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The ring of invariant real functions on the Brillouin zone

Jai Sam Kim[a], L. Michel[b,1], B.I. Zhilinskií[c,*]

[a]Department of Physics, Pohang University of Science and Technology, Pohang 790-784, South Korea
[b]Institut des Hautes Études Scientifiques, 91440 Bures-sur-Yvette, France
[c]Université du Littoral, BP 5526, 59379 Dunkerque Cédex, France

Contents

Abstract

With the coordinates chosen in the previous chapter, we show explicitly how to linearize the action of crystallographic space groups on the Brillouin zone. For two-dimensional crystallography it yields eight four-dimensional representations and five six-dimensional representations. For the 73 arithmetic classes in

* Corresponding author.
E-mail addresses: jsk@postech.ac.kr (J.S. Kim), zhilin@univ-littoral.fr (B.I. Zhilinskií).
[1]Deceased 30 December 1999.

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dimension three, it yields, respectively, 33, 24, 16 linear representations of dimension 6, 8, 12. We give the corresponding Molien functions. For the representations of dimensions four and six, we compute the invariants (up to 96 numerator invariants for the *R* lattices). We can even extend the results to the 16 hexagonal arithmetic classes. All obtained results are presented in the form of short tables. The comparison with the table of the previous chapter is instructive. Using the possibility to make plots of invariant function for the two-dimensional crystallography we exploit our corresponding results and also study the orbit spaces.

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1. Introduction

Many physical properties of periodic crystals of dimension $d = 2, 3$ are described or measured by functions on the Brillouin zone ($= BZ$) invariant by S, the symmetry group of the crystal (= space group). Physically it is very important to know the conditions imposed by S-invariance on these functions, because these symmetries are excellent physical approximations and their consequences are very strong. The periodic crystals of interest to physicists are of dimension[2] 3 or sometimes 2. The two-dimensional study is simpler, so it has also a pedagogical value. Finally, it is important to know the restrictions that must be satisfied by the S-invariant functions which are also invariant under the time reversal symmetry $\mathscr{T}$. That is for instance the case of the energy $E(\boldsymbol{k})$ of the Fermi surface of the electrons or of a one branch energy band (= simple band). The numbers of space groups S are, respectively, 17, 230 for the dimensions $d = 2, 3$. As for the Euclidean group Eu_d, their invariant subgroup of translation L acts trivially on the reciprocal space, and the Brillouin zone. So the space group S acts effectively through the quotient group $S/L = P$ which is the finite point group. As we showed in Chapter I, Section 3, for $d = 2, 3$, the set of crystallographic point groups forms, respectively, 9, 18 isomorphic classes, 10, 32 geometric classes (= conjugacy classes in $O(d)$) and 13, 73 arithmetic classes (= conjugacy classes in $GL(d, Z)$) (in Chapter IV, Section 4). In Chapter I, Section 5.4, Tables 4, 5 give the invariants on our Euclidean space for the geometric class actions.[3] Here for the need of microphysics, we study the action of the arithmetic classes. Indeed, as explained in Chapter I, Section 2, the effective actions of the groups P on L are given by an injective homomorphism (i.e. with trivial kernel) $P \to GL(3, Z) = \mathrm{Aut}\, L$. We denote the image by P^z. The contragradient action $(g \mapsto (g^{-1})^\top)$ of P^z is its action on $BZ = \hat{L}$, the dual group of L (i.e. the group on its set of unitary irreducible representations).

Given an arbitrary function $f(\boldsymbol{k})$ on BZ, by averaging over the group G we obtain an invariant function:

$$\bar{f}(\boldsymbol{k}) = \frac{1}{|G|} \sum_{g \in G} f(g^{-1} \cdot \boldsymbol{k}) \; . \tag{1}$$

This averaging is a projection operator on a vector space of functions on BZ and it has been used in the physics literature; for an impressive review of applications to crystals see e.g. (Cracknell, 1974) (for instance, starting from plane waves one works with “the augmented plane wave methods”).

The sum and the product of invariant functions are invariant functions; so they form a ring. The Schwarz (1975) theorem (mentioned in Chapter I, Section 5) applies to our problem and tells us that, for the global coordinate system we have chosen on BZ, every P^z-invariant smooth function is a smooth function of the P^z invariant polynomials.

So we can limit our study to the ring $\mathscr{R}^{P^z}$ of invariant polynomials. *The aim of this chapter is to compute these rings for the 13 + 73 arithmetic classes.* It is remarkable that for $d = 2$, these rings have only 2, 3 or 4 generators; for $d = 3$ and 62 arithmetic classes, the rings have 3, 4, 5 or

[2] We do know that modulated and aperiodic crystals can be considered as projections of higher-dimensional periodic crystals, but we do not study them here.

[3] We gave some more. To be very precise we gave the invariants for the conjugacy classes of the point groups in $GL(3, Q)$ where Q is the field of rational numbers. They are useful for symmetry breaking problems.

6 generators while 1 (Cm), 3 ($C2, R\bar{3}, F23$), 6 ($F222, Fmm2, R32, R3m, I4, I\bar{4}$), 1 ($R3$) have, respectively, at most 7, 9, 10, 15 generators. When time reversal is added the number of generators is always ≤ 6, except for $R\bar{3}$. It is also remarkable that, as it is the case for linear representations, these rings have a module structure (see Chapter I, Section 5). These results are new and very useful.

To explain the strategy we have used for solving our problem, we apply it to the easy one-dimensional case. The translation group is $L \sim Z$. There are only two space groups: $S_0 = Z$ and $S_1 = Z \rtimes Z_2(-I)$ where[4] the two-element point group $P = Z_2 = GL(1, Z)$ is generated by $-I$, the symmetry through the origin, so it is the automorphism of Z changing n into $-n$. In $d = 1$, with time reversal, it is the only group P we have to consider. A unirrep (= unitary irreducible representation) of $L = Z$ is of the form $Z \ni n \mapsto \exp(ink)$. Since n is an integer, k is a real number defined modulo 2π. So the set of unirreps of L forms a group (with the law of addition modulo 2π) which is called the dual group and denoted by $\hat{L}$ by the mathematicians while the physicists call it BZ (= Brillouin zone). This group $\hat{L} = BZ$ is isomorphic to U_1, the multiplicative group of norm 1 complex numbers. Its topology is that of a circle, S_1. The action of the point group P on BZ is defined by $(-I)\cdot k = -k$. Beware that this action, which is the linear representation σ on the "reciprocal space" (here the set of the real numbers k), is not linear on BZ; indeed it has two fixed points $k = 0$ and π.

Then we can use two methods for computing the ring of P^z invariant polynomials on BZ; since they complement each other, we shall use both of them.

(1) For the study of periodic functions of one variable $k \bmod 2\pi$, it is natural to introduce the trigonometric series in $c = \cos(k)$ and $s = \sin(k)$. The Schwarz (1975) theorem invites us to study first the polynomials $P[c, s]$. Using the algebraic relation $\cos^2 k + \sin^2 k = 1$, we can transform in each monomial $c^d s^{d'}$ the factor $(s^2)^{[d'/2]}$ into $(1 - c^2)^{[d'/2]}$ so an arbitrary polynomial in c, s becomes at most linear in s. In other words we have replaced the ring of polynomials $P[c, s]$ by the module of basis $(1, s)$ on the ring $P[c]$ that we denote by $P[c]\bullet(1, s)$ with the notation introduced in Chapter I, Section 5, Eq. (77). We computed in Chapter I, Section 5.4.3, Eq. (121) the four-dimensional module of polynomials on the 2-D torus; the eight-dimensional module for the 3-D torus is given in Section 5.1. For the point group P of the other (and larger) one-dimensional space group s is not an invariant, but only a pseudo-invariant. So the P-invariant polynomials form the one-dimensional submodule (= polynomial ring) $P[c]$.

(2) To apply the other method to P, we first linearize its action on BZ. To do it, we have to extend the linear representation σ to one acting on a two-dimensional orthogonal space V_2 with orthogonal coordinates s, c. With the relations: $s = \sin k$, $c = \cos k$, the equation of BZ in V_2 is that of the unit circle: $c^2 + s^2 - 1 = 0$. The action of P on BZ is deduced from the linear representation $\rho(P)$ on V_2 defined by

$$\rho(-I) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \equiv \sigma(-I) \oplus \gamma(-I) . \tag{2}$$

where γ is the trivial representation of Z_2 since $\cos(-k) = \cos k$. Notice that $\rho(-I)$ represents a reflection in the two-dimensional space; it leaves c invariant and changes the sign of s. As

[4] Let $\varepsilon = \pm 1$ the elements of the point group Z_2. The group law of the semi-direct product $Z \rtimes Z_2$ is $(n_1, \varepsilon_1)(n_2, \varepsilon_2) = (n_1 + \varepsilon_1 n_2, \varepsilon_1 \varepsilon_2)$.

explained in Chapter I, the ring of its invariant polynomials is the ring of two variable polynomials $P[c, s^2]$. The BZ equation defines an ideal of this polynomial ring; the quotient is the polynomial ring $\mathscr{P}[c]$ (its elements are all polynomial in the variable $c = \cos k$). Those are the P^z invariant polynomials on BZ that we were looking for; that result was obvious. We will follow exactly the same method for $d = 2, 3$. As the reader will see, computations become more and more complicated, several new difficulties appear and the results are less and less obvious. Their usefulness is equivalent to that of the one-dimensional result!

One has to choose a coordinate system for giving explicitly the invariant polynomials. That is done in Section 2 for the 13 + 73 P^z; we give their generating integral matrices in a basis of vectors generating the translation lattice L. This is done in ITC for the P (= primitive lattice). However, for the 16 I and the eight F arithmetic classes, it will appear that simpler results can be obtained with the use of non-primitive cell (as in ITC) by using the orthogonal axes of the corresponding primitive lattice.[5]

In Section 3 we build for each P^z the orthogonal representation ρ (whose existence has been proved by the Mostow theorem (Mostow, 1957) which linearizes its action on BZ. This representation is the direct sum:

$$\rho = \sigma \oplus \gamma \tag{3}$$

of two representations acting, respectively, on the variable s_i and c_i. The dimension of ρ is 4, 6 for 8, 5 two-dimensional arithmetic classes and for dimension three, 6, 8, 12 for the 33 orthogonal arithmetic classes, the sixteen P-hexagonal and sixteen I ones, the eight F ones, respectively. Then we compute the corresponding Molien functions. As we will explain, we need to compute the module of invariant polynomials of the ρ representations for only a few P^z; but we decided not to compute modules with dimension > 48. So we do not deal with I or F arithmetic classes in their natural basis. But, as we explain at the end of Section 5, we make the computation in the non-primitive orthogonal coordinates used by the ITC. That is done in Section 6; the results are simple and probably more useful for applications.

One needs to make a complete computation for few groups (generally the smallest groups in each family of modules on the same ring). The lengthiest computation is for $R3$. We obtain the other modules as submodules by using several simple theorems gathered at the end of Section 4.

It is also simpler to draw pictures for two-dimensional invariants; we do it in Section 7. In Section 8, to conclude, we emphasize the beauty and usefulness of our results and we suggest some applications.

2. Choice of representatives for the 13 and 73 arithmetic classes for $d = 2, 3$

In order to express the invariant polynomials we need to choose a coordinate system or, what is equivalent, to choose matrices v defining one of their groups for each of the 13 + 73 arithmetic classes. This choice will be made by the definition of the following matrices (Eqs. (4)–(11)).

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[5] For some groups, ITC consider several bases. In fact our results are given for all arithmetic classes, in one of the ITC bases.

For $d=2$: $(p1)=I_2$, $(p2)=-I_2$,

$$(p3)=\begin{pmatrix}0 & -1\\ 1 & -1\end{pmatrix}=-(p6),\quad (p4)=\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix},$$

$$(pm)=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},\qquad (cm)=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}. \tag{4}$$

Notice that $(p4)=(cm)(pm)$. The generator of the group $p6$ describes the rotation by $5\pi/3$, but it is convenient to introduce the pairs of $\pm$ matrices.

For $d=3$, $(P1)=I_3$, $(P\bar{1})=-I_3=-(P1)$,

$$(P2)=\begin{pmatrix}-1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & 1\end{pmatrix}=-(Pm), \tag{5}$$

$$(C2)=\begin{pmatrix}0 & -1 & 0\\ -1 & 0 & 0\\ 0 & 0 & -1\end{pmatrix}=-(Cm), \tag{6}$$

$$(P3)=\begin{pmatrix}0 & -1 & 0\\ 1 & -1 & 0\\ 0 & 0 & 1\end{pmatrix}=-(P\bar{3}),\quad (R3)=\begin{pmatrix}0 & 0 & 1\\ 1 & 0 & 0\\ 0 & 1 & 0\end{pmatrix}=-(R\bar{3}), \tag{7}$$

$(P6)=(P\bar{3})(Pm)=-(P\bar{6})$,

$$(P4)=\begin{pmatrix}0 & -1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 1\end{pmatrix}=-(P\bar{4}),\quad (I4)=\begin{pmatrix}0 & 1 & 0\\ 0 & 1 & -1\\ -1 & 1 & 0\end{pmatrix}=-(I\bar{4}). \tag{8}$$

The $7+16$ matrices we defined have been computed in Chapter IV, Section 4.4. Each one represents an arithmetic element (see Chapter IV, Section 4.2, 4.3) and the cyclic groups they generate are the cyclic arithmetic classes (their notation is identical to that of the element). From these matrices and some of their conjugate forms, we can define finite subgroups of $GL(d,Z)$, representatives of all non-cyclic arithmetic classes for $d=2,3$. It will be convenient to use the following three sets of three reflections:

$$(Pm)=m_3=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{pmatrix},\qquad m_1=\begin{pmatrix}-1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix},\qquad m_2=\begin{pmatrix}1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & 1\end{pmatrix}, \tag{9}$$

$$(Cm)=j_3=\begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 1\end{pmatrix},\qquad j_1=\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 1\\ 0 & 1 & 0\end{pmatrix},\qquad j_2=\begin{pmatrix}0 & 0 & 1\\ 0 & 1 & 0\\ 1 & 0 & 0\end{pmatrix}, \tag{10}$$

$$f_3 = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 1 & 1 & 1 \end{pmatrix}, \quad f_1 = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}, \quad f_2 = \begin{pmatrix} 0 & 0 & -1 \\ 1 & 1 & 1 \\ -1 & 0 & 0 \end{pmatrix}. \tag{11}$$

We check that

$$(R3) = j_3 j_1 = j_1 j_2 = j_2 j_3, \quad (P4) = m_1 j_3 = j_3 m_2 ,$$

$$(I4) = j_3 f_2^{\top} = f_1^{\top} j_3 , \tag{12}$$

$$(I4)^2 = -f_3^{\top}, \quad \prod_i m_i = -I_3 = \prod_i f_i . \tag{13}$$

Notice that the reflections j_i, f_i belong to the arithmetic class Cm; notice also that the j_i's generate $R3m$, the f_i's generate $Fmmm$ and the $f_i^{\top}$'s generate $Immm$ and (13) shows that $(I4)^2$ is an I rotation by π around axis 3. More generally, with the matrices of (4)–(13), we build a representation group P^z for all arithmetic classes in dimension $d = 2, 3$.

