $H(q)$; this is shown on the left- and right-hand parts of the figure. Note that in such a space, the lattice is periodic (that is, a $\mathbb{Z}$-module).

A symmetry operation acting on the Euclidean manifold is represented by a matrix and a translation part which may or may not correspond to the intrinsic translation of the operation. This is so, because the translation part does depend on the choice of the origin. Two questions then arise: (i) How can one determine the intrinsic translation of a symmetry operation? (ii) How can one derive the translation part in any coordinate system, if the intrinsic translation is known? These problems have already been treated in many books. We propose here an alternative way that is based on the tangent-space representation of a symmetry operation. Even if the final conclusions are the same, the point of view is interesting and the derivations will be instructive in their own right.

3.1. Finding the intrinsic translation

Let us consider an isometry ϕ in the Euclidean manifold; its representation in coordinates is given by

$$u \longmapsto u' = Fu + s,$$

where $F \in \mathrm{O}_n(\mathbb{R})$ and $s \in \mathbb{R}^n$. Note that in another coordinate system in the Euclidean manifold (in which the metric tensor is still constant everywhere), the relation above is the same, the only difference lies in the fact that F is no longer orthogonal, but still of determinant ± 1. In the tangent-space representation, this isometry is described by the linear map

$$\mathrm{d}\phi_q : \mathrm{T}_q\mathbb{R}^n \to \mathrm{T}_{\phi(q)}\mathbb{R}^n;$$

it carries vectors of the tangent space at a point q to vectors of the tangent space at the point $\phi(q)$.

Fig. 6 shows the equivalence of the two representations for an inversion operation in the one-dimensional Euclidean space. It also shows that if we consider the representation of the point p in the tangent space at the inversion centre $\overline{q}$, the differential map $\mathrm{d}\phi_{\overline{q}}$ is an endomorphism of $\mathrm{T}_{\overline{q}}\mathbb{R}$. In fact, we

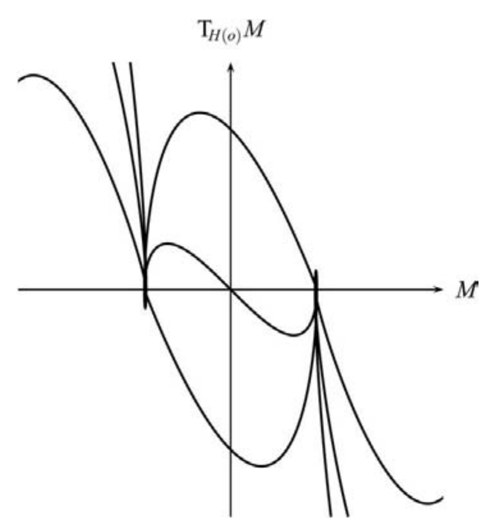

Figure 5
If H is not a one-to-one map from $\mathbb{R}^n$ to M (which is in fact $\mathbb{R}^n$ as well), M does in fact not have a manifold structure any more and the definition of equivalence relation on the 'tangent bundle' becomes absurd: two different 'equivalence classes' cross at least at one point, hence they are connected.

see that the 'distance' between $T_q\mathbb{R}$ and $T_{\phi(q)}\mathbb{R}$ decreases if the tangent point q approaches the symmetry element (inversion centre), and will be 0, if the chosen tangent point lies on the inversion centre.

There exist two kinds of isometries in the Euclidean manifold, those containing at least one fixed point and those without. For isometries with a fixed point, there exists a tangent space at a point for which the differential map of the isometry is an endomorphism of this tangent space. Let us now define the distance between two tangent spaces as the distance between the two associated tangent points (this is justified by the fact that the tangent bundle of $\mathbb{R}^n$ is the Cartesian product of $\mathbb{R}^n$ and $\mathbb{R}^n$). For isometries without a fixed point then, there exists a point such that the distance between the tangent space at this point and the tangent space at its image point (through the isometry) is minimal. In both cases, such a point may be found by minimizing, using derivative techniques, the distance between the two tangent spaces.

Thus, we need to find the distance function between a tangent point q and its image $q' = \phi(q)$ through the symmetry operation ϕ, and calculate its derivative. Since a function and its square have the same extrema, we shall rather calculate the derivative of the square of the distance function. In order to give a general formula, useful for crystallographic applications, we consider a more general, uncurved, coordinate system x in the Euclidean space, in which the metric tensor is still constant, but not necessarily diagonal. Such a situation occurs, *e.g.*, in the monoclinic or triclinic systems. In any coordinate system for which the metric tensor is constant, a Euclidean isometry ϕ may be written in components as

$$x'^i = \sum_{j=1}^{n} f^i_{\ j}\, x^j + s^i,$$

where $f^i_{\ j}$ is the component $(i;\ j)$ of a matrix F of determinant ± 1 and s^i is the component i of $s \in \mathbb{R}^n$. The distance between a point q and its image $q' = \phi(q)$ is simply the length of the straight line linking these two points; its square is

$$\begin{aligned}&\mathrm{dist}^2(q;\ \phi(q))\\ &\quad = \sum_{i,j=1}^{n}\left(\sum_{k=1}^{n}(f^i_{\ k} - \delta^i_{\ k})\, x_q^{\ k} + s^i\right)\left(\sum_{l=1}^{n}(f^j_{\ l} - \delta^j_{\ l})\, x_q^{\ l} + s^j\right) g_{ij},\end{aligned}$$

where g_{ij} is the component $(i;\ j)$ of the constant metric tensor. To find the minimum of this distance function, we need to calculate its directional derivative in the direction given by v, where v is the tangent vector at q of the straight line c linking q to $q' = \phi(q)$. This straight line, linearly parameterized between 0 and 1, is given by

$$\begin{aligned} c : [0;\ 1] &\to \mathbb{R}^n \\ t &\longmapsto c(t) = x_q + (x'_q - x_q)t. \end{aligned}$$

