A mathematical model for diamond-type crystals

1995 J. Phys. A: Math. Gen. 28 1371

(http://iopscience.iop.org/0305-4470/28/5/022)

J. Phys. A: Math. Gen. 28 (1995) 1371–1379. Printed in the UK

A mathematical model for diamond-type crystals

N Cotfas†

Department of Mathematics, Faculty of Physics, University of Bucharest, PO Box 76-54, *Bucharest, Romania*

Received 14 October 1994

Abstract. The physical phenomena occuring in a diamond-type crystal are usually described in terms of the invariants of some representations of the space group O_h^7. By choosing a new description, we obtain equivalent representations in which the expressions of the usual invariants are simpler.

The mathematical facilities obtained by using these representations offer new possibilities for elaborating improved variants of the usual theories or extensions from perfect crystals to crystals with impurities or defects.

1. Introduction

The diamond-type crystals are among the most widely discussed crystals in literature, and the usual theories supply results in good agreement with the experiment [1–24]. These theories are formulated in terms of the invariants of some representations of the space group O_h^7 [25–28], but generally the mathematical expressions of these invariants are not simple. We think that the crystals having diamond or zincblende structure are important enough to justify the utilization (beside the classical description) of a specific description in which the mathematical objects (equations, operators, etc) with physical significance have a simple obviously O_h^7-invariant form. To obtain this description we use a four-axes description very similar to the well known four-axes description one uses in the case of the hexagonal lattice [29].

To illustrate the mathematical facilities offered by the representations of O_h^7 obtained by using this description, we consider some classes of invariants which generalize certain invariants used in the actual theories.

We think that such mathematical objects allow us to obtain improved variants for the existing theories, new extensions of these theories from perfect crystals to crystals with impurities or defects, new theories, etc.

2. Some representations of the space group O_h^7

Let $\mathbb{Z}$ be the ring of integers, and let $\mathbb{N}$ be the set of all natural numbers. The metric space $(\mathbb{D}_\infty, \delta)$, where

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

† E-mail: cotfas@roifa.bitnet (or cotfas@ifa.ro).

0305-4470/95/051371+09$19.50

and

$$\delta : \mathbb{D}_\infty \times \mathbb{D}_\infty \to \mathbb{N}, \qquad \delta(n, n') = \sum_{j=0}^{3} |n_j - n'_j| \tag{2}$$

is a mathematical model for the 'infinite' crystal having the structure of diamond ($n' \in \mathbb{D}_\infty$ is a neighbour of order k of $n \in \mathbb{D}_\infty$ if $\delta(n, n') = k$) [30–32].

The group of all isometries of the space $(\mathbb{D}_\infty, \delta)$, that is, the group of all transformations $g : \mathbb{D}_\infty \to \mathbb{D}_\infty$ such that

$$\delta(g(n), g(n')) = \delta(n, n') \tag{3}$$

for all $n, n' \in \mathbb{D}_\infty$, is isomorphic to the space group O_h^7 [30]. This group, denoted also by O_h^7 (it can be regarded as a faithful representation of O_h^7 as a group of permutations of the set $\mathbb{D}_\infty$), is the group generated by the transformations

$$\begin{aligned} &\Lambda, \Lambda_\sigma : \mathbb{D}_\infty \to \mathbb{D}_\infty \\ &\Lambda(n_0, n_1, n_2, n_3) = (-n_0 + 1, -n_1, -n_2, -n_3) \\ &\Lambda_\sigma(n_0, n_1, n_2, n_3) = (n_{\sigma(0)}, n_{\sigma(1)}, n_{\sigma(2)}, n_{\sigma(3)}) \end{aligned} \tag{4}$$

where

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

that is,

$$O_h^7 = \{g_1 \circ g_2 \circ \ldots \circ g_j \mid j \in \mathbb{N} \setminus \{0\}, g_1, g_2, \ldots, g_j \in \{\Lambda\} \cup \{\Lambda_\sigma \mid \sigma \in \Sigma_4\}\}. \tag{5}$$

We will use the relation (5) as a definition for the space group O_h^7.