What we need here is to build for each P^z its contragradient representation $P^z \ni g \mapsto \sigma(g) = \tilde{g}$ with $\tilde{g} := (g^{-1})^{\top}$ since we are interested in the P^z action on BZ. The contragradient correspondence $g \to \tilde{g}$ is a duality on matrices which leaves fixed the orthogonal matrices. It induces a duality on the arithmetic classes; for $d = 2, 3$ the 8, 33 arithmetic classes which are $\leq \mathrm{O}(2, Z) = p4mm$, $\leq \mathrm{O}(3, Z) = Pm\bar{3}m$ are self-contragradient. That is also the case of 3, 14 other arithmetic classes which are transformed into themselves up to an equivalence. There are 2, 26 non-self-dual arithmetic classes; they form 1, 13 dual pairs:

$d = 2$: $p3m1 \leftrightarrow p31m$,

$d = 3$: $F222 \leftrightarrow I222$, $Fmm2 \leftrightarrow Imm2$, $Fmm \leftrightarrow Immm$, (14)

$I\bar{4}m2 \leftrightarrow I\bar{4}2m$, $P321 \leftrightarrow P312$, $P3m1 \leftrightarrow P31m$,

$P\bar{3}m1 \leftrightarrow P\bar{3}1m$, $P\bar{6}m2 \leftrightarrow P\bar{6}2m$. (15)

$F23 \leftrightarrow I23$, $Fm\bar{3} \leftrightarrow Im\bar{3}$, $F432 \leftrightarrow I432$, $F\bar{4}3m \leftrightarrow I\bar{4}3m$, $Fm\bar{3}m \leftrightarrow Im\bar{3}m$. (16)

Let us look at the two-dimensional case in more detail. The relation $\widetilde{(p3)} = (p4)(p3)(p4)^{-1}$ shows that $p3$ is self-contragradient (up to a conjugation); but $(p4)(cm)(p4)^{-1} = -(cm)$ shows that the arithmetic classes $p3m1$ and $p31m$ (defined in Chapter IV, Section 4.2) are in duality. The contragradient representation of $p3m1$ is generated by $\widetilde{(p3)}$ and (cm). The conjugation by $(p4)$ shows that the dual class of $p3m1$ is equivalent to $p31m$.

We give in Table 1 the generators of the contragradient representation σ for the chosen P^z for the 13 + 73 arithmetic classes. The corresponding bases coincide with that of ITC for the arithmetic classes whose labels begin by p, P, R, but not for the others. Later, at the end of Section 5 for the C, A classes and in Section 6 for the F, I classes, we will write the invariants in the "primitive bases".

Table 1
Generators of the contragradient representation $\tilde{\nu}(P^z)$ of the arithmetic class representatives P^{z}[a]

$p2$: $-I_2$	pm: (pm)	$p2mm$: $\pm(pm)$	cm: (cm)
$c2mm$: $\pm(cm)$	$p4$: $(p4)$	$p4mm$: $(pm),(cm)$	$p3$: $(\widetilde{p3})$
$p3m1$: $(\widetilde{p3}),(cm)$	$p31m$: $(\widetilde{p3}),-(cm)$	$p6$: $-(\widetilde{p3})$	$p6mm$: $-(\widetilde{p3}),(cm)$
$P\bar{1}$: $-I_3$	$P2$: $-m_3$	Pm: m_3	$P2/m$: $\pm m_3$
$C2$: $-j3$	Cm: j_3	$C2/m$: $\pm j_3$	$P222$: $-m_3,-m_1$
$Pmm2$: $-m_3,m_1$	$Pmmm$: m_i	$C222$: $-j_3,-m_3$	$Cmm2$: $j_3,-m_3$
$Amm2$: $-j_3,m_3$	$Cmmm$: $\pm j_3,m_3$	$F222$: $-f_3^{\top},-f_1^{\top}$	$Fmm2$: $-f_3^{\top},f_1^{\top}$
$Fmmm$: $f_i^{\top}$	$I222$: $-f_3,-f_1$	$Imm2$: $-f_3,f_1$	$Immm$: f_i
$P4$: $(P4)$	$P\bar{4}$: $-(P4)$	$P4/m$: $(P4),m_3$	$P422$: $(P4),-m_1$
$P4mm$: $(P4),m_1$	$P\bar{4}2m$: $-(P4),-m_1$	$P\bar{4}m2$: $-(P4),m_1$	$P4/mmm$: $(P4),m_i$
$I4$: $(\widetilde{I4})$	$I\bar{4}$: $-(\widetilde{I4})$	$I4/m$: $(\widetilde{I4}),f_3$	$I422$: $(\widetilde{I4}),-f_1$
$I4mm$: $(\widetilde{I4}),f_1$	$I\bar{4}m2$: $-(\widetilde{I4}),f_1$	$I\bar{4}2m$: $-(\widetilde{I4}),j_3$	$I4/mmm$: j_3,f_i
$R3$: $(R3)$	$R\bar{3}$: $-(R3)$	$R32$: $(R3),-j_i$	$R3m$: $(R3),j_i$
$R\bar{3}m$: $-(R3),\pm j_i$	$P3$: $(\widetilde{P3})$	$P\bar{3}$: $-(\widetilde{P3})$	$P312$: $(\widetilde{P3}),m_3j_3$
$P321$: $(\widetilde{P3}),-j_3$	$P3m1$: $(\widetilde{P3}),j_3$	$P\bar{3}m1$: $-(\widetilde{P3}),j_3$	$P31m$: $(\widetilde{P3}),-m_3j_3$
$P\bar{3}1m$: $-(\widetilde{P3}),m_3j_3$	$P6$: $(\widetilde{P6})$	$P\bar{6}$: $-(\widetilde{P6})$	$P6/m$: $(\widetilde{P6}),m_3$
$P622$: $(\widetilde{P6}),-j_3$	$P6mm$: $(\widetilde{P6}),j_3$	$P\bar{6}m2$: $-(\widetilde{P6}),j_3$	$P\bar{6}2m$: $-(\widetilde{P6}),-j_3$
$P6/mmm$: $(\widetilde{P6}),m_3,j_3$	$P23$: $-m_i,(R3)$	$Pm\bar{3}$: $m_i,(R3)$	$P432$: $-m_i,-j_i$
$P\bar{4}3m$: $-m_i,j_i$	$Pm\bar{3}m$: m_i,j_i	$F23$: $-f_i^{\top},(R3)$	$Fm\bar{3}$: $f_i^{\top},(R3)$
$F432$: $-f_i^{\top},-j_i$	$F\bar{4}3m$: $-f_i^{\top},j_i$	$Fm\bar{3}m$: $f_i^{\top},j_i$	$I23$: $-f_i,(R3)$
$Im\bar{3}$: $f_i,(R3)$	$I432$: $-f_i,-j_i$	$I\bar{4}3m$: $-f_i,j_i$	$Im\bar{3}m$: f_i,j_i

[a] The 12 + 72 non-trivial arithmetic classes are listed roughly in the order of ITC. The generating matrices are the ones listed in Eqs. (4)–(13) or, when they carry above a ~, they are their contragradient which are given in (17).

To use Table 1 we need only the matrices in Eqs. (4)–(13) and the contragradient matrices of the arithmetic elements $(p3)$, $(P3)$, $P(6)$, $(I4)$; they are

$$(\widetilde{p3}) = \begin{pmatrix} -1 & -1 \\ 1 & 0 \end{pmatrix}, \qquad (\widetilde{P3}) = \begin{pmatrix} -1 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$$(\widetilde{P6}) = \begin{pmatrix} 1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad (\widetilde{I4}) = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{pmatrix}. \tag{17}$$

We verify that $(\widetilde{I4})^2 = -f_3$.

3. Linearization $\rho(P^z)$ of the P^z action on BZ; its Molien function

In the preceding section we have defined the matrices of the $\tilde{\nu}$ representation of the arithmetic point groups P^z; that defines a basis in the reciprocal space and on BZ. On it the coordinates are given by the components $k_i \bmod 2\pi$ of the vector $\boldsymbol{k}$ in the reciprocal space E_d^*. We are interested in the action of P^z on functions on BZ, i.e. periodic functions on E_d^* whose lattice period is $2\pi L^*$. This action is given by

$$P^z \ni g, \quad (g \cdot f)(\boldsymbol{k}) = f(\tilde{g}^{-1} \cdot \boldsymbol{k}) = f(g^\top \cdot \boldsymbol{k}) . \tag{18}$$

Note that this action is a linear action on the vector space of such functions. The necessary and sufficient condition for such a function f on BZ to be invariant under P^z is

$$\forall g \in P^z, \quad f(\tilde{g} \cdot \boldsymbol{k}) = f(\boldsymbol{k}) . \tag{19}$$

The simplest functions of period 2π are the sine and cosine of the coordinates k_i's. For a given $\boldsymbol{k} \bmod 2\pi L^*$ we denote their values $s_j = \sin k_j$ and $c_j = \cos k_j$; they can be considered as $2d$ coordinates in a $2d$-dimensional space in which BZ is an algebraic manifold of equations:

$$1 \leq j \leq d, \quad c_j^2 + s_j^2 = 1 . \tag{20}$$

A smooth function on BZ can be written as a Fourier series

$$1 \leq i \leq d \quad f(k_i) = \prod_i \sum_{0 \leq n \in Z} (\alpha_{in} \cos(nk_i) + \beta_{in} \sin(nk_i)) . \tag{21}$$

Since the functions $\cos(n\omega)$ and $\sin(n\omega)$ are polynomials in $\cos\omega$ and $\sin\omega$, the function f is a polynomial series in $\cos k_i$, $\sin k_i$. That also suggests the interest of the polynomials themselves.

To linearize the P^z action we have several cases to consider for building the representation ρ of P^z.

3.1. *Case 1. P^z is orthogonal; we prove* $\dim \rho(P^z) = 2d$

That is the case of 8, 33 arithmetic classes for $d = 2, 3$. They are subgroups of the two maximal arithmetic classes:

$$O(2, Z) = p4m, \quad O(3, Z) = Pm\bar{3}m . \tag{22}$$

The matrices of $O(d, Z)$ have only one non-zero element per row and per column; this element is ± 1. When all elements are 1, it is a permutation matrix. So the group $O(d, Z)$ is generated by its diagonal and its permutation matrices; more precisely a matrix of $O(d, Z)$ is the product of one matrix of the Abelian group $\mathrm{diag}_d(\pm 1)$, the group of $d \times d$ diagonal matrices of elements ± 1, and one matrix of Π_d, the group of $d \times d$ permutation matrices. One verifies that $\mathrm{diag}_d(\pm 1)$ is an invariant subgroup of $O(d, Z)$ and

$$O(d, Z) \sim Z_2^d \rtimes \mathscr{S}_d, \quad |O_d(Z)| = 2^d d! . \tag{23}$$

For $d = 2, 3$ the groups $\mathrm{diag}_d(\pm 1)$ and Π_d define the arithmetic classes:

$$\mathrm{diag}_2(\pm 1) = p2mm, \quad \Pi_2 = cm, \quad \mathrm{diag}_3(\pm 1) = Pmmm, \quad \Pi_3 = R3m . \tag{24}$$

The orthogonal matrices permute up to a sign the three angles k_i so they transform linearly into themselves the three functions $\sin k_i$ on one hand and the three functions $\cos k_i$ on the other hand. Since the orthogonal matrices are self-contragradient, the three functions $\sin k_i$ transform under the representation $\tilde{v}$ of P^z which is in the present case the represention that we have called σ . Since

$\cos(-k_i) = \cos k_i$ the three functions $\cos k_i$ are permuted without changes of sign. The group $O(d, Z)$ operates on them through its quotient $O(3, Z)/\mathrm{diag}_d(\pm 1) = \Pi_d \sim \mathcal{S}_d$. That yields a linear representation $\gamma(P^z)$ obtained by keeping only the absolute value of the elements of the σ matrices. The direct sum of these two representations

$$\rho(P^z) = \sigma(P^z) \oplus \gamma(P^z), \quad \dim \rho = 2d \tag{25}$$

acts on the space of coordinates s_i, c_i and leaves invariant the algebraic equations (20) defining BZ. The restriction of the linear action of ρ on this manifold is the action of P^z on BZ; ρ is, by definition, the linearizing representation. From (24), the kernel of the representation γ is

$$d = 2,\ \gamma(G) = G/(G \cap p2mm), \quad d = 3,\ \gamma(G) = G/(G \cap Pmmm)\ . \tag{26}$$

Table 2 gives the image of $\gamma(P^z)$ in Π_d as another P^z.

As we explain in the introduction, we will compute the module of invariants of the representation $\rho(P^z)$. They contain three types of invariants; those of the representation γ are polynomials in c_i, those of σ are polynomials in s_i and the mixed ones, obtained from the products of two covariants of the same nature, one from σ, the other from γ. The next step of the program will be to use the d equations $s_i^2 = 1 - c_i^2$ of the BZ manifold to eliminate the s_i^2. We will find that the module structure is preserved and its ring on BZ is the ring of the module of the γ representation. These rings are simple since the $\mathrm{Im}\,\gamma$ (second column of Table 2) are all reflection groups (trivial for $p1, P1$) except for $R3$; but this group has the same denominator invariants as $R3m$. So for $d = 2, 3$ we will have only $2, 3$ polynomial rings for all the modules: those of dimension 3 are given in (50).