Notice that the distance function between q and $\phi(q)$ depends only on the coordinates of q, but not on those of $\phi(q)$. Thus, we can write $\mathrm{dist}(q;\ \phi(q)) \doteq \xi(u_q)$, where ξ is a function of u_q only. The directional derivative of ξ^2 in the direction v is thus

$$\begin{aligned} \partial_v \xi^2 &\doteq \frac{\mathrm{d}}{\mathrm{d}t}(\xi^2 \circ c)(t)\Big|_{t=0} \\ &= \sum_{m=1}^{n} \partial_m \xi^2\big(c(t)\big)\, \frac{\mathrm{d}c^m(t)}{\mathrm{d}t}\Big|_{t=0} \\ &= \sum_{m=1}^{n} \partial_m \xi^2(x_q)\,(x_{q'}^{\ m} - x_q^{\ m}), \end{aligned}$$

where

$$\begin{aligned} \partial_m \xi^2(x_q) &= \frac{\partial}{\partial x^m}\xi^2(x_q) \\ &= 2\sum_{i,j=1}^{n}(f^i_{\ m} - \delta^i_{\ m})\left(\sum_{k=1}^{n}(f^j_{\ k} - \delta^j_{\ k})\, x_q^{\ k} + s^j\right) g_{ij}, \end{aligned}$$

and

$$(x_{q'}^{\ m} - x_q^{\ m}) = \sum_{i=1}^{n}(f^m_{\ i} - \delta^m_{\ i})\, x_q^{\ i} + s^m.$$

Let us write $w^m = (x_{q'}^{\ m} - x_q^{\ m})$ and $a^i_{\ j} = (f^i_{\ j} - \delta^i_{\ j})$. Then

$$\partial_v \xi^2 = \sum_{i,j,m=1}^{n} a^i_{\ m} w^j g_{ij} w^m = \sum_{i,j,m=1}^{n} g_{ij} w^i a^j_{\ m} w^m.$$

To obtain the last equality, we have used the symmetry of the metric tensor, $g_{ij} = g_{ji}$, for all $1 \le i, j \le n$. The last expression may be written in compact matrix form:

$$\begin{aligned} \partial_v \xi^2 &= {}^{\mathrm{t}}\big(\nabla \xi^2(x_q)\big) w \\ &= {}^{\mathrm{t}}wGAw \\ &= {}^{\mathrm{t}}wG(F - I_n)w \\ &= {}^{\mathrm{t}}wGFw - {}^{\mathrm{t}}wGw, \end{aligned}$$

where $A = (a^i_{\ j})^n_{i,j=1}$, $w = (F - I_n)u_q + s$ and $G = {}^{\mathrm{t}}G$ is the matrix representing the constant metric tensor in the

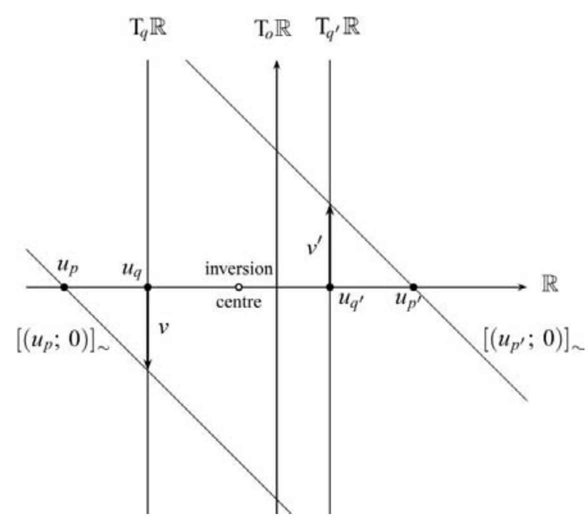

Figure 6
Illustration of the tangent-space representation of an isometry ϕ in the one-dimensional Euclidean space. Let ϕ be an inversion; then the differential map $\mathrm{d}\phi_q$ carries the vector v in the tangent space at q into the vector $v' = \mathrm{d}\phi_q(v)$ in the tangent space at $q' = \phi(q)$. With the tangent-bundle representation of p and p' (the equivalence classes $[(u_p;\ 0)]_\sim$ and $[(u_{p'};\ 0)]_\sim$), we see that the tangent-space representation of ϕ is completely equivalent to the usual manifold one.

coordinate system x. Indeed, $\sum_{m=1}^{n} a^j_m w^m = (Aw)^j$ (the component j of the vector Aw), hence $\sum_{i,j,m=1}^{n} g_{ij} a^j_m w^m w^i = \sum_{i,j=1}^{n} g_{ij} w^i (Aw)^j = {}^t wG(Aw) = {}^t wGAw$. The function ξ is minimal (it can never be maximal, unless in a pure translation, where it is constant) if

$$\partial_v \xi^2 = {}^t wGFw - {}^t wGw = {}^t wG(F - I_n)w = 0. \qquad (3)$$

Note that $(F - I_n)w$ can never be perpendicular to w unless $w = 0$. Let us find all the points satisfying this equation; several different cases may be distinguished:

(i) $w = 0$ and $F = I_n$. Then

$$w = s = 0.$$

The symmetry operation is the identity.

(ii) $w = 0$ and $F \neq I_n$. The symmetry operation has at least one fixpoint. Indeed, we have

$$w = (F - I_n)x_q + s = 0 \;\Leftrightarrow\; Fx_q + s = x_q,$$

the equation of the fixpoint(s) of the symmetry operation.

(iii) $w \neq 0$ and $F \neq I_n$. Then ${}^t wG(F - I_n)w = 0$ if and only if $(F - I_n)w = 0$. Let $P \in \mathrm{GL}_n(\mathbb{R})$ be a transformation matrix such that $PFP^{-1} \doteqdot U$ is an orthogonal matrix, which may be written in the irreducible form (Engel, 1986)

$$U = \left(\begin{array}{ccc|ccc} \pm 1 & & 0 & & & \\ & \ddots & & & 0 & \\ 0 & & \pm 1 & & & \\ \hline & & & U_1 & & 0 \\ & 0 & & & \ddots & \\ & & & 0 & & U_m \end{array}\right), \qquad (4)$$

where

$$U_i = \begin{pmatrix} \cos\theta_i & -\sin\theta_i \\ \sin\theta_i & \cos\theta_i \end{pmatrix}, \quad 1 \leq i \leq m.$$