Let $N \in \mathbb{N}$, $N > 3$, be a fixed natural number, and let $\mathbb{Z}_N$ be the quotient space $\mathbb{Z}/(N\mathbb{Z})$ whose elements are the cosets [33]

$$\begin{aligned} &0 = \{0 + kN \mid k \in \mathbb{Z}\} \\ &1 = \{1 + kN \mid k \in \mathbb{Z}\}, \ldots \\ &N - 1 = \{(N-1) + kN \mid k \in \mathbb{Z}\}. \end{aligned} \tag{6}$$

As usual, we denote

$$-k = N - k$$

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

We will obtain a mathematical model for the 'finite' crystal having the structure of diamond by using the set

$$\mathbb{D} = \{n = (n_0, n_1, n_2, n_3) \in (\mathbb{Z}_N)^4 \mid n_0 + n_1 + n_2 + n_3 \in \{0; 1\}\} \tag{7}$$

having $N' = 2N^3$ elements, instead of $\mathbb{D}_\infty$. The utilization of $\mathbb{Z}_N$ instead of $\mathbb{Z}$ is similar to the usual method based on the periodicity conditions.

For each $n \in \mathbb{D}$, we consider the elements

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

where

$$\varepsilon(n)=\begin{cases}1 & \text{if } n_0+n_1+n_2+n_3=0\\ -1 & \text{if } n_0+n_1+n_2+n_3=1\end{cases} \tag{9}$$

to be the first neighbours of n, the elements

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

where $j, k\in\{0, 1, 2, 3\}$, $j\neq k$, to be the second neighbours of n, the elements

$$n^{jkl}=((n^j)^k)^l$$

where $j, k, l\in\{0, 1, 2, 3\}$, $j\neq k\neq l$, to be the third neighbours of n, etc.

By using the formulae

$$\begin{aligned}&\Lambda, \Lambda_\sigma : \mathbb{D}\to\mathbb{D}\\ &\Lambda(n_0, n_1, n_2, n_3)=(-n_0+1, -n_1, -n_2, -n_3)\\ &\Lambda_\sigma(n_0, n_1, n_2, n_3)=(n_{\sigma(0)}, n_{\sigma(1)}, n_{\sigma(2)}, n_{\sigma(3)})\end{aligned} \tag{10}$$

we obtain a representation of O_h^7 as group of permutations of the set $\mathbb{D}$. The image of this representation will be also denoted by O_h^7, that is,

$$O_h^7=\{g_1\circ g_2\circ\ldots\circ g_j : \mathbb{D}\to\mathbb{D} \mid j\in\mathbb{N}\setminus\{0\}, g_1, \ldots, g_j\in\{\Lambda\}\cup\{\Lambda_\sigma \mid \sigma\in\Sigma_4\}\}. \tag{11}$$

The bijection

$$\begin{aligned}&\varphi : \mathbb{D}\to\varphi(\mathbb{D})\subset(\mathbb{Z}_N)^3\\ &\varphi(n_0, n_1, n_2, n_3)=(-n_0-n_1+n_2+n_3, -n_0+n_1-n_2+n_3, -n_0+n_1+n_2-n_3)\end{aligned} \tag{12}$$

establishes the correspondence between this description and a variant of the usual one [30, 31]. The usual description of O_h^7 in $\varphi(\mathbb{D})$ can be obtained by associating the transformation

$$\varphi\circ g\circ\varphi^{-1} : \varphi(\mathbb{D})\to\varphi(\mathbb{D}) \tag{13}$$

to each element $g\in O_h^7$, $g : \mathbb{D}\to\mathbb{D}$. The mathematical expression of the representation of O_h^7 in $\mathbb{D}$ is simpler than the expression of the corresponding representation in $\varphi(\mathbb{D})$.

The space $(\mathscr{H}, \langle .,. \rangle$, where

$$\begin{aligned}&\mathscr{H}=\{\psi : \mathbb{D}\to\mathbb{C} \mid \psi \text{ is a function}\}\\ &\langle\psi_1, \psi_2\rangle=\sum_{n\in\mathbb{D}}\psi_1(n)\,\overline{\psi_2(n)}\end{aligned} \tag{14}$$

is a Hilbert space isomorphic to the usual Hilbert space $\mathbb{C}^{N'}$. The formula

$$(T_g\psi)(n)=\psi(g^{-1}(n)) \tag{15}$$

where $n\in\mathbb{D}$, $g\in O_h^7$, defines a unitary representation of O_h^7 in $\mathscr{H}$.