We leave as an exercise to the reader to check that $\rho(R\bar{3})$ is equivalent to the regular representation of this six-element cyclic group.

From the definition given in Chapter I, Eq. (34) we calculate the Molien function of these $8 + 33$ representations ρ. They are listed, respectively, in Tables 4 and 5.

We remark that for the eight groups p^z representing the eight orthogonal arithmetic classes in dimension 2, correspond eight groups P^z obtained by adding the trivial one-dimensional representation; so for their ρ representation:

$$P^z = p^z \oplus I \ \Rightarrow \rho(P^z) = \rho(p^z) \oplus I_2\ . \tag{27}$$

Table 2
List of the orthogonal arithmetic classes whose γ representations have the same image; it is given in the second column

dim	$\mathrm{Im}\,\gamma(P^z)$	P^z							
$d = 2$	$p1$	$p1$	$p2$	pm	$p2mm$				
	cm	cm	$c2mm$	$p4$	$p4m$				
	$P1$	$P1$	$P\bar{1}$	$P2$	Pm	$P2/m$	$P222$	$Pmm2$	$Pmmm$
	Cm	$C2$	Cm	$C2/m$	$C222$	$Cmm2$	$Amm2$	$Cmmm$	
$d = 3$	”	$P4$	$P\bar{4}$	$P4/m$	$P422$	$P4mm$	$P\bar{4}2m$	$P\bar{4}m2$	$P4/mmm$
	$R3$	$R3$	$R\bar{3}$	$P23$	$Pm\bar{3}$				
	$R3m$	$R32$	$R3m$	$R\bar{3}m$	$P432$	$P\bar{4}3m$	$Pm\bar{3}m$		

These P^z have the same symbol in ITC except that the first letter p is replaced[6] by P. Their Molien functions are defined by

$$M_{P^z} = M_{p^z}(1-t)^{-2} . \tag{28}$$

3.2. Case 2. P^z is hexagonal or I; we prove $\dim \rho(P^z) = 2(d+1)$

This case splits into three subcases: the two-dimensional hexagonal system, and, for dimension 3, the hexagonal system and the sixteen I arithmetic classes. It contains $5 + 16 + 16 = 37$ arithmetic classes.

Case 2a: the five two-dimensional hexagonal classes.

The simplest arithmetic class belonging to this case is $p3$. Its σ representation is generated by $\widetilde{(p3)}$ given explicitly in (17). It transforms the coordinates of the vector $\boldsymbol{k} = k_1\boldsymbol{b}_1^* + k_2\boldsymbol{b}_2^*$ according to

$$\widetilde{p3}\begin{pmatrix} k_1 \\ k_2 \end{pmatrix} = \begin{pmatrix} -1 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} k_1 \\ k_2 \end{pmatrix} = \begin{pmatrix} -k_1 - k_2 \\ k_1 \end{pmatrix}, \quad \widetilde{p3}^2\begin{pmatrix} k_1 \\ k_2 \end{pmatrix} = \begin{pmatrix} k_2 \\ -k_1 - k_2 \end{pmatrix} . \tag{29}$$

Let us define k_0 by the relation

$$k_0 + k_1 + k_2 \equiv 0 \bmod 2\pi . \tag{30}$$

This equation is preserved by the action of $\widetilde{p3}$ since this matrix acts on the k_α, $\alpha = 0, 1, 2$ by a circular permutation: $k_0, k_1, k_2 \to k_2, k_0, k_1$. That is exactly the action of the matrix $(R3)$ of Eq. (7). This orthogonal matrix is self-contragradient and must have the same action on the direct space. Let us verify it. In the direct basis $i = 1, 2$, $(\boldsymbol{b}_i, \boldsymbol{b}_j) = (3\delta_{ij} - 1)/2$, we have

$$\boldsymbol{k} = k_1\boldsymbol{b}_1^* + k_2\boldsymbol{b}_2^* = \tfrac{2}{3}((2k_1 + k_2)\boldsymbol{b}_1 + (k_1 + 2k_2)\boldsymbol{b}_2) . \tag{31}$$

We can introduce in the direct space a third vector defined by

$$\boldsymbol{b}_0 + \boldsymbol{b}_1 + \boldsymbol{b}_2 = 0 , \tag{32}$$

these three vectors form a regular 3-branch star since the two vectors $\boldsymbol{b}_1, \boldsymbol{b}_2$ have the same length and form an angle of $2\pi/3$. Then with (29), $\boldsymbol{k}$ can be written in a unique way

$$\alpha = 0, 1, 2, \quad \boldsymbol{k} = \sum_\alpha k_\alpha \boldsymbol{b}_\alpha . \tag{33}$$

This concludes our verification; it shows that the linearization of the actions of the arithmetic classes $p3$ and $R3$ on BZ have the same ρ representation.

The third line of Table 1 shows that, besides $\pm\widetilde{(p3)}$, the other generators of the five groups representing the two-dimensional hexagonal arithmetic classes are $\pm(cm)$ which are orthogonal matrices. One verifies the identity of the σ representations and, therefore, of the six-dimensional ρ linear representations. This identity of the ρ representations can be extended to the four other natural pairs between the groups of the 2-D hexagonal Bravais class and the groups of the

[6] And $2mm$ is replaced by $mm2$; we do not know why this exception had been made by ITC.

rhombohedral Bravais class:

$$\rho(p3)=\rho(R3),\quad \rho(p3m1)=\rho(R3m),\quad \rho(p31m)=\rho(R32)\,,$$
$$\rho(p6)=\rho(R\bar{3}),\quad \rho(p6mm)=\rho(R\bar{3}m)\,. \tag{34}$$

Let us show it for $p3m1$ and $p31m$. The actions of $\pm(cm)$ on the coordinates k_α are

$$(cm)\cdot k_1=k_2,\quad (cm)\cdot k_0=k_0,\quad -(cm)\cdot k_1=-k_2,\quad -(cm)\cdot k_0=-k_0\;. \tag{35}$$

The Molien functions depend only on ρ and so the equalities given in (34) extend to the Molien functions; they are given in Table 4.

Case 2b: the three-dimensional hexagonal arithmetic classes.

There are 16 of them. Through the faithful contragradient representations of the two- and three-dimensional hexagonal arithmetic classes given in Table 1, one sees several relations subgroup $<$ group between the two- and three-dimensional classes.

The first one is obtained for the three-dimensional group acting trivially on the third component $k_3 \bmod 2\pi$ of the BZ:

$$h<H\colon\; p3<P3,\quad p3m1<P3m1,\quad p31m<P31m\,,$$
$$p6<P6,\quad p6mm<P6mm\,. \tag{36}$$

So the eight-dimensional linear representation $\rho(H)$ is defined by

$$\rho(H)=\rho(h)\oplus I_2\;, \tag{37}$$

where I_2 acts on the coordinates s_3, c_3. From these groups we can generate all other hexagonal arithmetic classes except for three of them and compute their ρ representations. That is done in Table 3.

It is easy to compute the Molien functions of the groups of the third and fourth lines from that of the first or second line groups (Tables 4 and 5)

$$M_H=M_h\frac{1}{(1-t)^2},\quad M_{H_h}=M_h\frac{1}{(1-t)(1-t^2)}\;. \tag{38}$$

Table 3
Construction of the representations $\rho(P^z)$ for the two and three-dimensional hexagonal systems, from the $\rho(P^z)$ of the rhombohedral system. The arithmetic classes $P321$, $P312$, $P622$ do not appear. In the last column the I_2, $-\sigma_3$ acts on s_3, c_3. The identity of the ρ representaions of the first two lines was established in (34)

l.s.	Group quintuplet					Generators	ρ representation
R	$R3$	$R3m$	$R32$	$R\bar{3}$	$R\bar{3}m$		$\rho(R)$
h	$p3$	$p3m1$	$p31m$	$p6$	$p6mm$		$\rho(h)=\rho(R)$
H	$P3$	$P3m1$	$P31m$	$P6$	$P6mm$	$h\oplus 1$	$\rho(h)\oplus I_2$
H_h	$P\bar{6}$	$P\bar{6}m2$	$P\bar{6}2m$	$P6/m$	$P6/mmm$	$\langle H, m_3\rangle$	$(\rho(h)\oplus I_2)\cup(\rho(h)\oplus -\sigma_3)$
H_-	$P\bar{3}$	$P\bar{3}m1$	$P\bar{3}1m$	$P6/m$	$P6/mmm$	$\langle H, -I_3\rangle$	$\rho(H)\cup(-\sigma(H)\oplus\gamma(H))$

Table 4
Molien functions of the ρ representations of the two-dimensional arithmetic groups[a]

AC	Generators	$D(t)$	$N(t)$
$p1$	I_2	$(1-t)^4$	1
$p2$	$-I_2$	$(1-t)^2(1-t^2)^2$	$1+t^2$
pm	(pm)	$(1-t)^3(1-t^2)$	1
$p2mm$	$\pm(pm)$	$(1-t)^2(1-t^2)^2$	1
cm	(cm)	$(1-t)^2(1-t^2)^2$	$1+t^2$
$c2mm$	$\pm(cm)$	$(1-t)(1-t^2)^3$	$1+t^3$
$p4$	$(p4)$	$(1-t)(1-t^2)^2(1-t^4)$	$1+2t^3+t^4$
$p4mm$	$(pm),(cm)$	$(1-t)(1-t^2)^2(1-t^4)$	$1+t^3$
$p3$	$(\widetilde{p3})$	$(1-t)^2(1-t^2)^2(1-t^3)^2$	$1+2t^2+6t^3+2t^4+t^6$
$p3m1$	$(\widetilde{p3}),(cm)$	$(1-t)^2(1-t^2)^2(1-t^3)^2$	$1+t^2+2t^3+t^4+t^6$
$p31m$	$(\widetilde{p3}),-(cm)$	$(1-t)(1-t^2)^3(1-t^3)^2$	$1+t^2+3t^3+5t^4+t^5+t^6$
$p6$	$-(\widetilde{p3})$	$(1-t)(1-t^2)^3(1-t^3)(1-t^6)$	$1+5t^3+6t^4+2t^5+3t^6+4t^7+2t^8+t^9$
$p6mm$	$-(\widetilde{p3}),(cm)$	$(1-t)(1-t^2)^3(1-t^3)(1-t^6)$	$1+2t^3+3t^4+t^5+t^6+2t^7+t^8+t^9$

[a]Their denominator and numerator are $D(t)$ and $N(t)$. The Molien functions of the 3D rhombohedral classes are those of the 2D hexagonal class with the correspondence: $\rho(p3)\leftrightarrow\rho(R3)$, $\rho(p3m1)\leftrightarrow\rho(R3m)$, $\rho(p31m)\leftrightarrow\rho(R32)$, $\rho(p6)\leftrightarrow\rho(R\bar{3})$, $\rho(p6mm)\leftrightarrow\rho(R\bar{3}m)$.

The new invariants are s_3, c_3 in the first case and s_3^2, c_3 in the second case. It will be also very easy to obtain for these 13 three-dimensional hexagonal arithmetic classes, the module of invariants on BZ from the correspondence of Table 3 with the two-dimensional hexagonal classes.

The arithmetic classes $P321, P312, P622$ must be treated separately (see Section 5).

Case 2c. The 16 I-arithmetic classes.

With the components k_i of the vector $\boldsymbol{k}$ we introduce

$$k_1 + k_2 + k_3 + k_4 = 0 \bmod 2\pi\ . \tag{39}$$

Then we obtain the tranformations of $\boldsymbol{k}$ by the matrices generating the contragradient representations of the I-tetragonal arithmetic classes:

$$f_1 \cdot \begin{pmatrix} k_1 \\ k_2 \\ k_3 \end{pmatrix} = -\begin{pmatrix} k_4 \\ k_3 \\ k_2 \end{pmatrix},\quad f_2 \cdot \begin{pmatrix} k_1 \\ k_2 \\ k_3 \end{pmatrix} = -\begin{pmatrix} k_3 \\ k_4 \\ k_1 \end{pmatrix}, \tag{40}$$

$$f_3 \cdot \begin{pmatrix} k_1 \\ k_2 \\ k_3 \end{pmatrix} = -\begin{pmatrix} k_2 \\ k_1 \\ k_4 \end{pmatrix},\quad (\widetilde{I4}) \cdot \begin{pmatrix} k_1 \\ k_2 \\ k_3 \end{pmatrix} = -\begin{pmatrix} k_4 \\ k_3 \\ k_1 \end{pmatrix}. \tag{41}$$

They induce permutations up to a sign, of the 4 k_α. In the classical cycle notation for the permutation they can be written with the change of sign:

$$f_1 \to -(14)(23),\quad f_2 \to -(13)(24),\quad f_3 \to -(12)(34),\quad (\widetilde{I4}) \to -(4231)\ . \tag{42}$$

Table 5
Molien functions of the ρ representations of the three-dimensional arithmetic groups of P, C, A lattices[a]