θ_i is supposed to be different from $k\pi$, $k \in \mathbb{Z}$, as otherwise U_i would be equal to $\pm I_2$ and would in fact be a part of the first block of the matrix U. In our case, at least one of the values of this first block is necessarily +1, as otherwise U would be invertible and this would correspond to the previous case, where $w = 0$. Suppose that the number of values +1 is r. Thus, we have

$$\begin{aligned} (F - I_n)w = 0 &\Leftrightarrow P(F - I_n)P^{-1}Pw = 0 \\ &\Leftrightarrow (U - I_n)Pw = 0, \end{aligned}$$

with

$$U - I_n = \left(\begin{array}{c|c} 0_r & 0_{r\times(n-r)} \\ \hline 0_{(n-r)\times r} & B \end{array}\right),$$

where B is an invertible $(n-r)\times(n-r)$ matrix. Right multiplication of the last equation above by P gives

$$\begin{aligned} &(F - I_n)w = 0 \\ &\Leftrightarrow P(F - I_n)w = 0 \\ &\Leftrightarrow P(F - I_n)\big((F - I_n)x_q + s\big) = 0 \\ &\Leftrightarrow P(F - I_n)P^{-1}\big(P(F - I_n)P^{-1}Px_q + Ps\big) = 0 \\ &\Leftrightarrow (U - I_n)^2 Px_q + (U - I_n)Ps = 0. \end{aligned}$$

Let us now write the following decomposition:

$$Px_q = \begin{pmatrix} (Px_q)_\parallel \\ (Px_q)_\perp \end{pmatrix}, \quad Ps = \begin{pmatrix} (Ps)_\parallel \\ (Ps)_\perp \end{pmatrix},$$

where $(Px_q)_\parallel$ and $(Ps)_\parallel$ contain the first r components of Px_q and Ps, respectively, and $(Px_q)_\perp$ and $(Ps)_\perp$ the last $n - r$ ones. From the last equation above, we obtain the following condition:

$$B(Px_q)_\perp + (Ps)_\perp = 0. \qquad (5)$$

Thus, it can be concluded that every point q of which the coordinates x_q satisfy the expression

$$(Px_q)_\perp = B^{-1}(Ps)_\perp \qquad (6)$$

has a minimal distance to its image. Note that relation (6) consists of $n - r$ linearly independent equations which can be seen as constraints on the n coordinates of the point; this means that r of the n coordinates of the point are free, they may be chosen arbitrarily. Equation (5) shows that each of these constraints may be written as $f(x) = 0$ (where f is a function of x). As P and B are invertible matrices, all the gradients of each of these functions are linearly independent. Thus, we can say that the set

$$N = \{q \in \mathbb{R}^n \mid B(Px_q)_\perp + (Ps)_\perp = 0\}$$

is a submanifold of $\mathbb{R}^n$ of dimension r. Every point q of N is such that its image under the symmetry operation stays in N. Indeed, if $x_{q'} = Fx_q + s$, then

$$Px_{q'} = PFx_q + Ps = PFP^{-1}Px_q + Ps = UPx_q + Ps$$

and

$$\begin{aligned} (Px_{q'})_\perp &= (UPx_q)_\perp + (Ps)_\perp \\ &= (B + I_{(n-r)})(Px_q)_\perp + (Ps)_\perp \\ &= -(Ps)_\perp + (Px_q)_\perp + (Ps)_\perp \\ &= (Px_q)_\perp; \end{aligned}$$

the coordinates of the point $q \in N$ and its image are such that $(Px_{q'})_\perp = (Px_q)_\perp$, which means that both satisfy relation (5). The corresponding symmetry operation has no fixed point and it is not a pure translation either, as the matrix part is not supposed to be equal to the identity.

(iv) $w \neq 0$ and $F = I_n$. The corresponding symmetry operation is a pure translation. Indeed, we have

$$w = s \neq 0.$$

The derivations just presented here are treated in several textbooks, for instance in the monograph written by D. Schwarzenbach and G. Chapuis (Schwarzenbach & Chapuis, 2006), or that of H. Burzlaff and H. Zimmermann (Burzlaff &

Zimmermann, 1977). However, the concepts used to obtain them are completely different. Thus, some new definitions of notions commonly used in crystallography may be proposed:

Definition 1. A symmetry element of a Euclidean symmetry operation is the submanifold N of the Euclidean manifold consisting of all points such that the distance between one of these points and its image is minimal. This submanifold is invariant under the symmetry operation (it corresponds to its image).

Definition 2. The intrinsic translation of a Euclidean symmetry operation is the element $w = x_{q'} - x_q = (F - I_n)\,x_q + s$, where $q \in N$ and $q' = \phi(q)$. It may be considered the tangent vector at q of the straight line linearly parameterized between 0 and 1, linking q to $q' = \phi(q)$.

(i) A symmetry operation ϕ for which

$$\min_{q\in\mathbb{R}^n} \operatorname{dist}\big(q;\ \phi(q)\big) = 0$$

is called a fixed-point operation.

(ii) A symmetry operation ϕ for which

$$\min_{q\in\mathbb{R}^n} \operatorname{dist}\big(q;\ \phi(q)\big) = c > 0$$

is called an operation without a fixed point.

Consequence. As $\phi(q) = q' \in N$ when $q \in N$, the intrinsic translation $w = x_{q'} - x_q$ can never be perpendicular to N, it is always contained in N. Roughly speaking, we can say that it is the 'minimal vector of translation'. Any point q which is not in N is such that the distance between itself and its image $\phi(q)$ is bigger than the length of w. Any point in N is not under the effect of the matrix part of the operation, but only under the translation part, whereas a point out of N is under the effect of both.

These definitions are particularly interesting if we consider the tangent-space representation of a symmetry operation ϕ. Indeed, let us select a point q in the symmetry element N as a tangent point; then, the differential map $\mathrm{d}\phi_q : \mathrm{T}_q\mathbb{R}^n \to \mathrm{T}_{\phi(q)}\mathbb{R}^n$ carries vectors of the tangent space at a point of N to the tangent space at another point of N, and $x_{q'} - x_q$ corresponds to the intrinsic translation of ϕ. Thus, we obtain the precise intrinsic characteristics of the operation in a clear and simple way, without resorting to any change of coordinates! We therefore understand why the translation part s does not correspond to the intrinsic translation when the origin of the coordinate system is not in the symmetry element N. Indeed, every point p of $\mathbb{R}^n$ may be seen as the tip of a vector v linking the origin to itself. The image of p is then simply the image of v (through the differential map of the operation) the initial point of which is at the image of the origin point. When the origin point is in N, it is only under the effect of the intrinsic translation of the symmetry operation and it is this translation which appears in the image of the point p:

$$x_o = 0 \quad \text{and} \quad x_{o'} = w$$
$$x_p = v \quad \text{and} \quad x_{p'} = Fv + w.$$