The relations

$$\begin{aligned}&\Lambda(X_0, X_1, X_2, X_3)=(-X_0, -X_1, -X_2, -X_3)\\ &\Lambda_\sigma(X_0, X_1, X_2, X_3)=(X_{\sigma(0)}, X_{\sigma(1)}, X_{\sigma(2)}, X_{\sigma(3)})\end{aligned} \tag{16}$$

define a linear representation of the group O_h^7 in the vector space

$$\mathbb{L}=\{(X_0, X_1, X_2, X_3) \mid X_0+X_1+X_2+X_3=0\}$$

and the formula

$$(R_g X)(t, n) = g(X(t, g^{-1}(n))) \tag{17}$$

defines a linear representation of O_h^7 in the space of functions

$$\mathcal{V} = \left\{ X : \mathbb{R} \times \mathbb{D} \to \mathbb{L} \;\middle|\; \begin{array}{c} X \text{ is a function differentiable} \\ \text{with respect to } t \end{array} \right\}.$$

A mathematical object defined on a representation of O_h^7 is O_h^7-invariant if and only if it is invariant under the transformations corresponding to Λ and Λ_σ, for any $\sigma \in \Sigma_4$.

3. An application to lattice dynamics of diamond-type crystals

Let A be the equilibrium position of an atom of a crystal having the structure of diamond, and let A_0, A_1, A_2, A_3 be the equilibrium positions of the first neighbours of A. Since the point A is the centre of the regular tetrahedron $A_0A_1A_2A_3$, it follows that the unitary vectors e_0, e_1, e_2, e_3 corresponding to the oriented segments AA_0, AA_1, AA_2, AA_3 verify the relation

$$e_0 + e_1 + e_2 + e_3 = 0. \tag{18}$$

To describe the position P' at time t of the atom of the crystal whose equilibrium position is P, we use the element

$$(e_0 \cdot \boldsymbol{PP'}, e_1 \cdot \boldsymbol{PP'}, e_3 \cdot \boldsymbol{PP'}, e_2 \cdot \boldsymbol{PP'}) \in \mathbb{L}$$

that is, the orthogonal projections of the vector $\boldsymbol{PP'}$ on the four axes corresponding to the vectors e_0, e_1, e_2, e_3.

To describe the time evolution of the atoms of the crystal with respect to their equilibrium positions, we use a function $X \in \mathcal{V}$.

Let Φ_{jl}^{p}, Φ_{jl}^{pq} be real constants such that

$$\Phi_{jl}^{p} = \Phi_{\sigma(j)\sigma(l)}^{\sigma(p)} \qquad \Phi_{jl}^{pq} = \Phi_{\sigma(j)\sigma(l)}^{\sigma(p)\sigma(q)} \tag{19}$$

for all $j, l, p, q \in \{0, 1, 2, 3\}$, $p \neq q$, $\sigma \in \Sigma_4$, and let $m \in (0, \infty)$. The system of equations

$$m \frac{d^2}{dt^2} X_j(t, n) = \sum_{p=0}^{3} \sum_{l=0}^{3} \Phi_{jl}^{p} [X_l(t, n^p) - X_l(t, n)] + \sum_{p \neq q} \sum_{l=0}^{3} \Phi_{jl}^{pq} [X_l(t, n^{pq}) - X_l(t, n)] \tag{20}$$

where $j \in \{0, 1, 2, 3\}$, $n \in \mathbb{D}$, and

$$X : \mathbb{R} \times \mathbb{D} \to \mathbb{L}, \qquad X(t, n) = (X_0(t, n), X_1(t, n), X_2(t, n), X_3(t, n))$$

is an O_h^7-invariant system of equations. Indeed, it is invariant under the transformation Λ, and since

$$\Lambda_\sigma (X_j(t, \Lambda_\sigma^{-1}(n))) = (X_{\sigma(j)}(t, \Lambda_{\sigma^{-1}}(n))) \tag{21}$$

$$\Lambda_{\sigma^{-1}}(n^j) = (\Lambda_{\sigma^{-1}}(n))^{\sigma(j)} \tag{22}$$

for all $\sigma \in \Sigma_4$, $n \in \mathbb{D}$, $j \in \{0, 1, 2, 3\}$, it follows that the system (20) is invariant under the transformations Λ_σ.