AC	Generators	$D(t)$	$N(t)$
$P1$	I_3	$(1-t)^6$	1
$P\bar{1}$	$-I_3$	$(1-t)^3(1-t^2)^3$	$1+3t^2$
$P2$	$-m_3$	$(1-t)^4(1-t^2)^2$	$1+t^2$
Pm	m_3	$(1-t)^5(1-t^2)$	1
$P2/m$	$\pm m_3$	$(1-t)^3(1-t^2)^3$	$1+t^2$
$C2$	$-j_3$	$(1-t)^3(1-t^2)^3$	$1+3t^2$
Cm	j_3	$(1-t)^4(1-t^2)^2$	$1+t^2$
$C2/m$	$\pm j_3$	$(1-t)^2(1-t^2)^4$	$1+t^2+2t^3$
$P222$	$-m_3, -m_1$	$(1-t)^3(1-t^2)^3$	$1+t^3$
$Pmm2$	$-m_3, m_1$	$(1-t)^4(1-t^2)^2$	1
$Pmmm$	m_i	$(1-t)^3(1-t^2)^3$	1
$C222$	$-j_3, -m_3$	$(1-t)^2(1-t^2)^4$	$1+t^3$
$Cmm2$	$j_3, -m_3$	$(1-t)^3(1-t^2)^3$	$1+t^3$
$Amm2$	$-j_3, m_3$	$(1-t)^3(1-t^2)^3$	$1+t^2$
$Cmmm$	$\pm j_3, m_3$	$(1-t)^2(1-t^2)^4$	$1+t^3$
$P4$	$(P4)$	$(1-t)^3(1-t^2)^2(1-t^4)$	$1+2t^3+t^4$
$P\bar{4}$	$-(P4)$	$(1-t)^2(1-t^2)^3(1-t^4)$	$1+t^2+4t^3+t^4+t^6$
$P4/m$	$(P4), m_3$	$(1-t)^2(1-t^2)^3(1-t^4)$	$1+2t^3+t^4$
$P422$	$(P4), -m_1$	$(1-t)^2(1-t^2)^3(1-t^4)$	$1+t^3+t^4+t^5$
$P4mm$	$(P4), m_1$	$(1-t)^3(1-t^2)^2(1-t^4)$	$1+t^3$
$P\bar{4}2m$	$-(P4), -m_1$	$(1-t)^2(1-t^2)^3(1-t^4)$	$1+2t^3+t^6$
$P\bar{4}m2$	$-(P4), m_1$	$(1-t)^2(1-t^2)^3(1-t^4)$	$1+t^2+2t^3$
$P4/mmm$	$(P4), m_i$	$(1-t)^2(1-t^2)^3(1-t^4)$	$1+t^3$
$P3$	$(\widetilde{P3})$	$(1-t)^4(1-t^2)^2(1-t^3)^2$	$1+2t^2+6t^3+2t^4+t^6$
$P\bar{3}$	$-(\widetilde{P3})$	$(1-t)^2(1-t^2)^4(1-t^3)(1-t^6)$	$1+t^2+7t^3+10t^4+5t^5+5t^6+10t^7+7t^8+t^9+t^{11}$
$P312$	$(\widetilde{P3}), m_3 j_3$	$(1-t)^3(1-t^2)^3(1-t^3)^2$	$1+t^2+3t^3+5t^4+t^5+t^6$
$P321$	$(\widetilde{P3}), -j_3$	$(1-t)^2(1-t^2)^4(1-t^3)^2$	$1+2t^2+4t^3+10t^4+4t^5+2t^6+t^8$
$P3m1$	$(\widetilde{P3}), j_3$	$(1-t)^4(1-t^2)^2(1-t^3)^2$	$1+t^2+2t^3+t^4+t^6$
$P\bar{3}m1$	$-(\widetilde{P3}), j_3$	$(1-t)^2(1-t^2)^4(1-t^3)(1-t^6)$	$1+t^2+3t^3+5t^4+2t^5+2t^6+5t^7+3t^8+t^9+t^{11}$
$P31m$	$(\widetilde{P3}), -m_3 j_3$	$(1-t)^3(1-t^2)^3(1-t^3)^2$	$1+t^2+3t^3+5t^4+t^5+t^6$
$P\bar{3}1m$	$-(\widetilde{P3}), m_3 j_3$	$(1-t)^2(1-t^2)^4(1-t^3)(1-t^6)$	$1+3t^3+5t^4+3t^5+2t^6+5t^7+4t^8+t^9$
$P6$	$(\widetilde{P6})$	$(1-t)^3(1-t^2)^3(1-t^3)(1-t^6)$	$1+5t^3+6t^4+2t^5+3t^6+4t^7+2t^8+t^9$
$P\bar{6}$	$-(\widetilde{P6})$	$(1-t)^3(1-t^2)^3(1-t^3)^2$	$1+2t^2+6t^3+2t^4+t^6$
$P6/m$	$(\widetilde{P6}), m_3$	$(1-t)^2(1-t^2)^4(1-t^3)(1-t^6)$	$1+5t^3+6t^4+2t^5+3t^6+4t^7+2t^8+t^9$
$P622$	$(\widetilde{P6}), -j_3$	$(1-t)^2(1-t^2)^4(1-t^3)(1-t^6)$	$1+2t^3+6t^4+4t^5+2t^6+4t^7+3t^8+2t^9$
$P6mm$	$(\widetilde{P6}), j_3$	$(1-t)^3(1-t^2)^3(1-t^3)(1-t^6)$	$1+2t^3+3t^4+t^5+t^6+2t^7+t^8+t^9$
$P\bar{6}m2$	$-(\widetilde{P6}), j_3$	$(1-t)^3(1-t^2)^3(1-t^3)^2$	$1+t^2+2t^3+t^4+t^6$
$P\bar{6}2m$	$-(\widetilde{P6}), -j_3$	$(1-t)^2(1-t^2)^4(1-t^3)^2$	$1+t^2+3t^3+5t^4+t^5+t^6$
$P6/mmm$	$(\widetilde{P6}), m_3, j_3$	$(1-t)^2(1-t^2)^4(1-t^3)(1-t^6)$	$1+2t^3+3t^4+t^5+t^6+2t^7+t^8+t^9$

Table 5
Continued

AC	Generators	$D(t)$	$N(t)$
$P23$	$(R3), -m_i$	$(1-t)(1-t^2)^2(1-t^3)^2(1-t^4)$	$1+3t^3+2t^4+2t^5+3t^6+t^9$
$Pm\bar{3}$	$(R3), m_i$	$(1-t)(1-t^2)^2(1-t^3)(1-t^4)(1-t^6)$	$1+3t^3+2t^4+2t^5+3t^6+t^9$
$P432$	$-m_i, -j_i$	$(1-t)(1-t^2)^2(1-t^3)^2(1-t^4)$	$1+t^4+t^5+3t^6$
$P\bar{4}3m$	$-m_i, j_i$	$(1-t)(1-t^2)^2(1-t^3)^2(1-t^4)$	$1+t^3+t^4+t^5+t^6+t^9$
$Pm\bar{3}m$	m_i, j_i	$(1-t)(1-t^2)^2(1-t^3)(1-t^4)(1-t^6)$	$1+t^3+t^4+t^5+t^6+t^9$

[a]Their denominator and numerator are $D(t)$ and $N(t)$. The Molien functions of the 3D rhombohedral Bravais system are those of the 2D hexagonal system; the correspondence which gives these functions are given in the caption of Table 4.

The matrices in (40), (41) and the three j_i of (10) generate the contragradient representations of the I-cubic arithmetic classes. The matrices j_i generate the permutation group $\mathscr{S}_3$ which is a subgroup of $\mathscr{S}_4 \times Z_2$ of permutations up to a sign and this group is isomorphic to O_h. So the σ representation of $Im\bar{3}m$ is the natural four-dimensional representation of $\mathscr{S}_4 \times Z_2(I_4)$, and the γ representation is obtained by forgetting the factor $-I_4$. We have solved the linearization of the action of $Im\bar{3}m$ on BZ and also for the 15 other I-groups P^z; indeed their ρ representation is obtained by restriction to these subgroups.

It is straightforward to compute the corresponding Molien functions. They are given in the first $\frac{2}{3}$ of Table 6.

3.3. *Case 3*: *the eight F-arithmetic classes* $\dim \rho(P^z) = 12$

The contragradient representations of the P^z groups of the eight F arithmetic classes are generated by the matrices $\pm f_i^{\top}$ and j_i. The matrices $f_i^{\top}$ transform the coordinates k_i of a vector of the reciprocal space either into themselves or into the difference of two coordinates. To linearize the action on BZ we are led to introduce the following expressions:

$$k_4 = k_2 - k_3, \quad k_5 = k_3 - k_1, \quad k_6 = k_1 - k_2, \quad \text{so } k_4 + k_5 + k_6 = 0 . \tag{43}$$

The action of the $f_i^{\top}$ on the k_i, $i = 1,2,3$ induces an orthogonal action on the k_α, $\alpha = 1,2,3,4,5,6$; indeed the corresponding orthogonal symmetric matrices $\sigma(f_i^{\top})$ are:

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} . \tag{44}$$

Similarly, the σ representation of the j_i is

$$\sigma(j_i) = j_i \oplus -j_i \ . \tag{45}$$

Table 6
Molien functions of the ρ representations of the three-dimensional arithmetic groups of I and F lattices[a]

AC	Generators	$D(t)$	$N(t)$
$I222$	$-f_3, -f_1$	$(1-t)^2(1-t^2)^4(1-t^4)^2$	$1+4t^2+10t^3+11t^4+12t^5+11t^6+10t^7+4t^6+t^{10}$
$Imm2$	$-f_3, f_1$	Same as $I222$	Same as $I222$
$Immm$	f_i	$(1-t)(1-t^2)^7$	$1+7t^3+7t^4+t^7$
$I4$	$(I\tilde{\bar{4}})$	$(1-t)^2(1-t^2)^4(1-t^4)^2$	$1+3t^2+12t^3+12t^4+8t^5+12t^6+12t^7+3t^8+t^{10}$
$I\bar{4}$	$-(I\tilde{\bar{4}})$	Same as $I4$	Same as $I4$
$I4/m$	$(I\tilde{\bar{4}}), f_3$	$(1-t)(1-t^2)^5(1-t^4)^2$	$1+9t^3+14t^4+8t^5+8t^6+14t^7+9t^8+t^{11}$
$I422$	$(I\tilde{\bar{4}}), -f_1$	$(1-t)(1-t^2)^5(1-t^4)^2$	$1+t^2+8t^3+11t^4+11t^5+11t^6+11t^7+8t^8+t^9+t^{11}$
$I4mm$	$(I\tilde{\bar{4}}), f_1$	$(1-t)^2(1-t^2)^4(1-t^4)^2$	$1+2t^2+6t^3+5t^4+4t^5+5t^6+6t^7+2t^8+t^{10}$
$I\bar{4}m2$	$-(I\tilde{\bar{4}}), f_1$	Same as $I422$	Same as $I422$
$I\bar{4}2m$	$-(I\tilde{\bar{4}}), j_3$	Same as $I4$mm	Same as $I4$mm
$I4/mmm$	j_3, f_i	$(1-t)(1-t^2)^5(1-t^4)^2$	$1+5t^3+6t^4+4t^5+4t^6+6t^7+5t^8+t^{11}$
$I23$	$-f_i, (R3)$	$(1-t)^2(1-t^2)^3(1-t^3)^2$ $(1-t^4)$	$1+2t^3+7t^4+4t^5+7t^6+2t^7+t^{10}$
$Im\bar{3}$	$f_i, (R3)$	$(1-t)(1-t^2)^3(1-t^3)$ $(1-t^4)^2(1-t^6)$	$1+2t^3+5t^4+8t^5+12t^6+14t^7+12t^8+14t^9+12t^{10}+8t^{11}$ $+5t^{12}+2t^{13}+t^{16}$
$I432$	$-f_i, -j_i$	$(1-t)(1-t^2)^3(1-t^3)^2$ $(1-t^4)^2$	$1+t^3+6t^4+7t^5+9t^6+9t^7+7t^8+6t^9+t^{10}+t^{13}$
$I\bar{4}3m$	$-f_i, j_i$	$(1-t)^2(1-t^2)^2(1-t^3)^2$ $(1-t^4)^2$	$1+t^2+2t^3+4t^4+2t^5+4t^6+2t^7+4t^8+2t^9+t^{10}+t^{12}$
$Im\bar{3}m$	f_i, j_i	$(1-t)(1-t^2)^3(1-t^3)$ $(1-t^4)^2(1-t^6)$	$1+2t^3+4t^4+4t^5+4t^6+6t^7+6t^8+6t^9+4t^{10}+4t^{11}$ $+4t^{12}+2t^{13}+t^{16}$
$F222$	$-f_3^\top, -f_1^\top$	$(1-t)^3(1-t^2)^9$	$1+9t^2+27t^3+27t^4+27t^5+27t^6+9t^7+t^9$
$Fmm2$	$-f_3^\top, f_1^\top$	$(1-t)^5(1-t^2)^7$	$1+6t^2+9t^3+9t^4+6t^5+t^7$
$Fmmm$	$f_i^\top$	$(1-t)^3(1-t^2)^9$	$1+3t^2+13t^3+15t^4+15t^5+13t^6+3t^7+t^9$
$F23$	$-f_i^\top, (R3)$	$(1-t)(1-t^2)^7(1-t^3)^4$	$1+21t^3+58t^4+70t^5+104t^6+178t^7+178t^8+104t^9$ $+70t^{10}+58t^{11}+21t^{12}+t^{15}$
$Fm\bar{3}$	$f_i^\top, (R3)$	$(1-t)(1-t^2)^5(1-t^3)^2$ $(1-t^4)^2(1-t^6)^2$	$1+13t^3+33t^4+58t^5+127t^6+221t^7+332t^8+501t^9+641t^{10}$ $+726t^{11}+803t^{12}+803t^{13}+726t^{14}+641t^{15}+501t^{16}$ $+332t^{17}+221t^{18}+127t^{19}+58t^{20}+33t^{21}+13t^{22}+t^{25}$
$F432$	$-f_i^\top, -j_i$	$(1-t)(1-t^2)^4(1-t^3)^4$ $(1-t^4)^3$	$1+t^2+10t^3+32t^4+67t^5+135t^6+220t^7+335t^8+447t^9$ $+494t^{10}+480t^{11}+422t^{12}+329t^{13}+231t^{14}+144t^{15}$ $+66t^{16}+29t^{17}+11t^{18}+2t^{19}$
$F\bar{4}3m$	$-f_i^\top, j_i$	Same as $F432$	Same as $F432$
$Fm\bar{3}m$	$f_i^\top, j_i$	$(1-t)(1-t^2)^4(1-t^3)^2$ $(1-t^4)^3(1-t^6)^2$	$1+7t^3+18t^4+35t^5+75t^6+137t^7+233t^8+364t^9+484t^{10}$ $+613t^{11}+730t^{12}+770t^{13}+759t^{14}+714t^{15}+614t^{16}$ $+489t^{17}+358t^{18}+226t^{19}+142t^{20}+85t^{21}+36t^{22}+15t^{23}$ $+6t^{24}+t^{25}$

[a]Their denominator and numerator are $D(t)$ and $N(t)$.

To obtain the matrices of the γ representations one replaces the elements -1 of the σ matrices of (44), (45) by 1. We have thus obtained the $\rho = \sigma \oplus \gamma$ linearizing representation; it has dimension 12.

The corresponding Molien functions are given in the last part of Table 6.