When the origin is not in N, it is under the effect of both parts of the operation, hence the origin and its image are not linked by 'the minimal vector of translation' w. The intrinsic translation neither appears in the image of the origin, nor in the image of any point p:

$$x_o = 0 \quad \text{and} \quad x_{o'} = s$$
$$x_p = v \quad \text{and} \quad x_{p'} = Fv + s.$$

As an example, let us consider the symmetry operation ϕ of the three-dimensional Euclidean space $\mathbb{R}^3$, written as

$$\underbrace{\begin{pmatrix} u'^1 \\ u'^2 \\ u'^3 \end{pmatrix}}_{u'} = \underbrace{\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}}_{F} \underbrace{\begin{pmatrix} u^1 \\ u^2 \\ u^3 \end{pmatrix}}_{u} + \underbrace{\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}}_{s}, \qquad (7)$$

where $(u^1;\ u^2;\ u^3)$ is the natural coordinate system of $\mathbb{R}^n$. Some algebra shows that

$$w = (F - I_3)u + s = \begin{pmatrix} -u^1 + u^2 + 1 \\ u^1 - u^2 + 1 \\ -2u^3 + 1 \end{pmatrix}$$

is never equal to 0. We also see that $F \neq I_3$. This corresponds typically to the third case described above. For determining the symmetry element and the intrinsic translation, we can either use the technique developed above or, equivalently, calculate the set of points q such that the distance between q and $\phi(q)$ is minimal. Following the first method, we first need to derive the matrix P such that $U = PFP^{-1}$ has the form of the matrix in expression (4). This matrix is

$$P = \frac{1}{2}\begin{pmatrix} \sqrt{2} & \sqrt{2} & 0 \\ -\sqrt{2} & \sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Thus, we have

$$U = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

and

$$(U - I_n) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & -2 \end{pmatrix} \quad \text{with} \quad B \doteqdot \begin{pmatrix} -2 & 0 \\ 0 & -2 \end{pmatrix}.$$

Equation (5) becomes in this case:

$$\begin{pmatrix} \sqrt{2}(-u^1 + u^2) \\ 2u^3 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

We obtain $u^1 = u^2$ and $u^3 = \frac{1}{2}$. The symmetry element of this operation is then

$$N = \big\{q \in \mathbb{R}^3 \mid {u_q}^1 = {u_q}^2 \quad \text{and} \quad {u_q}^3 = \tfrac{1}{2}\big\}.$$

Finally, the intrinsic translation is

$$w = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}.$$

Thus, the symmetry operation given by relation (7) corresponds to a screw rotation, the submanifold N is the screw axis and w is the screw vector. It is quite likely that these results could have been derived faster using relation (3) directly.

3.2. Referring symmetry operations to any origin

After having obtained a general method for calculating the intrinsic translation of a symmetry operation, let us now derive the expression of a particular operation in a (natural) coordinate system with an arbitrary origin. Assuming that the matrix and translation parts are known, we shall use the tangent-bundle representation of a point for this task. Recall that in the Euclidean manifold a point p of coordinates u_p is represented, in the tangent bundle, as

$$(u_p - v;\ v),$$

where $v \in \mathbb{R}^n$ is a parameter which is in fact a vector of the tangent space at the point q of coordinates $u_p - v$. Also remember (Kocian *et al.*, 2009) that the image of a point p under a Euclidean symmetry operation ϕ may be written as

$$\phi(u_p) = \phi(u_p - v + v) = \phi(u_p - v) + \mathrm{d}\phi_q(v). \qquad (8)$$

If we consider v and $\mathrm{d}\phi_q(v)$ as elements of tangent spaces, relation (8) must be written as

$$\mathrm{d}\phi_q : (u_p - v;\ v) \longmapsto \big(\phi(u_p - v);\ \mathrm{d}\phi_q(v)\big).$$

As v is a free parameter, $\mathrm{d}\phi_q$ (where $u_q = u_p - v$) is a map not only between one but between any tangent space and its image. We then write $\mathrm{d}\phi$ instead of $\mathrm{d}\phi_q$, which thus becomes a map on the tangent bundle. Interestingly, it carries the equivalence class of any point to the equivalence class of its image. Indeed, this can be shown by considering the representation of ϕ and $\mathrm{d}\phi_q$ in coordinates:

$$u' = Fu + s \quad \text{and} \quad v' = Fv.$$

Then

$$\mathrm{d}\phi : \begin{pmatrix} u_p - v \\ v \end{pmatrix} \longmapsto \begin{pmatrix} F(u_p - v) + s \\ Fv \end{pmatrix}, \qquad (9)$$

where $F(u_p - v) + s = (Fu_p + s) - Fv$. Thus

$$\big(F(u_p - v) + s;\ Fv\big)$$

belongs to the equivalence class of $(Fu_p + s;\ 0)$. $\mathrm{d}\phi$, such as represented in expression (9), is called the tangent-bundle representation of the symmetry operation ϕ, since it carries the tangent-bundle representation of a point (the equivalence class of a point) into the tangent-bundle representation of its image (the equivalence class of the image). In matrix notation $\mathrm{d}\phi$ becomes

$$\begin{pmatrix} u_p - v \\ v \end{pmatrix} \longmapsto \begin{pmatrix} F & 0_n \\ 0_n & F \end{pmatrix} \begin{pmatrix} u_p - v \\ v \end{pmatrix} \begin{pmatrix} s \\ 0 \end{pmatrix}. \qquad (10)$$