Looking for solutions of the form

$$X_j(t,n)=\begin{cases} A_j \exp\left[i\left(\sum_{y=0}^{3} K_j n_j-\omega t\right)\right] & \text{if } \varepsilon(n)=1 \\ B_j \exp\left[i\left(\sum_{j=0}^{3} K_j n_j-\omega t\right)\right] & \text{if } \varepsilon(n)=-1 \end{cases} \tag{23}$$

where

$$K\in\mathscr{L}=\{K=(K_0,K_1,K_2,K_3)\in\mathbb{L}\,|\,K_j\in\{2\pi l/N|\,l\in\{0,1,2,\ldots,N-1\}\}\} \tag{24}$$

and (A_j), $(B_j)\in\mathbb{L}$, the system (18) becomes

$$\begin{aligned} m\omega^2 A_j &= -\sum_{p=0}^{3}\sum_{l=0}^{3}\Phi_{jl}^{p}[B_l\exp(iK_p)-A_l]-\sum_{p\neq q}\sum_{l=0}^{3}\Phi_{jl}^{pq}A_l[\exp(i(K_p-K_q))-1] \\ m\omega^2 B_j &= -\sum_{p=0}^{3}\sum_{l=0}^{3}\Phi_{jl}^{p}[A_l\exp(-iK_p)-B_l]-\sum_{p\neq q}\sum_{l=0}^{3}\Phi_{jl}^{pq}B_l[\exp(i(K_q-K_p))-1] \end{aligned} \tag{25}$$

where $j\in\{0,1,2,3\}$.

Since only six of these equations are independent and $\Sigma_{j=0}^{3}A_j=0$, $\Sigma_{j=0}^{3}B_j=0$, the system (25) is equivalent to the system

$$\begin{aligned} m\omega^2 A_j &= -\sum_{p=0}^{3}\sum_{l=1}^{3}(\Phi_{jl}^{p}-\Phi_{j0}^{p})[B_l\exp(iK_p)-A_l] \\ &\quad -\sum_{p\neq q}\sum_{l=1}^{3}(\Phi_{jl}^{pq}-\Phi_{j0}^{pq})A_l[\exp(i(K_p-K_q))-1] \\ m\omega^2 B_j &= -\sum_{p=0}^{3}\sum_{l=1}^{3}(\Phi_{jl}^{p}-\Phi_{j0}^{p})[A_l\exp(-iK_p)-B_l] \\ &\quad -\sum_{p\neq q}\sum_{l=1}^{3}(\Phi_{jl}^{pq}-\Phi_{j0}^{pq})B_l[\exp(i(K_q-K_p))-1] \end{aligned} \tag{26}$$

where $j\in\{1,2,3\}$.

The system of equations (20) corresponds to the system of equations used in lattice dynamics of diamond-type crystals (the model of Born–von Karman type) [1, 24, 34].

Particularly, for Φ_{jl}^{p}, Φ_{jl}^{pq} determined by using (19) and

$$\begin{bmatrix}\Phi_{00}^{0}\ldots\Phi_{03}^{0}\\ \Phi_{30}^{0}\ldots\Phi_{33}^{0}\end{bmatrix}=\begin{bmatrix}243.91 & 0 & 0 & 0\\ 0 & 157.17 & 43.37 & 43.37\\ 0 & 43.37 & 157.17 & 43.37\\ 0 & 43.37 & 43.37 & 157.17\end{bmatrix} \tag{27}$$

$$\begin{bmatrix}\Phi_{00}^{03}\ldots\Phi_{03}^{03}\\ \Phi_{30}^{03}\ldots\Phi_{33}^{03}\end{bmatrix}=\begin{bmatrix}22.8 & 7.28 & 7.28 & -14.8\\ 15.28 & 0 & 0 & 7.28\\ 15.28 & 0 & 0 & 7.28\\ -30.8 & 15.28 & 15.28 & 22.8\end{bmatrix} \tag{28}$$

the system of equations (20) corresponds to the system of equations used in the article

of Patel *et al.* [24] for the description of the lattice dynamics of the diamond crystal (the constants are in units of $N\,m^{-1}$.