4. The module of invariants on *BZ* for the two-dimensional arithmetic classes

We have established the linear four-dimensional ρ representations of the eight orthogonal two-dimensional arithmetic classes in Section 3.1 and given the corresponding Molien functions in Table 4. It is easy to write the module of $\rho(P^z)$ invariants. Then, using the algebraic equations (20) of the BZ we can eliminate the s_i variables from the module ring (after it has been made into a form containing only s_i^2's). We find that the final result is still a module of invariants.

Let us illustrate the general method by the simplest case: $p2 = Z_2(-I_2)$. Since $\rho(-I_2)c_i = c_i$, $\rho(-I_2)s_i = -s_i$, as suggested by the Molien function in Table 4, the corresponding module is $R^{p2} = P[c_1, c_2, s_1^2, s_2^2] \bullet (1, s_1 s_2)$. Using the BZ equations: $s_i^2 = 1 - c_i^2$ we obtain for the module of invariants on the BZ: $\mathscr{R}^{p2} = P[c_1, c_2] \bullet (1, s_1 s_2)$. That is the generalization of the one-dimensional case studied at the end of the introduction; because of the existence of a non-trivial numerator invariant in the module corresponding to $\rho(p2)$, the module on the BZ, $\mathscr{R}^{p2}$ has dimension 2.

The trivial case $p1 = 1$ is slightly more complicated! Corresponding to the trivial ρ representation $R = P[c_1, c_2, s_1, s_2]$ (obviously, all polynomials). But, to use the BZ equations we have to transform the polynomial ring R into a four-dimensional module over a sub polynomial ring, repeating twice the transformation explained in Chapter I, Section 5: $R^{p1} = P[c_1, c_2, s_1^2, s_2^2] \bullet (1, s_1)(1, s_2)$. We obtain on the BZ:

$$\mathscr{R}^{p1} = P[c_1, c_2] \bullet (1, s_1)(1, s_2) . \tag{46}$$

That is Eq. (121) from Chapter I, Section 5.5.3, obtained from a different point of view, of the module of polynomial on a 2-D torus. The two other cases of the first line of Table 2, the γ representations are trivial so the ring of the modules on BZ are the same: $P[c_1, c_2]$; so we have to obtain a submodule of $\mathscr{R}^{P1}$. For *pm* we want to treat together the two groups $pm_{(i)}$, $i = 1, 2$ depending on whether the symmetry axis is the axis 1 or 2. Then s_i is invariant. The group *p2mm* is generated by the two groups $pm_{(1)}$ and $pm_{(2)}$ so its ring of invariants is the intersection of the two rings. It is $P[c_1, c_2]$, i.e. a polynomial ring; it is the direct generalization of the one-dimensional case. Notice that *p2mm* is a group generated by reflection.

The four arithmetic classes of the second line of Table 2 have the same γ representation; its image is *cm*, a reflection group. The ring of its invariant is $P[c_1 + c_2, c_1 c_2]$. On this module we obtain for $P1$ (i.e. for all polynomials on BZ):

$$\mathscr{R}^{p1} = P[c_1 + c_2, c_1 c_2] \bullet (1, s_1)(1, s_2) . \tag{47}$$

We want again to compute the invariants for both of the two-element reflection groups $Z_2(cm)$; we denote them by $cm_{(\pm)}$ ($cm_{(+)}$ is the *cm* of Table 1). With $\varepsilon = \pm 1$ we make both computations together:

$$\begin{aligned} R^{cm} &= P[c_1 + c_2, c_1 c_2, s_1 + \varepsilon s_2, (s_1 - \varepsilon s_2)^2] \bullet (1, (c_1 - c_2)(s_1 - \varepsilon s_2)) \\ &= P[c_1 + c_2, c_1 c_2, s_1^2 + s_2^2, s_1 s_2] \bullet (1, s_1 + \varepsilon s_2)(1, (c_1 - c_2)(s_1 - \varepsilon s_2)) \\ &= P[c_1 + c_2, c_1 c_2, s_1^2 + s_2^2, s_1^2 s_2^2] \bullet (1, s_1 + \varepsilon s_2)(1, s_1 s_2)(1, (c_1 - c_2)(s_1 - s_2)) . \end{aligned}$$

Table 7
Modules of invariant polynomials on the Brillouin zone for the 13 arithmetic classes in dimension 2[a]

	Class	θ_1	θ_2	φ_1	φ_2	φ_3	dim
	$p1$	c_1	c_2	s_1	s_2	$s_1 s_2$	4
B	$p2$	c_1	c_2	$s_1 s_2$			2
	$pm_{(i)}$	c_1	c_2	$s_{(i)}$			2
B	$p2mm$	c_1	c_2				1
	$cm_{(+)}$	$c_1 + c_2$	$c_1 c_2$	$s_1 + s_2$	$s_1 s_2$	$c_1 s_2 + c_2 s_1$	4
	$cm_{(-)}$	$c_1 + c_2$	$c_1 c_2$	$s_1 - s_2$	$s_1 s_2$	$-c_1 s_2 + c_2 s_1$	4
B	$c2mm$	$c_1 + c_2$	$c_1 c_2$	$s_1 s_2$			2
T	$p4$	$c_1 + c_2$	$c_1 c_2$	$(c_1 - c_2) s_1 s_2$			2
B	$p4mm$	$c_1 + c_2$	$c_1 c_2$				1
	$p3$	$c_1 + c_2 + c_1 c_2 - s_1 s_2$	$c_1 c_2 (c_1 c_2 - s_1 s_2)$	ϕ_1^{-+}	ϕ_2^{--}	$\phi_3^{+-} = \phi_1^{-+} \phi_2^{--}$	4
	$p3m1$	$c_1 + c_2 + c_1 c_2 - s_1 s_2$	$c_1 c_2 (c_1 c_2 - s_1 s_2)$	ϕ_1^{-+}			2
	$p31m$	$c_1 + c_2 + c_1 c_2 - s_1 s_2$	$c_1 c_2 (c_1 c_2 - s_1 s_2)$	ϕ_2^{--}			2
T	$p6$	$c_1 + c_2 + c_1 c_2 - s_1 s_2$	$c_1 c_2 (c_1 c_2 - s_1 s_2)$	ϕ_3^{+-}			2
B	$p6mm$	$c_1 + c_2 + c_1 c_2 - s_1 s_2$	$c_1 c_2 (c_1 c_2 - s_1 s_2)$				1

[a]Time reversal restricts to the seven cases indicated in the 1st column by T, or B when it is a Bravais group. The dimension of the modules is given in the last column. As rings, all the modules of the table have from 2 to 4 generators.
$\phi_1^{-+} = s_1 + s_2 - (c_1 s_2 + c_2 s_1)$,
$\phi_2^{--} = s_1 - s_2 + c_1 s_2 - c_2 s_1 + 2(c_1 - c_2)(c_1 s_2 + c_2 s_1)$,
$(\phi_1^{-+})^2 = 1 - 2\theta_1 + \theta_1^2 - 4\theta_2$.
$(\phi_2^{--})^2 = 2 + 4\theta_1 + \theta_1^2 + 20\theta_2 - 2\theta_1^3 + 20\theta_1\theta_2 - \theta_1^4 + 4\theta_1^2\theta_2 - 4\theta_2^2$.

Using the two equations $s_i^2 = 1 - c_i^2$ of the BZ, we obtain

$$P[c_1 + c_2, c_1 c_2]\bullet(1, s_1 + \varepsilon s_2, s_1 s_2, (c_1 - c_2)(s_1 - \varepsilon s_2)) . \tag{48}$$

This is indeed a submodule of (47) and could have been obtained directly. In Table 7 we give a different expression for the last numerator invariant by using the relation: $(c_1 - c_2)(s_1 - \varepsilon s_2) = (c_1 + c_2)(s_1 + \varepsilon s_2) - 2(\varepsilon c_1 s_2 + c_2 s_1)$.

Since $c2mm$ is generated by the groups $cm_{(\pm)}$, its module of polynomial invariants is the intersection of the module of these two groups.

Let us compute the module of invariants of $\rho(p4)$ as a submodule of (47). The matrix $(p4)$ transforms s_1 into s_2 and s_2 into $-s_1$. So s_1, s_2 form the basis of a two-dimensional, irreducible on the real, representation of the group $p4$ and $s_1 s_2$ is a pseudoinvariant. As we saw, from Table 2, the γ representation of $(p4)$ is the matrix (cm) which exchanges c_1, c_2; hence $c_1 - c_2$ is a pseudo-invariant and the module of $p4$ is

$$\mathscr{R}^{p4} = P[c_1 + c_2, c_1 c_2]\bullet(1, (c_1 - c_2) s_1 s_2) . \tag{49}$$

The group $p4mm$ is generated by its two subgroups $c2mm$ and $p4$; hence the module of invariant polynomials of $p4mm$ is the intersection of the modules of its two generating subgroups. Thus we have finished the second part of Table 7.

The results for the five hexagonal arithmetic classes are obtained from the modules of the five rhombohedral classes and given in Table 7. They are modules of invariants, but with inhomogenous polynomials. The four generators of $\mathscr{R}^{p3}$ have been obtained through brute force computations. Then it is easy to find the submodules corresponding to the four other hexagonal groups. The invariants of $p3m1$ must be invariant by its subgroup $cm_{(+)}$; that choose ϕ_1^{-+}. Similarly the invariants of $p31m$ must be invariant by its subgroup $cm_{(-)}$; that choose ϕ_2^{--}. The group $p2$ leaves invariant c_i and changes the sign of s_i. So it changes the sign of ϕ_1^{-+} and ϕ_2^{--} and leaves invariant their product ϕ_3^{+-}; hence the basis of the module of $p6$, submodule of that of $p3$. The group $p6mm$ is generated by the four other hexagonal groups; its module is the intersection of their modules.

In Table 7 the module structure for each group is verified by forming all equations (Chapter I, Section 5, Eq. (78)) for the φ_α polynomials. The verification is easy for the orthogonal classes; it is given in the caption of Table 7 for the hexagonal ones.

4.1. General remarks

We want to gather different remarks we made for the construction of the Table 7; indeed they are very general and allow us to build a strategy for making the tables of the 3-D arithmetic classes.

(i) Study together the P^z whose modules have the same ring $P[\theta_1(c_i), \theta_2(c_i), \theta_3(c_i)]$; e.g. for the 33 orthogonal arithmetic classes, that gives three families which are given in Table 2. The ring depends only on the image of the representation γ and for the last two lines of Table 2, $R3$ and $R3m$ have the same denominator invariants (cf. Chapter I, Section 5, Table 4). Then we have to compute the module of the ρ representations of the smallest groups in each family as well as those not generated by their subgroups in the family and take their quotient by the ideal defined by the equations of BZ. It is remarkable that in our case the module structure passes to the quotient (notice that the ideal is contained in the ring of the module of ρ), but we do know from the first method that the ring of invariant of any P^z is a submodule of $\mathscr{R}^{P1}$.

(ii) The module of invariants of a P^z is a submodule of the modules of its subgroups. More precisely, when P^z is generated by some subgroups its module is the intersection of the modules of the generating subgroups. The intersection is very easily made inside a family with a common ring for the modules.

(iii) When a small P'^z is an invariant subgroup of P^z in the same family and the quotient P^z/P'^z is Abelian (e.g. P'^z is a subgroup of index 2 of P^z) we can generally choose the basis of its module of P'^z-invariants on BZ such that the basis polynomials are either invariants or pseudo-invariants (i.e. change of sign) for the larger group P^z. Then the module of P^z is the submodule of that of P'^z whose basis is made of the P'^z basis polynomials invariant by P^z.

(iv) The weak condition that the invariants of the groups containing P^z as a subgroup must be invariant by P^z is a good check for the consistency of the tables and can even help to build them!

5. The module of invariants on BZ for the three-dimensional P, C, A, R arithmetic classes

The results of this section are summarized in the four Tables 8–10, 12. We begin first with the 33 orthogonal classes. Table 2 shows that there are only 4 different γ representations. The groups $P1$

Table 8
Bases of the modules of invariant polynomials on the three-dimensional *BZ* for the eight arithmetic classes *P* triclinic, monoclinic, orthorhombic[a]

	Class	s_1	s_2	s_3	s_2s_3	s_3s_1	s_1s_2	$s_1s_2s_3$	d
	$P1$	x	x	x	x	x	x	x	8
B	$P\bar{1}$				x	x	x		4
	$P2$			x			x	x	4
	Pm	x	x				x		4
B	$P2/m$						x		2
	$P222$							x	2
	$Pmm2$			x					2
B	$Pmmm$								1

[a]The common ring of these modules is $P[c_1, c_2, c_3]$. The module dimensions are 1, 2, 4, 8 (last column). Their bases contain 1 and the polynomials marked by the x's. Time reversal restricts to the three cases indicated by a B (for Bravais group) in the 1st column. Four of these groups are invariant subgroups of $Pm\bar{3}m$, the symmetry group of the cube. In this group, for each of the four other classes, there are three groups, labelled by the preferred axis $i = 1, 2, 3$, forming one conjugacy class. With i, j, k as a permutation of 1, 2, 3, here are their modules:
$\mathscr{R}(Pm_{(i)}) = P[c_1, c_2, c_3]\bullet(1,\ s_j,\ s_k,\ s_js_k)$,
$\mathscr{R}(P2_{(i)}) = P[c_1, c_2, c_3]\bullet(1,\ s_i,\ s_j\ s_k,\ s_1s_2s_3)$,
$\mathscr{R}(P2/m_{(i)}) = P[c_1, c_2, c_3]\bullet(1,\ s_js_k)$, $\mathscr{R}(Pmm2_{(i)}) = P[c_1, c_2, c_3]\bullet(1,\ s_i)$.
As rings the modules of the table have from 3 to 6 generators.

(trivial), *Cm*, *R3m* are reflection groups. Their rings of invariants are, respectively,

$$\mathscr{R}^{P_1} = P[c_1, c_2, c_3], \quad \mathscr{R}^{Cm} = P[c_1 + c_2, c_1c_2, c_3] ,$$
$$\mathscr{R}^{R3m} = P[c_1 + c_2 + c_3,\ c_1^2 + c_2^2 + c_3^2,\ c_1c_2c_3] . \tag{50}$$

The group *R*3 is a unimodular subgroup of the reflection group *R3m*, so its module of invariants has the same ring. The three rings of (50) are also the ring of the module of invariants over *BZ*.