In order to motivate and illustrate the considerations above, we take the example of an isometry ϕ in the two-dimensional Euclidean manifold $\mathbb{R}^2$ endowed with the natural coordinate system $u = (u^1;\ u^2)$. Let ϕ be a glide plane, *i.e.* a reflection through the mirror line $(u^1;\ u^1)$ cutting u^1 at a, followed by the translation $(b;\ b)$. As the translation is parallel to the mirror line, it corresponds to the intrinsic translation. The aim is to derive the matrix and translation part of this glide plane in the coordinate system $(u^1;\ u^2)$. The matrix part F is

$$F = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

To obtain the translation part, we could perform a change of coordinates in order to have the new origin on the symmetry element, work out the expression of the isometry in this new coordinate system, and return to the previous one. This traditional method is perfectly correct, but long and cumbersome. By using the tangent-bundle representations of points and symmetry operations, we can reach the same result without carrying out any change of coordinates at all. Indeed, let o be the origin of the coordinate system, the coordinates of which are $u_o = (0;\ 0)$. Its tangent-bundle representation is $(-v^1,\ -v^2;\ v^1,\ v^2)$, $v = (v^1;\ v^2) \in \mathbb{R}^2$. Through $\mathrm{d}\phi$, it becomes

$$\begin{pmatrix} -v^1 \\ -v^2 \\ v^1 \\ v^2 \end{pmatrix} \longmapsto \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} -v^1 \\ -v^2 \\ v^1 \\ v^2 \end{pmatrix} + \begin{pmatrix} s^1 \\ s^2 \\ 0 \\ 0 \end{pmatrix}.$$

Let $-v = (a;\ 0)$. The point q, such that $u_q = -v = (a;\ 0)$, lies on the glide plane; its image is then obtained by adding the intrinsic translation to its coordinates: $u_{q'} = (a;\ 0) + (b;\ b) = (a + b\,;\ b)$. Thus, we have the equation

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ 0 \end{pmatrix} + \begin{pmatrix} s^1 \\ s^2 \end{pmatrix} = \begin{pmatrix} a + b \\ b \end{pmatrix},$$

from which we derive

$$\begin{pmatrix} s^1 \\ s^2 \end{pmatrix} = \begin{pmatrix} a + b \\ -a + b \end{pmatrix},$$

the translation part of the isometry in the coordinate system under consideration.

This example shows the importance of the points defining the symmetry element of a Euclidean isometry. Thanks to them, it is possible to obtain the image of any point without knowing the translation part s. Moreover, a relation between the translation part s and the intrinsic translation w can easily be derived. Indeed, for any point q with coordinates u_q, lying on the symmetry element of an isometry ϕ, its image through this isometry can be written as $Fu_q + s$, as well as $u_q + w$, where F, s and w are, respectively, the matrix part, the translation part and the intrinsic translation of ϕ. The first expression is the usual one for the image of any point under the isometry, while the second is a consequence of the fact that q belongs to the symmetry element. Thus, equalizing these two forms, we obtain

$$
\begin{aligned}
Fu_q + s &= u_q + w \\
&\Leftrightarrow s = (I_n - F)u_q + w. \qquad (11)
\end{aligned}
$$

The coordinates of the image of any point p, with coordinates u_p, are then

$$Fu_p + (I_n - F)u_q + w.$$

Indeed,

$$
\begin{aligned}
Fu_p + s = F(u_q + v) + s &= Fu_q + s + Fv \\
&= u_q + w + Fv = u_q + w + F(u_p - u_q) \\
&= Fu_p + (I_n - F)u_q + w.
\end{aligned}
$$

The tangent-bundle representations of points and Euclidean isometries are very useful tools, because they offer a framework which is independent of the choice of origin. Even without performing any change of origin, we can obtain the representation of an isometry as if the origin lay at any other place, *e.g.* on the symmetry element. We have already seen that any isometry appears not only as a map in the Euclidean manifold, but also as a linear map between two tangent spaces. In the tangent-bundle formalism, it now also manifests itself as a map from a tangent space into itself. Indeed, let p be a point with coordinates u_p and ϕ an isometry. The tangent-bundle representation of p is given by $(u_p - v;\ v)$, where $v \in \mathbb{R}^n$, and is transformed, through $d\phi$, according to

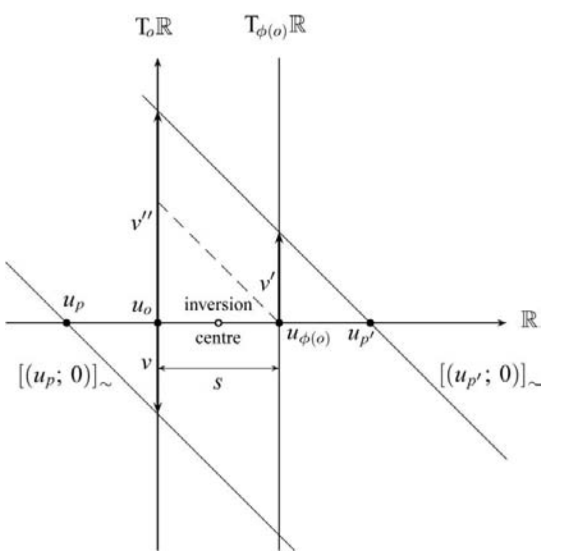

Figure 7
In coordinates, the inversion operation ϕ, with inversion centre at $(a;\,0)$ (in the tangent bundle), is written as $u' = -u + s$, where $s\ (= 2a \in \mathbb{R}_+)$ is the translation part, which in fact corresponds to the distance between the tangent space $T_o\mathbb{R}$ at the origin o and the tangent space $T_{\phi(o)}\mathbb{R}$ at the image of the origin $\phi(o)$. In the tangent-space representation of this operation, the vector $v \in T_o\mathbb{R}$ is carried into the vector $v' \in T_{\phi(o)}\mathbb{R}$. Thanks to the equivalence relation $\sim$ on the tangent bundle, $v' \in T_{\phi(o)}\mathbb{R}$ is equivalent to the vector $v'' \in T_o\mathbb{R}$. The length of this vector v'' is nothing else than the sum of the length of v' (which is equal to the length of v) and the translation part s. The value of v'' then corresponds to that of u_p. Thus, we can write $v'' = -v' + s$, which is the same formula as for the coordinate u in the manifold.