By using (26) and the bijection

$$\begin{aligned}&\mathbb{R}^3\to\mathbb{L}\\&k=(x,y,z)\to K\\&\quad=((-x-y-z),(-x+y+z),(x-y+z),(x+y-z))\end{aligned}\tag{29}$$

we can re-obtain the dispersion curves for diamond in good agreement with experiment (see the figure presented in Patel's article).

In the usual description, the symmetry conditions (19) for the interaction constants and the system of equations (20) have complicated mathematical expressions, even in the case when we consider only interaction with first neighbours (one can see this case presented in detail in [34]).

We can extend our formalism to include interactions with the third, fourth, etc, neighbours without important complications.

4. An application to quasi-bound electron theory

Let $\alpha,\beta\in\mathbb{R}$ be two real constants. The operator

$$V:\mathscr{H}\to\mathscr{H}\qquad (V\psi)(n)=\alpha\psi(n)+\beta\sum_{j=0}^{3}\psi(n^j)\tag{30}$$

is a self-adjoint O_h^7-invariant operator. Indeed,

$$\begin{aligned}\langle V\psi_1,\psi_2\rangle&=\sum_{n\in\mathbb{D}}\left[\alpha\psi_1(n)+\beta\sum_{j=0}^{3}\psi_1(n^j)\right]\overline{\psi_2(n)}\\&=\sum_{n\in\mathbb{D}}\alpha\psi_1(n)\,\overline{\psi_2(n)}+\beta\sum_{j=0}^{3}\sum_{n\in\mathbb{D}}\psi_1(n^j)\,\overline{\psi_2(n)}\\&=\sum_{n\in\mathbb{D}}\alpha\psi_1(n)\,\overline{\psi_2(n)}+\beta\sum_{j=0}^{3}\sum_{n\in\mathbb{D}}\psi_1(n)\,\overline{\psi_2(n^j)}=\langle\psi_1,V\psi_2\rangle\end{aligned}\tag{31}$$

and since

$$\Lambda^{-1}(n^j)=(\Lambda^{-1}(n))^j\qquad \Lambda_\sigma^{-1}(n^j)=(\Lambda_\sigma^{-1}(n))^{\sigma(j)}\tag{32}$$

we get

$$T_g\circ V=V\circ T_g\tag{33}$$

for any $g\in O_h^7$.

In the case of an electron lying inside a diamond-type crystal and considered in the tight-binding approximation [35], one assume that the only possible positions of the electron are in the proximity of an atom of the crystal.

Denoting by $|n\rangle$ the wavefunction corresponding to the electron lying in the proximity of atom n, the general wavefunction is a superposition

$$\sum_{n\in\mathbb{D}}\psi(n)|n\rangle\tag{34}$$

where $\psi\in\mathscr{H}$.

For $\alpha=-4$ and $\beta=1$, the operator V considered above is similar to the discrete Laplacean one considers [36] on the space $l^2(\mathbb{Z}^3)$ used in the case of the crystals having the structure of a cubic lattice. In this sense, the operator V defined above is an operator of Schrödinger type.

Looking for eigenfunctions of V having the form

$$\psi_K:\mathbb{D}\to\mathbb{C}$$

$$\psi_K(n)=\begin{cases} a\exp\left(\mathrm{i}\sum_{j=0}^{3}K_jn_j\right) & \text{if } \varepsilon(n)=1 \\ b\exp\left(\mathrm{i}\sum_{j=0}^{3}K_jn_j\right) & \text{if } \varepsilon(n)=-1 \end{cases} \tag{35}$$

where $K=(K_0, K_1, K_2, K_3)\in\mathscr{L}$, $a, b\in\mathbb{C}$ are constants, the relation

$$V\psi_K=\lambda_K\psi_K$$

is equivalent with the system of equations

$$\begin{aligned} &\alpha a+\beta b\sum_{j=0}^{3}\exp(\mathrm{i}K_j)=\lambda_K a \\ &\alpha b+\beta a\sum_{j=0}^{3}\exp(-\mathrm{i}K_j)=\lambda_K b. \end{aligned} \tag{36}$$