5.1. The triclinic, P-monoclinic, P-orthorhombic classes

So the first polynomial ring of (50) (all polynomials in c_i) is the ring of the modules of the eight arithmetic classes of line 3 (first line for $d = 3$) of Table 2. We give the eight corresponding modules in Table 8. We have already explained in the previous section the construction of the module for the trivial group: $\mathscr{R}^{P1} = P[c_1, c_2, c_3]\bullet(1, s_1)(1, s_2)(1, s_3)$; this is the eight-dimensional module of the polynomials on a 3-D torus. The seven other modules of Table 8 are submodules of $\mathscr{R}^{P1}$. Since the σ representations of the seven other groups of Table 8 are diagonal, the eight elements of $\mathscr{R}^{P1}$ are either invariants or pseudoinvariants for each of these groups. Hence we can apply the strategy of Section 4.1(iii): The three elements s_1, s_2, s_3 of the basis of the module $\mathscr{R}^{P1}$ generate the four following elements in Table 8; to construct the other modules one needs only the action of P^z on the s_i: *Pm* changes the sign of s_3, *P*2 that of s_1 and s_2, $P\bar{1}$ changes the signs of the three s_i. Hence the next three lines of Table 8 are obtained by keeping only the invariants of these three groups.

P2/m is generated by all previous groups in Table 8; so its module is the intersection of the four previous ones: its basis is $(1, s_1s_2)$. The next two groups, *P*222, *Pmm*2, contain *P*2 and do not

Table 9
Bases of the modules of invariant polynomials on the three-dimensional BZ for the 15 arithmetic classes whose label begins with $C, A, P4$: monoclinic C, orthorhombic C, tetragonal P[a]

	arith. cl.	s_3	s_+	s_-	s_{3+}	s_{12}	s_{123}	c_-s_3	c_-s_+	c_-s_-	c_-s_{3-}	c_-s_{12}	c_-s_{123}	d
	$C2$			x	x	x		x	x		x		x	8
	Cm	x	x		x	x	x			x	x			8
B	$C2/m$				x	x					x			4
	$C222$					x		x					x	4
	$Cmm2$	x				x	x							4
	$Amm2$			x		x			x					4
B	$Cmmm$					x								2
	$P4$	x										x	x	4
	$P\bar{4}$						x	x				x		4
T	$P4/m$											x		2
	$P422$												x	2
	$P4mm$	x												2
	$P\bar{4}2m$						x							2
	$P\bar{4}m2$							x						2
B	$P4/mmm$													1

[a]These modules are over the polynomial ring $P[c_+, c_{12}, c_3] \equiv P[c_1 + c_2, c_1c_2, c_3]$. The P^z groups of the Table have 2, 4, 8, 16 elements and the dimension of the corresponding modules are, respectively, 8, 4, 2, 1. Time reversal restricts to the arithmetic classes indicated in the first column by T or by B for the Bravais groups of lattices. In order to make easier the verification that the module of an arithmetic class G is a submodule of the modules of the smaller classes ($< G$), we add to the table the eight-dimensional module of $C2'$, represented by the matrix m_3j_3 and Cm' represented by $-m_3j_3$.

$\mathscr{R}^{C2'} = P[c_1 + c_2, c_1c_2, c_3]\bullet(1, s_+, c_-s_3, c_-s_-, s_{12}, s_{3-}, c_-s_{3+}, c_-s_{123})$,

$\mathscr{R}^{Cm'} = P[c_1 + c_2, c_1c_2, c_3]\bullet(1, s_3, s_-, c_-s_+, s_{12}, s_{3-}, c_-s_{3+}, s_{123})$.

As rings, the number of generators of these 15 modules is 3 (for $P4/mmm$), 4, 5 (for $C222, Cmm2, P4$), 6 (for $C2/m, Amm2, P\bar{4}$), 7 (for Cm), 9 (for $C2$).

We use the following shorthands:

a_i for c_i or s_i: $a_\pm = a_1 \pm a_2$, $a_{12} = a_1a_2$, $a_{3\pm} = a_3(a_1 \pm a_2)$, $a_{123} = a_1a_2a_3$.

contain $P2/m$; so each one keeps one of the two invariants of $P2$ not invariants of $P2/m$. By its definition, $Pmm2$ leaves s_3 invariant. Finally, since $Pmmm$ contains all seven previous groups, its module has dimension one, i.e. it is the polynomial ring in the c_i's. This is also obvious from the fact that $\sigma(Pmmm)$ is a reflection group containing three reflections changing the sign of each s_i separately. These results are gathered in Table 8.

5.2. The C-monoclinic, C-orthorhombic, P-tetragonal classes

The 15 orthogonal arithmetic classes of the fourth and fifth lines of Table 2 have the same γ representation, that of Cm; the ring of their modules of invariants is the second of (50). On this ring we have for the module of polynomials on BZ:

$$\mathscr{R}^{P1} = P[c_1 + c_2, c_1c_2, c_3]\bullet(1, c_1 - c_2)(1, s_1)(1, s_2)(1, s_3) . \quad (51)$$

The two smallest groups in this list are C_2 and C_m. Table 1 gives their σ representations: $Z_2(-j_3)$ and $Z_2(j_3)$, respectively. The eigen polynomials of the γ and σ representations are linear

Table 10
Bases of the modules of invariant polynomials on the three-dimensional BZ for the 10 arithmetic classes of the rhombohedral and the P-cubic Bravais classes[a]

	arith. cl.	s	$s.s$	$s.s.s$	cs	$c.s.s$	c^2s	$c^2.s.s$	ζ	$(s)(\zeta)$	$(s.s)(\zeta)$	$(s.s.s)(\zeta)$	$c[s]$	$c^2[s]$	$cs[s]$	$c^2s[s]$	d
	$R3$	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	16
T	$R\bar{3}$		x			x		x	x		x			x		x	8
	$R32$		x			x		x		x		x	x		x		8
	$R3m$	x	x	x	x	x	x	x									8
B	$R\bar{3}m$		x			x		x									4
	$P23$			x					x			x					4
T	$Pm\bar{3}$								x								2
	$P432$											x					2
	$P\bar{4}3m$			x													2
B	$Pm\bar{3}m$																1

[a]These modules are over the ring $P[c, c^2, c.c.c] \equiv P[c_1 + c_2 + c_3,\ c_1^2 + c_2^2 + c_3^2,\ c_1c_2c_3]$.

The groups P^z of 3, 6, 12, 24, 48 elements have modules of dimensions 16, 8, 4, 2, 1, respectively. The arithmetic classes satisfying time reversal are indicated in the first column by T or, when it is a Bravais class of lattices, by B.

The invariant polynomials of $R\bar{3}m, R\bar{3}$ (respectively, those of $R3m, R32$ not invariant by $R\bar{3}m$) are of even (odd) degree in the variables s_i; the invariant polynomials of $R\bar{3}m, R3m$ (respectively, those of $R\bar{3}, R32$ not invariant by $R\bar{3}m$) are even (odd) under permutations of the variable indices. As rings, the numbers of generators of these modules are 3, 4, 5, 6, 8 (for $R\bar{3}$), 9 (for $R3m$), 10 (for $R32$), 14 (for $R3$). For $R3$ notice that three invariants are a product of two other invariants and that $s.s = \frac{1}{2}((s)^2 + c^2 - 3)$.

Notations. We use a short code for labelling the invariant polynomials. Let i, j, k a circular permutation of 1,2,3. $\sum'$ is the sum over circular permutations. a_i, b_i are expressions with index i, e.g. $c_i, c_i^2, s_i, c_is_i, c_i^2s_i$; we introduce the shorthands: $a = \sum_i a_i$, $ab = \sum_i a_ib_i$, $a.a = \sum' a_ia_j$, $a.a.a = a_1a_2a_3$, $a.b = \sum'(a_ib_j + b_ia_i)$, $a.b.b = \sum' a_ib_jb_k = b.b.a$, $a[b] = \sum' a_i(b_j - b_k) = -b[a]$. If the obtained polynomial is multiplied by an overall integer factor $\neq 1$, drop it. For product or power of these invariants, we write each factor between ( ).

Example for the code: $\zeta = :c[c^2] = \sum' c_i(c_j^2 - c_k^2)$.

combination of c_i's and s_i's. To write them, it is convenient to use the following shorthands:

$$a_i \text{ for } c_i \text{ or } s_i\text{: } a_\pm = a_1 \pm a_2,\ a_{12} = a_1a_2,\ a_{3\pm} = a_3a_\pm,\ a_{123} = a_{12}a_3\ . \tag{52}$$

Then (51) can be written as

$$\mathscr{R}^{P1} = P[c_+, c_{12}, c_3]\bullet(1, c_-)(1, s_+, s_-, s_{12})(1, s_3)\ . \tag{53}$$

The eigen polynomials of the common γ representation are c_+, c_3, as invariants and c_- as pseudoinvariants. For $\sigma(Cm)$, change c by s in the previous statement. For $\sigma(C2)$ exchange the words invariants and pseudoinvariants from $\sigma(Cm)$. This leads to the module of these two groups; their basis are, respectively,

$$N_{Cm} = 1, s_3, s_+, s_{3+}, s_{12}, s_{123}, c_-s_-, c_-s_{3-}\ ,$$

$$N_{C2} = 1, s_-, s_{3+}, s_{12}, c_-s_3, c_-s_+, c_-s_{3-}, c_-s_{123}\ . \tag{54}$$

These results form the first two lines of Table 9. The third line of the table is their intersection since $C2/m$ is generated by $C2$ and Cm. The three next groups of Table 9 are generated by the following pairs of groups (see Table 1):

$$C222 = \langle C2, P2 \rangle, \quad Cmm2 = \langle Cm, P2 \rangle, \quad Amm2 = \langle C2, Pm \rangle \ . \tag{55}$$

As we show in (51), one transforms the modules of Table 8, into modules with the ring of Table 9 by multiplying their module basis by $(1, c_-)$; that yields for $P2$ and Pm:

$$\mathscr{R}^{P2} = P[c_+, c_{12}, c_3] \bullet (1, c_-)(1, s_3, s_{12}, s_{123}) \ ,$$
$$\mathscr{R}^{Pm} = P[c_+, c_{12}, c_3] \bullet (1, c_-)(1, s_1, s_2, s_{12}) \ . \tag{56}$$

Thus, from (55), we obtain the modules for $C222, Cmm2, Amm2$ by taking the intersections of the modules in (56) with those of the first two lines of Table 9. The group $Cmmm$ contains the first six groups of Table 9; they generate it. So the $Cmmm$ module is the intersection of the six modules of the lines above it.

We have noted earlier that the groups $Cmm2, P4, P4mm$ are, respectively, the direct sums $c2mm \oplus I$, $p4 \oplus I$, $p4mm \oplus I$. So the basis polynomials of their respective modules are s_3 for all of them, and for $Cmm2, P4$, respectively, s_{12}, $c_- s_{12}$ from Table 7 and their products with s_3. The cyclic group $P\bar{4}$ is generated by the matrix $(P\bar{4})^{-1} = p4 \oplus -I$. So, as for $P4$, $c_- s_{12}$ is one of its basis invariant polynomial while s_3 is a pseudoinvariant; since c_- and s_{12} are also pseudoinvariant, the two other invariants are $s_3 c_-$ and $s_3 s_{12}$.

From Fig. 2 of Chapter I, Section 3 we verify that the next five groups of Table 9 are each generated by two subgroups of the same table:

$$P4/m = \langle P4, P\bar{4} \rangle, \quad P422 = \langle P4, C222 \rangle, \quad P4mm = \langle P4, Cmm2 \rangle \ ,$$
$$P\bar{4}2m = \langle P\bar{4}, Cmm2 \rangle, \quad P\bar{4}m2 = \langle P\bar{4}, C222 \rangle \ . \tag{57}$$

So the module of invariants of these five groups is the intersection of the modules of invariants of the two subgroups.

The group $P4/mmm$ contains the 14 other groups of Table 9 as subgroups; they generate it. So its module of invariants is of dimension 1.

5.3. The rhombohedral and P-cubic classes

The module $\mathscr{R}^{R3}$ of invariant polynomials on BZ, has dimension 16. This module is reproduced in the first line of Table 10.

$R\bar{3} = R3 \times Z_2(-I_3)$ where $-I_3$ is the symmetry through the origin, changes the sign of s_i and leaves invariant c_i in its ρ representation. So the module of $R\bar{3}$ is the submodule of $R3$ whose basis elements (= numerator invariants) are of even degree in s_i.

The group $R3m$ is the group of permutation of coordinates of both, the direct and the reciprocal space; $R3$ is the subgroup of even permutations. So the module of $R3m$ is the submodule of $R3$ whose basis elements are also invariant by odd permutations (i.e they do not contain expressions of the type $a[b]$).

Similarly the module of $R32$ is the submodule of $R3$ whose basis elements are invariant under the product of an odd permutation and a change of sign of s_i. The module of $R\bar{3}m$ is the intersection of the four previous modules.

Table 2 shows that the *P*-cubic groups belong to the same family. The five cubic-P groups are generated by their common invariant subgroup *P*222 and their respective rhombohedral subgroup (see for instance Chapter 1, Section 3, Fig. 2). The module of invariants of *P*222 is given in Table 8: $\mathscr{R}^{P222} = \mathscr{P}[c_1, c_2, c_3]\bullet(1, s.s.s)$. As a direct application of Chapter I, Section 5, Theorem Chevalley 2 the ring of polynomials in the three variables c_i is a dimension $|P3m| = 6$ module on the polynomial ring $\mathscr{P}[c, c^2, c.c.c]$ of the family we study, so $\mathscr{R}^{P222}$ is a dimension 12 module on the family polynomial ring. Its intersection with $\mathscr{R}^{R3}$ is $\mathscr{P}[c, c^2, c.c.c]\bullet(1, c[c^2])(1, s.s.s) = \mathscr{R}^{P23}$, the 6th line of Table 10. The intersection of this module with those of $R\bar{3}$, *R*32, *R*3*m*, $R\bar{3}m$ can be read directly from the first six lines of the table and yields its last four lines.

5.4. The three-dimensional hexagonal system

This system has 16 arithmetic classes. Between the maximal one: $|P6/mmm| = 24$ and the minimal one $|P3| = 3$ there are two sets of seven classes whose groups have 12 and six elements, respectively.