$$
\begin{array}{ccc}
T_q\mathbb{R}^n & \longrightarrow & T_{\phi(q)}\mathbb{R}^n \\
\begin{pmatrix} u_q \\ v \end{pmatrix} & \longmapsto & \begin{pmatrix} Fu_q + s \\ Fv \end{pmatrix},
\end{array}
$$

where $u_q = u_p - v$, and F and s are, respectively, the matrix and translation parts of ϕ. With the equivalence relation $\sim$, we obtain the equivalent image point in the tangent space at q:

$$
\begin{pmatrix} Fu_q + s \\ Fv \end{pmatrix} \sim \begin{pmatrix} Fu_q + s - \big((F - I_n)u_q + s\big) \\ Fv + \big((F - I_n)u_q + s\big) \end{pmatrix} = \begin{pmatrix} u_q \\ Fv + s' \end{pmatrix},
$$

where $s' = (F - I_n)u_q + s$. Thus, we effectively obtain a map which transforms a vector $v \in T_q\mathbb{R}^n$ into the element $Fv + s' \in T_q\mathbb{R}^n$. In particular, in the case of the tangent space at the real origin o of the coordinate system, we obtain

$$
\begin{array}{ccc}
T_o\mathbb{R}^n & \longrightarrow & T_{\phi(o)}\mathbb{R}^n \\
\begin{pmatrix} 0 \\ v \end{pmatrix} & \longmapsto & \begin{pmatrix} s \\ Fv \end{pmatrix},
\end{array}
$$

and the equivalence relation $\sim$ affords

$$
\begin{pmatrix} s \\ Fv \end{pmatrix} \sim \begin{pmatrix} 0 \\ Fv + s \end{pmatrix},
$$

whence $Fv + s$ is seen to be the image of v in $T_o\mathbb{R}^n$. So, an important corollary emerges: Since the image of v *in the tangent space* $T_o\mathbb{R}^n$, namely $Fv + s$, has exactly the same form as the image, under ϕ, of an arbitrary point p of coordinates u_p *in the manifold* $\mathbb{R}^n$, namely $Fu_p + s$, the Euclidean manifold and its tangent space at the origin become truly indistinguishable! A conceptual difference remains, however: the Euclidean space is a manifold and its tangent space at the origin is a vector space. Euclidean isometries are affine maps in the Euclidean manifold and linear maps between tangent spaces. The translation part s appearing in the expression above is due to the equivalence relation $\sim$, which offers the possibility of going back to the original tangent space. Fig. 7 illustrates this point for a one-dimensional Euclidean manifold.

3.3. The modulated case

Recall that for the geometrical description of modulated structures we consider a manifold M, parameterized by the one-to-one function $H : \mathbb{R}^n \to M$, such that $M \subset \mathbb{R}^n$ and $\mathbb{R}^n \subset M$. Any symmetry operation of a modulated structure $\tilde{\mathcal{S}}$ can be written as $\tilde{\phi} \doteqdot H \circ \phi \circ H^{-1}$, where ϕ is a Euclidean isometry, thus a symmetry operation of the corresponding average structure $\mathcal{S}$ in the Euclidean manifold. There is no need, therefore, for developing a formalism for finding the symmetry element and the intrinsic translation of an operation in this case; they are simply obtained by applying, respectively, the parameterization H to the symmetry element and the intrinsic translation of the corresponding Euclidean isometry ϕ. Indeed, since a symmetry operation of a modulated structure is given by $\tilde{\phi} = H \circ \phi \circ H^{-1}$, where ϕ is a Euclidean isometry with symmetry element N and intrinsic translation w, then $H(N)$ is the symmetry element of $\tilde{\phi}$ and

$H(u_q + w) - H(u_q)$, where $q \in N$, its intrinsic translation. Thus, symmetry elements such as axes or mirrors are not straight lines or planes any more, and the intrinsic translation is not constant: it depends on the point $q \in N$. Note that this holds not only for symmetry operations of a structure $\tilde{\mathcal{S}}$, but also for any transformation from M to M which can be written as $H \circ \phi \circ H^{-1}$, where ϕ is a Euclidean isometry.

Let ϕ be a Euclidean symmetry operation of a structure $\mathcal{S}$ in the Euclidean space and $\tilde{\phi} = H \circ \phi \circ H^{-1} : M \to M$ be a symmetry operation of the corresponding modulated structure $\tilde{\mathcal{S}} = H(\mathcal{S})$ in the manifold M. Also let $H(q) \in M$ be a point with coordinates $H(u_q)$. Recall that the differential map $\mathrm{d}\tilde{\phi} = \mathrm{d}H \circ \mathrm{d}\phi \circ \mathrm{d}H^{-1}$ carries any vector $\tilde{v}$ in the tangent space at $H(q)$ to the vector $\mathrm{d}\tilde{\phi}(\tilde{v})$ in the tangent space at the point $H(q')$ with coordinates $H(u_{q'}) = H(Fu_q + s)$, where F and s are, respectively, the matrix and translation parts of the isometry ϕ (see Fig. 8). Suppose that the point $\big(H(u_q);\ \tilde{v}\big)$ belongs to the equivalence class of $\big(H(u_p);\ 0\big)$, where p is a point with coordinates $H(u_p)$. This means that $\tilde{v} = \Omega(u_q)(u_p - u_q)$, where Ω is the matrix representing the differential map $\mathrm{d}H$. Considering $v \doteq u_p - u_q$ as a free n-dimensional parameter, $\mathrm{d}\tilde{\phi}_q$ becomes a function on the tangent bundle; as in the Euclidean case, we shall write $\mathrm{d}\tilde{\phi}$ instead of $\mathrm{d}\tilde{\phi}_q$. Fig. 8 illustrates the situation in the case where ϕ is an inversion operation.

The differential map $\mathrm{d}\tilde{\phi} = \mathrm{d}H \circ \mathrm{d}\phi \circ \mathrm{d}H^{-1}$ of $\tilde{\phi}$ carries the tangent-bundle representation (equivalence class) of any point of M to the tangent-bundle representation (equivalence class) of its image through $\tilde{\phi}$. Indeed,