It follows that the solutions

$$\lambda_K=\alpha\pm\beta\left|\sum_{j=0}^{3}\exp(\mathrm{i}K_j)\right| \tag{37}$$

of the equation

$$\begin{vmatrix} \alpha-\lambda_K & \beta\Sigma_{j=0}^{3}\exp(\mathrm{i}K_j) \\ \beta\Sigma_{j=0}^{3}\exp(-\mathrm{i}K_j) & \alpha-\lambda_K \end{vmatrix}=0 \tag{38}$$

are eigenvalues of V for any $K\in\mathscr{L}$. Particularly, if $K\in\mathscr{L}$ satisfies the relation

$$\sum_{j=0}^{3}\sin K_j=0 \tag{39}$$

then

$$\lambda_K=\alpha\pm\beta\sum_{j=0}^{3}\cos K_j \tag{40}$$

are eigenvalues of V.

The result obtained is in concordance with the existence of the energy bands. To include the interaction with the second neighbours, we can use the operator

$$V:\mathscr{H}\to\mathscr{H}\qquad (V\psi)(n)=\alpha\psi(n)+\beta\sum_{j=0}^{3}\psi(n^j)+\gamma\sum_{j\neq l}\psi(n^{jl}). \tag{41}$$

A more detailed description, is obtained by choosing the Hilbert space

$$\mathscr{H}'=\left\{\Psi:\mathbb{R}^3\times\mathbb{D}\to\mathbb{C}\;\middle|\;\sum_{n\in\mathbb{D}}\int_{\mathbb{R}^3}|\Psi(r,n)|^2\mathrm{d}r<\infty\,;\,\Psi(r,n)=0\text{ if }\|r\|\geqslant\frac{d}{2}\right\}\tag{42}$$

$$\langle\Psi_1,\Psi_2\rangle=\sum_{n\in\mathbb{D}}\int_{\mathbb{R}^3}\Psi_1(r,n)\,\overline{\Psi_2(r,n)}\,\mathrm{d}r\tag{43}$$

where d is the distance between the nearest atoms of the crystal, $\|(x,y,z)\|=(x^2+y^2+z^2)^{1/2}$ is the usual norm on $\mathbb{R}^3$, and by using a Hamiltonian of the form $H=H_a+V$, where H_a is the Hamiltonian of the isolated atom and

$$(V\Psi)(r,n)=\alpha\Psi(r,n)+\beta\sum_{j=0}^{3}\Psi(r,n^j)\tag{44}$$

describes the interaction with the neighbouring atoms.

If $K\in\mathscr{L}$, $\psi_a:\mathbb{R}^3\to\mathbb{C}$ is an eigenfunction of H_a

$$H_a\psi_a=E_a\psi_a\tag{45}$$

such that $\psi_a(r)=0$ for $\|r\|>d/2$, and $\psi_K:\mathbb{D}\to\mathbb{C}$ is an eigenfunction of V corresponding to the eigenvalue λ_K, then

$$\Psi:\mathbb{R}^3\times\mathbb{D}\to\mathbb{C}\qquad\Psi(r,n)=\psi_a(r)\cdot\psi_K(n)\tag{46}$$

is an eigenfunction of H corresponding to the eigenvalue $E=E_a+\lambda_K$. Hence the operator H has eigenvalues of the form

$$E=E_a+\alpha\pm\beta\left|\sum_{j=0}^{3}\exp(\mathrm{i}K_j)\right|\tag{47}$$

that is, each level E_a corresponds in the crystal to a band of levels of width $8|\beta|$ translated with α.

5. Conclusions

The considered representations of O_h^7 are more advantageous than the usual ones as regards the possibility of defining mathematical objects with a simple O_h^7-invariant form and their physical significance.