Fig. 4 of Chapter I gives the incidence relations between these two sets of seven groups; for the convenience of the reader we give these data in an easier form in Table 11.

We know from Table 3 that the γ representation of these 16 groups is either $R3\oplus I$ or $R3m\oplus I$; that leads to the same ring for all the modules of Table 12: $P[\theta_1, \theta_2, c_3]$, where the θ_i are the two invariants of the polynomial ring of the modules of the 2-D hexagonal groups. Table 3 also tells us how to proceed for constructing the module bases for the 3-D hexagonal family.

To pass from the line *h* to the line *H* of Table 3 we add the invariant s_3 and its products with the ϕ's. This gives the invariants of the module basis of *P*3. This group is an invariant subgroup of the 15 other groups of Table 12. Their modules are strict submodules of the eight-dimensional module of *P*3. The rest of the line *H* of Table 3 gives the module of *P*3*m*1, *P*31*m*, *P*6, *P*6*mm*. To pass to the line H_h, since m_3 changes the sign of s_3 independently, keep only the ϕ_i invariants. This gives the module of $P\bar{6}$, $P\bar{6}m2$, $P\bar{6}2m$, *P*6/*m*, *P*6/*mmm*.

To pass from line *H* to H_-, one has to keep only the invariants quadratic in the s_i: $\phi_1 s_3$, $\phi_2 s_3$, $\phi_1\phi_2$. That gives the modules of $P\bar{3}$, $P\bar{3}m1$, $P\bar{3}1m$ and again of *P*6/*m*, *P*6/*mmm*.

Table 11
Partial order of 14 hexagonal arithmetic classes for $d = 3$[a]

	$P\bar{3}$	*P*312	*P*321	*P*6	*P*31*m*	*P*3*m*1	$P\bar{6}$
*P*622		x	x	x			
$P\bar{3}1m$	x	x			x		
$P\bar{3}m1$	x		x			x	
*P*6/*m*	x			x			x
$P\bar{6}m2$		x				x	x
$P\bar{6}2m$			x		x		x
*P*6*mm*				x	x	x	

[a]For a given six-element group, each column gives the three 12-element group containing it. For a given 12-element group, each line gives the three 6-element groups that it contains. This table has to be symmetric through its first diagonal.

Table 12
Module of polynomial invariants of the three-dimensional hexagonal arithmetic classes[a]

	arithm. cl.	ϕ_1	ϕ_2	$\phi_1\phi_2$	s_3	$\phi_1 s_3$	$\phi_2 s_3$	$\phi_1\phi_2 s_3$	d
	P3	x	x	x	x	x	x	x	8
T	$P\bar{3}$			x		x	x		4
	$P312$	x					x	x	4
	$P321$		x			x		x	4
	$P6$			x	x			x	4
	$P31m$		x		x		x		4
	$P3m1$	x			x	x			4
	$P\bar{6}$	x	x	x					4
	$P622$							x	2
T	$P\bar{3}1m$						x		2
T	$P\bar{3}m1$					x			2
T	$P6/m$			x					2
	$P\bar{6}m2$	x							2
	$P\bar{6}2m$		x						2
	$P6mm$				x				2
B	$P6/mmm$								1

[a]The ring of the module is:
$P[\theta_1, \theta_2, \theta_3]$ with $\theta_1 = c_1 + c_2 + c_1c_2 - s_1s_2$, $\theta_2 = c_1c_2(c_1c_2 - s_1s_2)$, $\theta_3 = c_3$. The ϕ's polynomials are those of Table 7:
$\phi_1 = s_1 + s_2 - (c_1s_2 + c_2s_1)$, $\phi_2 = (c_1 - c_2)(s_1 + s_2) - (c_1 + c_2 - 2c_1c_2)(s_1 - s_2)$.
The arithmetic classes with groups of 3, 6, 12, 24 elements have modules of invariants of dimension 8, 4, 2, 1, respectively. Time reversal is satisfied by the five classes indicated in the first column by T or by B for the Bravais class of the hexagonal lattice. As rings, all the modules of the table have from 3 to 6 generators.

As we noted at the end of Section 3.3, case 2b, using this systematic method, we have solved the problem for 13 out of the 16 hexagonal classes. Since the seven invariants must distinguish the seven classes of 12-element group, $\phi_1\phi_2 s_3$ has to be the numerator invariant of $P622$.

The numerator invariant of any 12-element group P^z is also a numerator invariant of its three 6-element subgroups: they are given in Table 11. With this remark we obtain the modules of $P312$ and $P321$; thus we have completed Table 12.

5.5. Modules of C and A arithmetic groups over BZ of primitive lattices

For all groups P^z we have studied up to now, we have used one of the coordinate systems used in ITC[7] except for the groups of C-lattices. For the orthorhombic, tetragonal and cubic system, the 4, 2, 3 Bravais classes of lattices have three orthogonal symmetry axes; it is very tempting to use them as coordinate axes and it has some advantages (and some drawbacks). We shall conclude this

[7] For some groups, these tables propose several sytems of coordinates (e.g. for the rhombohedral groups).

section by computing the modules of invariants of the 7 C and A Bravais classes in a system of coordinates used by ITC.

Beware that we are studying the invariants of a group P^z not on its Brillouin zone but on the BZ of another group whose BZ of P^z is a submanifold but not a subgroup!.

Let us first show the method for a two-dimensional lattice. Let us consider a lattice *p2mm*. In an orthogonal system of coordinates the lattice points have integer coordinates: $i = 1,2$, $\mu_i \in Z$. As we explained in Chapter IV, Section 3.3, we obtain the orthorhombic *c2mm*, sublattice of index 2 of *p2mm*, by imposing the supplementary condition on the integral coordinates of vectors: $\mu_1 + \mu_2 \in 2Z$, i.e. the sum of the vector coordinates is even. By duality the lattice *p2mm* becomes a sublattice of index 2 of *c2mm*; i.e., in the reciprocal space, the *c2mm* lattice has a "centring", i.e. a point at the center of the fundamental rectangle $0 \le k_1,\ k_2 < 2\pi$ of *p2mm*. The *c2mm* and *p2mm* lattices have the same axes of symmetry; since the mid-point between two lattice points is a symmetry center of the lattice, *c2mm* has moreover four symmetry centers in a fundamental rectangle. They form an orbit of the point group of *p2mm* since one orbit point has coordinates $k_1 = k_2 = \pi/2$. By the symmetry through this point, k_i is transformed into $\pi - k_i$ so c_i are changed into $-c_i$. With this new symmetry, the module of invariants of *c2mm* on *BZ* becomes a submodule of the module of *p2mm*-invariants which is given in Table 7:

$$\mathscr{R}^{p2mm} = \mathscr{P}^{p2mm}[c_1, c_2] \equiv \mathscr{P}^{p2mm}[c_1^2, c_2^2]\bullet(1, c_1)(1, c_2)\ . \tag{58}$$

So

$$\text{on } BZ(p2mm), \mathscr{R}^{c2mm} = \mathscr{P}[c_1^2, c_2^2]\bullet(1, c_1 c_2)\ . \tag{59}$$

Similarly, from the module of invariants of *pm* given in Table 7 and the fact that *pm* changes the sign of s_2:

$$\text{on } BZ(pm), \mathscr{R}^{cm} = \mathscr{P}[c_1^2, c_2^2]\bullet(1, c_1 c_2, c_1 s_2, c_2 s_2)\ . \tag{60}$$

We can easily pass to the three-dimensional C-Bravais classes. Nothing is changed for the orthogonal third axis; indeed the centring of the three-dimensional C-lattices is in the plane of the coordinates 1, 2. Crystallographers call it a *one face centring*. We want to consider this situation in the reciprocal space; we showed how to obtain it in dimension two to form a *c2mm* sublattice of *p2mm*. Similarly in the reciprocal space one obtains the reciprocal lattices of the Bravais groups *C2/m*, *Cmmm* from those of *P2/m*, *Pmmm* by adding a new period of coordinates $\boldsymbol{w}(\pi, \pi, 0)$. That imposes the transformations:

$$\begin{aligned} &c_1 \leftrightarrow -c_1, \quad c_2 \leftrightarrow -c_2, \quad s_1 \leftrightarrow -s_1\ , \\ &s_2 \leftrightarrow -s_2, \quad c_3 \leftrightarrow c_3, \quad s_3 \leftrightarrow s_3\ . \end{aligned} \tag{61}$$

On the Brillouin zone of *Pmmm* we have the equivalence of modules:

$$\mathscr{R}^{Pmmm} = P[c_1, c_2, c_3] \equiv P[c_1^2, c_2^2, c_3]\bullet(1, c_1)(1, c_2)\ . \tag{62}$$

The module of *Cmmm* on this *BZ* is obtained by adding conditions (61):

$$\text{on } BZ(Pmmm)\text{: } \mathscr{R}^{Cmmm} = P[c_1^2, c_2^2, c_3]\bullet(1, c_1 c_2)\ . \tag{63}$$

For the Bravais group *P2/m* one has to choose a preferred axis: the rotation axis by π which is also, from the convention $m \equiv \bar{2}$ the direction normal to the reflection plane. For the *P*-lattices the consensus chooses the axis 3. For the C-lattices, ITC pp. 114–121 present many possible choices. Using the module presentations given in the caption of Table 8, it is easy to make the computations corresponding to any of these choices. As an illustration we choose the first (and most used later) choice given by ITC, "unique axis b, cell choice one"; it corresponds to the definition of the matrices m_3, j_3. The preferred axis (that of the rotation by π) is 2:

$$\mathscr{R}^{(P2/m)_{(2)}} = P[c_1, c_2, c_3] \bullet (1, s_1 s_3)$$
$$\equiv P[c_1^2, c_2^2, c_3] \bullet (1, c_1)(1, c_2)(1, s_1 s_3) . \qquad (64)$$

It is then straightforward to compute the module of the subgroups of $C2/m$. For the other three larger groups, we need to know two of their generating subgroups (see Table 1):

$$C222 = \langle C2, P2_{(3)} \rangle, \quad Cmm2 = \langle Cm, P2_{(3)} \rangle, \quad Amm2 = \langle C2, Pm_{(3)} \rangle . \qquad (65)$$

6. The modules of invariants of the *F*, *I* arithmetic classes

6.1. The eight F arithmetic classes

In a Molien function the value $N(1)$ (of the numerator for $t = 1$) gives the dimension of the module of invariants. In Tables 4 and 5, for the ρ representations, the highest value of $N(1)$ is, respectively, 24 (for $p6$) and 48 (for $P\bar{3}$); in Table 6, the highest value is 6912 (for four of the five F-cubic groups). So we cannot make the similar computations done up to now for finding the module of invariants in a generating basis. As we did in the previous case (Table 13), we will use the orthogonal bases used in ITC.

For the *Pmmm* (= *primitive*) lattices, there is a basis with three orthogonal vectors: $(\boldsymbol{b}_i, \boldsymbol{b}_j) = \lambda_i \delta_{ij}$. In this basis the P-lattice vectors have arbitrary integer coordinates μ_i while the

Table 13
Bases of the modules of invariant polynomials on the three-dimensional BZ of primitive P-lattices for the seven arithmetic classes whose label begins with C, A: monoclinic C, orthorhombic C[a]

	arith. cl.	c_{12}	s_{13}	$c_1 s_1$	$c_1 s_2$	$c_1 s_3$	$c_2 s_1$	$c_2 s_2$	$c_2 s_3$	$c_{12} s_{12}$	$c_1 s_{123}$	$c_2 s_{123}$	d
	*C*2	x	x		x			x		x	x	x	8
	Cm	x	x	x		x	x		x	x			8
B	*C*2/*m*	x	x							x			4
	*C*222	x									x	x	4
	*Cmm*2	x				x			x				4
	*Amm*2	x			x			x					4
B	*Cmmm*	x											2

[a]These modules are over the ring $P[c_1^2, c_2^2, c_3]$.

The P^z groups of the table have 2, 4, 8 elements and the dimension of the corresponding modules are respectively 8, 4, 2. Time reversal restricts to the arithmetic classes indicated in the first column by B for the Bravais groups of lattices. As rings, all the modules of the table have from 3 to 10 generators.

Notations: $a = c, s$, $a_{ij} = a_i a_j$, $a_{123} = a_1 a_2 a_3$.

Table 14
Modules of the F-orthorhombic arithmetic classes. Bases of the modules of invariant polynomials on the three-dimensional BZ of $Pmmm$ 3 F arithmetic classes of the orthorhombic system[a]

	arith. cl.	c_{12}	c_{23}	c_{31}	$c_1 s_i$	$c_2 s_i$	$c_3 s_i$	$c_{123} s_i$	$c_1 s_{123}$	$c_2 s_{123}$	$c_3 s_{123}$	$c_{123} s_{123}$	d
	$F222$	x	x	x					x	x	x	x	8
	$Fmm2_{(i)}$	x	x	x	x	x	x	x					8
B	$Fmmm$	x	x	x									4

[a]The modules are over the ring $P[c_1^2, c_2^2, c_3^2]$.
The P^z groups of the table have 4, 8 elements and the dimension of the corresponding modules are respectively 8, 4. Time reversal restricts to the arithmetic classes indicated in the first column by B for the Bravais group of lattices. As rings, all the modules of the table have from 3 to 9 generators.
Notations: $a = c, s, a_{ij} = a_i a_j, a_{123} = a_1 a_2 a_3$.

coordinates of the vectors of the F-lattices must satisfy: $\sum_i \mu_i \in 2Z$ (i.e. their sum is even). That gives the F-lattices as sublattice of index 2 of the corresponding primitive lattice. By duality, up to the scaling of the basis vectors: $\boldsymbol{b}_i^* = \lambda_i^i nv \boldsymbol{b}_i$, the primitive lattice is transformed into itself and becomes a sublattice of $F^* = P^* \cup \boldsymbol{w} + P^*$, with $\boldsymbol{w} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; that is exactly the "body centring"[8] used in ITC for the I-lattices. We had already explained this $F \leftrightarrow I$ duality. We have also explained how to pass from the corresponding primitive lattice to the reciprocal lattice of an F lattice: one has to introduce a new period for the invariant functions $2\pi \boldsymbol{w} = (\pi, \pi, \pi)$. That condition changes the signs of c_i and s_i, so the invariant polynomials are homogeneous of even degrees in these six variables. That leads us to use for the module of invariants of $Pmmm$ the equivalent form (see Table 8):

$$\mathscr{R}^{Pmmm} = P[c_1, c_2, c_3] \equiv P[c_1^2, c_2^2, c_3^2] \bullet (1, c_1)(1, c_2)(1, c_3) . \tag{66}$$

Using the last three lines of Table 8 we write with the same polynomial ring the modules of $P222, Pmm2$; then we keep only the even degree polynomials to obtain Table 14.