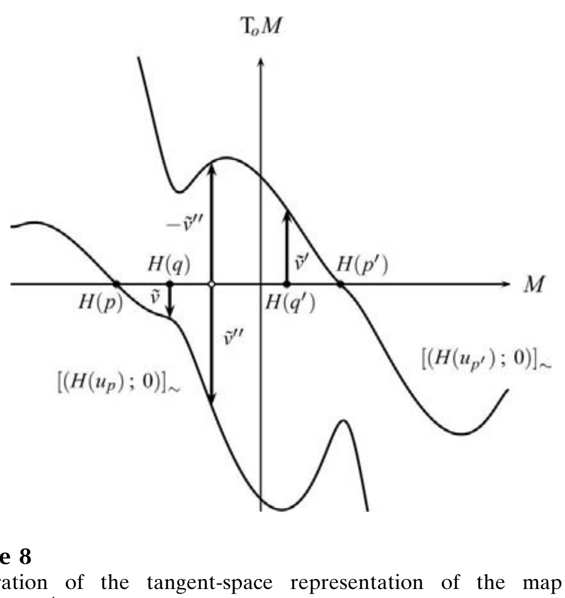

Figure 8
Illustration of the tangent-space representation of the map $\tilde{\phi} = H \circ \phi \circ H^{-1}$ in the one-dimensional manifold M parameterized by the map H, in the case where ϕ is an inversion operation. The differential map $\mathrm{d}\tilde{\phi}_q$ carries the vector $\tilde{v}$ in the tangent space at $H(q)$ into the vector $\tilde{v}' = \mathrm{d}\tilde{\phi}_{q'}(\tilde{v})$ in the tangent space at $H(q')$, the image point of q through $\tilde{\phi}$. When $H(q)$ is on the symmetry element, $\mathrm{d}\tilde{\phi}$ is an endomorphism of $\mathrm{T}_q M$, which implies that the image of the vector $\tilde{v}''$ is simply $-\tilde{v}''$. With the tangent-bundle representation of $H(p)$ and $H(p')$, we notice that the tangent-space representation of $\tilde{\phi}$ is completely equivalent to the usual manifold one.

$$\mathrm{d}\tilde{\phi} : \begin{pmatrix} H(u_p - v) \\ \Omega(u_p - v)v \end{pmatrix} \longmapsto \begin{pmatrix} H\big(F(u_p - v) + s\big) \\ \Omega\big(F(u_p - v) + s\big)Fv \end{pmatrix}, \qquad (12)$$

where F and s are, respectively, the matrix and translation parts of ϕ, and Ω is the matrix representing $\mathrm{d}H$. Then, writing $F(u_p - v) + s = (Fu_p + s) - Fv$, we have

$$\begin{pmatrix} H\big(F(u_p - v) + s\big) \\ \Omega\big(F(u_p - v) + s\big)Fv \end{pmatrix} \sim \begin{pmatrix} H\big(F(u_p - v) + s + Fv\big) \\ \Omega\big(F(u_p - v) + s + Fv\big)(Fv - Fv) \end{pmatrix};$$

the first component is equal to $H(Fu_p + s)$ and the second is 0. Thus

$$\big(H(Fu_p + s);\ \Omega\big(F(u_p - v) + s\big)Fv\big)$$

belongs to the equivalence class of $\big(H(Fu_p + s);\ 0\big)$.

4. Tangent-bundle representation of space groups

The choice of the origin in the representation of space groups is a recurring problem in crystallography. For any symmetry operation, it is convenient to place the origin on its symmetry element. Unfortunately, the different symmetry elements of the operations constituting a space group do not, in general, all intersect at one point. Therefore, one privileged point does not exist and compromises must be made. As mentioned in the introduction, privileged points do exist, namely those corresponding to sites of high symmetry (Niggli, 1919; Burzlaff & Zimmermann, 1980) but there might remain some symmetry elements not containing the high-symmetry points chosen as an origin. With the formalism developed in the previous section, this problem disappears, since any point can be selected as an origin, without changing the real origin of the coordinate system. Each symmetry operation can then be described with respect to its own 'origin' point lying on its symmetry element. Let us illustrate our method by the example of the specific space group $P2_1/c$.

In the second monoclinic setting, the space group considered is generated by a twofold screw axis along the b axis and a c-glide plane normal to b. In the coordinate system x adapted to the unit cell, the matrix and intrinsic translation parts of these two operations are

$$2_1 : \left\{ F_1 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix};\ w_1 = \begin{pmatrix} 0 \\ \frac{1}{2} \\ 0 \end{pmatrix} \right\}$$

and

$$c : \left\{ F_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix};\ w_2 = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix} \right\}.$$

We search for a point onto which to place the origin of our coordinate system. For this purpose, let us consider the origin point o, with coordinates $x_o = 0$, and the point q, of coordinates x_q lying at the intersection of the symmetry elements associated with the 2_1 and c operations. The tangent-bundle representation of o is simply $(-v;\ v)$, where $v \in \mathbb{R}^3$ is a parameter. Consider the case where $-v = x_q$. The image of the point $(x_q;\ -x_q)$ through the tangent-bundle representation of the 2_1 operation is

$$\begin{pmatrix} F_1 & 0_3 \\ 0_3 & F_1 \end{pmatrix}\begin{pmatrix} x_q \\ -x_q \end{pmatrix} + \begin{pmatrix} s_1 \\ 0 \end{pmatrix} = \begin{pmatrix} F_1 x_q + s_1 \\ -F_1 x_q \end{pmatrix},$$

where s_1 is the translation part of the operation 2_1 in the chosen coordinate system (with the chosen origin o). As q is in the symmetry element of 2_1, the coordinates of its image are simply $x_q + w_1$. We then have

$$\begin{pmatrix} F_1 x_q + s_1 \\ -F_1 x_q \end{pmatrix} = \begin{pmatrix} x_q + w_1 \\ -F_1 x_q \end{pmatrix},$$

which is equivalent to

$$\begin{pmatrix} x_q \\ -F_1 x_q + w_1 \end{pmatrix},$$

and write the equivalence as

$$\begin{pmatrix} x_q + w_1 \\ -F_1 x_q \end{pmatrix} \sim \begin{pmatrix} x_q \\ -F_1 x_q + w_1 \end{pmatrix}.$$

The image of this last point of the tangent bundle, through the tangent-bundle representation of the c-glide plane is

$$\begin{pmatrix} F_2 & 0_3 \\ 0_3 & F_2 \end{pmatrix}\begin{pmatrix} x_q \\ -F_1 x_q + w_1 \end{pmatrix} + \begin{pmatrix} s_2 \\ 0 \end{pmatrix} = \begin{pmatrix} F_2 x_q + s_2 \\ -F_2 F_1 x_q + F_2 w_1 \end{pmatrix},$$

where s_2 is the translation part of c in the chosen coordinate system. As q is in the mirror plane, the coordinates of its image are $x_q + w_2$. We then obtain

$$\begin{pmatrix} F_2 x_q + s_2 \\ -F_2 F_1 x_q + F_2 w_1 \end{pmatrix} = \begin{pmatrix} x_q + w_2 \\ -F_2 F_1 x_q + F_2 w_1 \end{pmatrix}$$

and

$$\begin{pmatrix} x_q + w_2 \\ -F_2 F_1 x_q + F_2 w_1 \end{pmatrix} \sim \begin{pmatrix} x_q + w_2 + F_2 w_1 \\ -F_2 F_1 x_q \end{pmatrix}.$$