Generally speaking, the ideas presented can immediately be extended to zincblende-type crystals.

The correspondence between the proposed description and the usual one has a simple form, and we can choose in each situation the most convenient of them. These descriptions used together may offer significant advantages.

Acknowledgments

The author is grateful to Professor Stere Ianus (Bucharest University) and to Dr Jean-Louis Verger-Gaugry (LTPCM–Grenoble) for useful suggestions.

References

[1] Smith H M J 1948 *Phil. Trans. R. Soc.* A **241** 105
[2] Herman F 1952 *Phys. Rev.* **88** 1210
[3] Herman F 1954 *Physica* **20** 801
[4] Bassani F 1959 *Nuovo Cimento* **13** 244
[5] Cochran W 1959 *Proc. R. Soc.* A **253** 260
[6] Herman F 1959 *J. Phys. Chem. Solids* **8** 405
[7] Woods A D B, Cochran W, and Brockhouse B N 1960 *Phys. Rev.* **119** 980
[8] Kleinman L and Phillips J C 1960 *Phys. Rev.* **118** 1152
[9] Cowley R A 1962 *Proc. Roy. Soc.* A **268** 109
[10] Maradudin A, Montroll E W, and Weiss G H 1963 *Solid State Physics* suppl 3 (New York: Academic) pp 5–21
[11] Bassani F and Yoshimine M 1963 *Phys. Rev.* **130** 20
[12] Bassani F and Brust D 1963 *Phys. Rev.* **131** 1524
[13] Woods A D B, Brockhouse B N, Cowley R A, and Cochran W 1963 *Phys. Rev.* **131** 1025
[14] Cowley R A, Cochran W, Brockhouse B N, and Woods A D 1963 *Phys. Rev.* **131** 1030
[15] Brust D 1964 *Phys. Rev.* **134** A1337
[16] Dolling G and Cowley R A 1966 *Proc. Phys. Soc.* **88** 463
[17] Warren J L, Yarnell J L, Dolling G, and Cowley R A 1967 *Phys. Rev.* **158** 805
[18] Saravia L R and Brust D 1968 *Phys. Rev.* **176** 915
[19] Cochran W 1971 *CRC Crit. Rev. Solid State Sci.* **2** 1
[20] Price D L, Rowe J M, and Nicklow R M 1971 *Phys. Rev.* B **3** 1268
[21] Sinha S K 1973 *CRC Crit. Rev. Solid State Sci.* **3** 273
[22] Sham L J 1974 *Dynamical Properties of Solids* vol 1, ed G K Horton and A A Maradudin (New York: Elsevier) pp 303–42
[23] Weber W 1977 *Phys. Rev.* B **15** 4789
[24] Patel C, Sherman W F, and Wilkinson G R 1984 *J. Phys. C: Solid State Phys.* **17** 6063–9
[25] Streitwolf H W 1971 *Group Theory in Solid-State Physics* (London: Macdonald) pp 68–74
[26] Janssen T 1973 *Crystallographic Groups* (Amsterdam: North-Holland) pp 124–7
[27] Michel L 1977 *Group Theoretical Methods in Physics* (New York: Academic)
[28] Jaric M V, Michel L and Sharp R T 1984 *J. Physique* **45** 1
[29] Burns G and Glazer A M 1978 *Space Groups for Solid State Scientists* (New York: Academic)
[30] Cotfas N 1991 *J. Phys.: Condens. Matter* **3** 9279
[31] Cotfas N 1992 *J. Geom. Phys.* **10** 107
[32] Cotfas N 1993 *J. Phys. I (France)* **3** 2269
[33] Lang S 1970 *Algebra* (Reading, MA: Addison-Wesley) p 63
[34] Ghatak A K and Kothari L S 1972 *An Introduction to Lattice Dynamic* (London: Addison-Wesley) pp 77–87, 217–225
[35] Kireev P S 1974 *Semiconductor Physics* (Moscow: Mir) pp 103–16
[36] Cycon H L, Froese R G, Kirsch W, and Simon B 1987 *Schrödinger Operations with Applications to Quantum Mechanics and Global Geometry* (Berlin: Springer) pp 164–5