Scrutinizing the vector part of the equivalence class, we see that $-x_q$ is transfered to $-F_2 F_1 x_q = x_q$. This shows that the composition of the two operations corresponds to an inversion operation $\overline{1}$. Its symmetry element is located halfway between q and the point of coordinates $x_q + w_2 + F_2 w_1$. Crystallographers favour the inversion centre at the origin. In this case, $x_q + w_2 + F_2 w_1$ must be equal to $-x_q$. The coordinates of q must then be

$$x_q = -\frac{1}{2}(F_2 w_1 + w_2) = \begin{pmatrix} 0 \\ \frac{1}{4} \\ -\frac{1}{4} \end{pmatrix};$$

they indicate the intersection of the axis and the mirror plane. A comparison with *International Tables for Crystallography* Volume A (2002) shows that our result is in agreement with the space-group information. Note that the coordinates of the point q were obtained without calculating s_1 and s_2, namely by simply exploiting the intrinsic characteristics of each symmetry operation. If we require the full symmetry operations in the chosen coordinate system, however, we need to know the translations part s. This can be found using relation (11). We have

$$s_1 = -(F_1 - I_3)x_q + w_1 = \begin{pmatrix} 0 \\ \frac{1}{2} \\ -\frac{1}{2} \end{pmatrix},$$

$$s_2 = -(F_2 - I_3)x_q + w_2 = \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix};$$

and the translation part s_3 of the inversion operation is, of course, zero. We can now write the tangent-bundle representation of these three symmetry operations. For any point p, with coordinates u_p, we have

$$\begin{aligned} 2_1 \ : \ \begin{pmatrix} u_p - v \\ v \end{pmatrix} &\longmapsto \begin{pmatrix} F_1 & 0_3 \\ 0_3 & F_1 \end{pmatrix}\begin{pmatrix} u_p - v \\ v \end{pmatrix} + \begin{pmatrix} s_1 \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} F_1(u_p - v) + s_1 \\ F_1 v \end{pmatrix}, \\ c \ : \ \begin{pmatrix} u_p - v \\ v \end{pmatrix} &\longmapsto \begin{pmatrix} F_2 & 0_3 \\ 0_3 & F_2 \end{pmatrix}\begin{pmatrix} u_p - v \\ v \end{pmatrix} + \begin{pmatrix} s_2 \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} F_2(u_p - v) + s_2 \\ F_2 v \end{pmatrix}, \\ \overline{1} \ : \ \begin{pmatrix} u_p - v \\ v \end{pmatrix} &\longmapsto \begin{pmatrix} -I_3 & 0_3 \\ 0_3 & -I_3 \end{pmatrix}\begin{pmatrix} u_p - v \\ v \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} -(u_p - v) \\ -v \end{pmatrix}. \end{aligned}$$

In these representations, any point p is seen as the tip of a tangent vector at the 'origin' point q, with coordinates $u_q = u_p - v$. As $v \in \mathbb{R}^3$ is a free parameter, we can choose any point q as an origin of the manifold and then apply this tangent-bundle representation of symmetry operations. In each case, the final result, the image in the manifold, is always the same. This viewpoint is particularly friendly if for each operation an appropriate origin point is selected. Indeed, if for each symmetry operation we consider as an origin a point on its symmetry element, the image of any point has a very simple expression where only the intrinsic characteristics of the operation appear. In our example, selecting q, with coordinates $u_q = (0;\ \frac{1}{4};\ -\frac{1}{4})$, as an origin for the 2_1 and c operations, and the point o, with coordinates $u_o = (0;\ 0;\ 0)$, as an origin for the $\overline{1}$ operation, we obtain

$$\begin{aligned} 2_1 \ &: \ \begin{pmatrix} u_q \\ u_p - u_q \end{pmatrix} \longmapsto \begin{pmatrix} u_q + w_1 \\ F_1(u_p - u_q) \end{pmatrix}, \\ c \ &: \ \begin{pmatrix} u_q \\ u_p - u_q \end{pmatrix} \longmapsto \begin{pmatrix} u_q + w_2 \\ F_2(u_p - u_q) \end{pmatrix}, \\ \overline{1} \ &: \ \begin{pmatrix} 0 \\ u_p \end{pmatrix} \longmapsto \begin{pmatrix} 0 \\ -u_p \end{pmatrix}. \end{aligned}$$

Not one, but two different origins are chosen for the tangent-bundle representation of our three symmetry operations. This does not create a problem whatsoever; on the contrary, it furnishes the possibility of describing each symmetry operation in a representation in which only its intrinsic characteristics appear.

Finally, note that in the space group $P2_1/c$, there are more than one inversion centre, more than one twofold axis and more than one glide plane per cell. The others are products of the three operations above with lattice translations, and their symmetry elements are obtained by using the technique of minimizing the distance between a point and its image.

5. Conclusion

As concluded in our previous article (Kocian *et al.*, 2009), differential geometry is the tool of choice for treating geometrical and symmetry aspects of crystals. The notion of tangent space is truly fundamental, because it provides an infinity of different origin points, being devoid of the necessity to change the real origin of the coordinate system.

The equivalence relation defined on the tangent bundle of a manifold is also an essential concept for the transition from the representation in one tangent space to that in another one. In fact, in the Euclidean case, the tangent-space representation of a point can be interpreted as the position of the point in the Euclidean manifold with respect to a Cartesian coordinate system with any other origin. This is the reason why we say that an infinity of different possible origins exist.

Owing to the tangent-space representation of symmetry operations, we can propose novel, more general definitions of a symmetry element and the intrinsic translation part of a symmetry operation. These definitions are simple, as they rely only on the concept of the minimization of the distance between a point and its image.

Finally, the combination of the equivalence class of a point and the tangent-space representation of a symmetry operation creates a formalism in which symmetry operations can be expressed relative to any origin. Several symmetry operations can be referred to different origin points without causing any difficulties. Thus, each symmetry operation can be written in such a way that its intrinsic characteristics (notably the intrinsic translation part) are revealed without effectively changing the real origin of the chosen coordinate system. We therefore have an ‘origin-less’ description of symmetry operations and space groups.

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