The same method applies for the F-cubic arithmetic classes. First we have to choose for the polynomial ring of $Pm\bar{3}m$ a polynomial ring of even degree polynomials (see Table 10):

$$\begin{aligned} \mathscr{R}^{Pm\bar{3}m} &= P[c_1 + c_2 + c_3, c_1^2 + c_2^2 + c_3^2, c_1 c_2 c_3] \\ &= P[c_1^2 + c_2^2 + c_3^2, c_1 c_2 + c_2 c_3 + c_3 c_1, c_1 c_2 c_3] \bullet (1, c_1 + c_2 + c_3)(1, c_1 c_2 c_3) . \end{aligned} \tag{67}$$

With this presentation we write, from Table 10, the modules of the other P-cubic arithmetic classes. In each module, keeping only the even degree polynomials, we obtain the modules of the F-cubic classes (Table 15).

6.2. The eight I arithmetic classes of the orthorhombic and cubic systems

The dual of these lattices are F-lattices. In ITC they are presented as P-lattices with *three face centrings* added: $(\frac{1}{2}, \frac{1}{2}, 0), (\frac{1}{2}, 0, \frac{1}{2}), (0, \frac{1}{2}, \frac{1}{2})$. So to pass to the reciprocal lattices we have to add the three

[8] In German "Inner zenntrit".

Table 15
Modules of the F-cubic arithmetic classes. Bases of the modules of invariant polynomials on the three-dimensional BZ of $Pm\bar{3}m$ for the 5 F arithmetic classes of the cubic system[a]

	Class	$c.c_{123}$	$c.s_{123}$	$c^3[c]$	$c_{123}.c[c^2]$	$s_{123}.c[c^2]$	$c_{123}s_{123}$	$c_{123}s_{123}.c^3[c]$	d
	$F23$	x	x	x	x	x	x	x	8
T	$Fm\bar{3}$	x		x	x				4
	$F432$	x				x		x	4
	$F\bar{4}3m$	x	x				x		4
B	$Fm\bar{3}m$	x							2

[a]These modules are over the ring $P[c_1^2 + c_2^2 + c_3^2, c_1c_2 + c_2c_3 + c_3c_1, c_1c_2c_3]$.

The groups P^z of 12, 24, 48 elements have modules of dimensions 8,4,2, respectively. The arithmetic classes satisfying time reversal are indicated, in the first column, by T or by B when it is a Bravais class of lattices. As rings, all the modules of the table have from 3 to 9 generators.

Notations. Let i, j, k be a circular permutation of 1, 2, 3. We use a short code for labelling the invariant polynomials (listed here by increasing degree): $c = \sum_i c_i$, $c_{123} = c_1c_2c_3$, $s_{123} = s_1s_2s_3$, $c[c^2] = \sum_i c_i(c_j^2 - c_k^2)$, $c^3[c] = \sum_i c_i^3(c_j - c_k)$.

periods $(\pi, \pi, 0)$, $(\pi, 0, \pi)$, $(0, \pi, \pi)$. That corresponds for the c_i, s_i to the simultaneous changes of sign for each of the three possible pairs of indices. Remark that each square c_i^2, s_j^2 is invariant for any of the three transformations; that is also the case for the products $a_1a'_2a''_3$ when each a, a', a'' is either c or s.

For the orthorhombic system, the presentations of the module of $Pmmm$ invariants given in Eq. (66) is exactly what we need; the only basis element ($\neq 1$) which is invariant for $Immm$ is $c_1c_2c_3$. So

$$\mathscr{R}^{Immm} = P[c_1^2, c_2^2, c_3^2]\bullet(1, c_1c_2c_3)\ . \tag{68}$$

From Table 8 we obtain immediately:

$$\mathscr{R}^{I222} = P[c_1^2, c_2^2, c_3^2]\bullet(1, c_1c_2c_3)(1, s_1s_2s_3)\ ,$$
$$\mathscr{R}^{(Imm2)_{(i)}} = P[c_1^2, c_2^2, c_3^2]\bullet(1, c_1c_2c_3)(1, c_is_i)\ . \tag{69}$$

The presentation of the module of $Pm\bar{3}m$ invariants we need is

$$\mathscr{R}^{Pm\bar{3}m} \equiv P[\textstyle\sum c_i^2, c_1c_2c_3, \sum c_i^4]\bullet(1, \sum c_i)(1, c_1c_2 + c_2c_3 + c_3c_1)\ . \tag{70}$$

No basis element of this module is invariant under the three changes of pairs of signs. So the ring of $Im\bar{3}m$ invariants is the polynomial ring in (70); remark that it is formally that of the reflection group T_d in Table 4 of invariants of Chapter I. The basic element of degree 3 in (70) can be transformed, modulo the polynomial ring, into $(\sum c_i)(c_1c_2 + c_2c_3 + c_3 + c_1) - c_1c_2c_3$. The product of this expression with the ϕ invariant of $Pm\bar{3}$ in Table 10 [$\phi = \sum_i c_i(c_j^2 - c_k^2)$] is the sixth degree invariant $(c_1^2 - c_2^2)(c_2^2 - c_3^2)(c_3^2 - c_1^2)$ which coincides with the ϕ of T_h in Table 4 of Chapter I where x, y, z should be replaced by c_1, c_2, c_3. We verify that no other similar product satisfies the three changes of pairs of signs. This completes the construction of the modules of the cubic I arithmetic classes:

$$\mathscr{R}^{I23} = P[\textstyle\sum c_i^2, c_1c_2c_3, \sum c_i^4]\bullet(1, s_1s_2s_3)(1, (c_1^2 - c_2^2)(c_2^2 - c_3^2)(c_3^2 - c_1^2))\ . \tag{71}$$

$$\mathscr{R}^{Im\bar{3}} = P[\textstyle\sum c_i^2, c_1c_2c_3, \sum c_i^4]\bullet(1, (c_1^2 - c_2^2)(c_2^2 - c_3^2)(c_3^2 - c_1^2))\ . \tag{72}$$

$$\mathscr{R}^{I432} = P[\sum c_i^2, c_1c_2c_3, \sum c_i^4] \bullet (1, s_1s_2s_3(c_1^2 - c_2^2)(c_2^2 - c_3^2)(c_3^2 - c_1^2)) \; . \tag{73}$$

$$\mathscr{R}^{I\bar{4}3m} = P[\sum c_i^2, c_1c_2c_3, \sum c_i^4] \bullet (1, s_1s_2s_3) \; . \tag{74}$$

$$\mathscr{R}^{Im\bar{3}m} = P[\sum c_i^2, c_1c_2c_3, \sum c_i^4] \; . \tag{75}$$

6.3. *The eight I arithmetic classes of the tetragonal system*

We recall that these classes are self-dual except for the following pair of classes $I\bar{4}m2 \leftrightarrow I\bar{4}2m$ which are exchanged. In ITC they are presented as the primitive tetragonal ones with the centring $\boldsymbol{w} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. We can use this presentation directly on the reciprocal lattice (replacing $\boldsymbol{w}$ by $2\pi\boldsymbol{w}$). That seems to fulfill the needs of the user; but one should be aware that it means that in the direct space, the coordinates used are not (up to a scale) the ones of ITC.

With the centring $2\pi\boldsymbol{w}$ the I invariant polynomials are homogeneous in c_i, s_i and of even degree, a convenient presentation of the $P4/mmm$ module is (see Table 9)

$$\begin{aligned}\mathscr{R}^{P4/mmm} &= P[c_1 + c_2, c_1c_2, c_3] \\ &= P[c_1^2 + c_2^2, c_1c_2, c_3^2] \bullet (1, c_1 + c_2, c_3, (c_1 + c_2)c_3) \; .\end{aligned} \tag{76}$$

Then $\mathscr{R}^{I4/mmm}$ is the two-dimensional module of even degree polynomials. From the bottom half of Table 9, it is straightforward to build the next Table 16.

7. Study of the $d = 2$ invariant polynomials on BZ; the orbit spaces

In Section 4 we established the structure of the module of the invariant polynomials for each of the 13 arithmetic classes; the results are given in Table 7. We noticed that, as rings, these modules

Table 16
Bases of the modules of invariant polynomials on the three-dimensional BZ of $P4/mmm$ for the eight arithmetic classes I-tetragonal[a]

	arith. cl.	c_{+3}	c_3s_3	c_+s_3	c_-s_3	$c_{+-3}s_3$	$c_{+-}s_{12}$	$c_{-3}s_{12}$	c_+s_{123}	c_3s_{123}	c_-s_{123}	$c_{+-3}s_{123}$	d
	I4	x	x	x			x	x			x	x	8
	$I\bar{4}$	x			x	x	x	x	x	x			8
T	$I4/m$	x					x	x					4
	$I422$	x									x	x	4
	$I4mm$	x	x	x									4
	$I\bar{4}2m$	x							x	x			4
	$I\bar{4}m2$	x			x	x							4
B	$I4/mmm$	x											2

[a]These modules are over the ring $P[c_1^2 + c_2^2, c_1c_2, c_3^2]$.

The P^z groups of the table have 4, 8, 16 elements and the dimension of the corresponding modules are, respectively, 8, 4, 2. Time reversal restricts to the arithmetic classes indicated in the first column by T or by B for the Bravais group of lattices.

As rings, all the modules of the table have from 3 to 9 generators.

Notations: $c_{\pm} = c_1 \pm c_2$, $c_{\pm 3} = (c_1 \pm c_2)c_3$, $c_{+-} = (c_1^2 - c_2^2)$, $c_{+-3} = (c_1^2 - c_2^2)c_3$, $s_{12} = s_1s_2$, $s_{123} = s_1s_2s_3$.

have from 2 to 4 generators. Here, from the explicit knowledge of these generators, we build some of the orbit spaces $BZ|P^z$; they are orbifolds whose singularities are related to the critical orbits. We recall in Table 17 (Michel, 1996), the critical orbits for the actions of the P^z's on the Brillouin zone (we add also $\mathscr{T}$ invariance) and the positions and nature of the extrema for the simplest Morse functions (i.e. those with the minimal number of extrema); Chapter IV, Section 6 explains the building of this table.

One can "show" an invariant function by drawing its level lines on BZ. It is interesting to do it for the generators of some rings of invariants. Fig. 1 shows the level lines of the three functions $\theta_1 = \cos(k_1) + \cos(k_2)$, $\theta_2 = \cos(k_1)\cos(k_2)$, $\varphi = \sin(k_1)\sin(k_2)$ which generate the ring $\mathscr{R}^{c2mm}$. To abbreviate the notation we will write $\cos(k_i) \equiv c_i$ and $\sin(k_i) \equiv s_i$. Thus $\theta_1 = c_1 + c_2$, $\theta_2 = c_1 c_2$, and $\varphi = s_1 s_2$.

Table 17 shows that *c2mm* has three critical orbits on BZ: O, R, AB. The 6-side Brillouin cell has four sides of same length; their middle represents the 2 points A, B on the same orbits. Morse perfect functions have only 4 extrema on the 2-torus: one maximum ($= M$), one minimum ($= m$) and two saddle points ($= sp$). For the perfect Morse functions invariant by *c2mm* on BZ, since A, B belong to the same orbit, they must be saddle points; that is the case of θ_1. The functions θ_2 and φ in Fig. 1 have eight extrema on BZ: $2M, 2m, 4sp$; notice that φ has saddle points not only at A, B but also at O, R while for θ_2, the points O, R are maxima and the points A, B form an orbit of minima.

Table 17
Extrema common to all functions on the two dimensional Brillouin zone, invariant by the crystallographic group and time reversal[a]

cr. syst.	BZ	sg	arithm. class		$k=0$	$2k=0$	$3k=0$	Nb	0,2	1	2,0	$Q(t)$
Diclinic	6	2	*p2*	*p1*	O	R, A, B		4	1	1,1	1	0
Orthorhombic	4	5	*p2mm*	*pm*	O	R, A, B		4	1	1,1	1	0
	6	2	*c2mm*	*cm*	O	R, AB		4	1	2	1	0
Square	4	1	*p4*		$[O]$	$[R], AB$		4	[1]	2	[1]	0
	4	2	*p4mm*		$[O]$	$[R], AB$		4	[1]	2	[1]	0
Hexagonal	6	2	*p6*	*p3*	$[O]$	RAB	$[CC']$	6	[2]	3	[1]	$1, t$
	6	3	*p6mm*	*p3m1*	$[O]$	RAB	$[CC']$	6	[2]	3	[1]	$1, t$
				p31m								

[a]Column 1 gives the crystallographic system; each contains one Bravais class except the orthorhombic one which contains two: *pmm* and *cmm*. Column 2 indicates the number of sides of the Brillouin cell. Column 3 gives the number of corresponding space groups. Columns 4, 5 list, respectively, the arithmetic class containing $-I$, (so $\mathscr{T}$ = time reversal is implied) and those which yield that arithmetic classes when $-I$ is added to them. Columns 6, 7, 8 list the critical orbits for the arithmetic classes of column 4. When the Brillouin cell has six sides, the three points satisfying $2k = 0$ are R, A, B, the middle of the sides. We choose R to be a fixed point for *c2mm* and to correspond to the pair of shrinking symmetric edges (for *pm* or *c2mm*) when the Brillouin cell is transformed into a 4-side one (rectangle). Then R is represented by the four vertices and is invariant by the full point group. In the hexagonal system, the two points C, C' satisfy $3k = 0$ and represent the six vertices of the Brillouin cell. The points of the orbits between [ ] have to be maxima or minima because the stabilizer acts as a two-dimensional representation irreducible on the real. Column 9 gives the minimal number of extrema. Columns 10–12 give, for the simplest Morse functions, the orbits of extrema with a given Morse index. Column 13 gives the corresponding polynomial $Q(t)$ (defined in Chapter I, Eq. (132)).

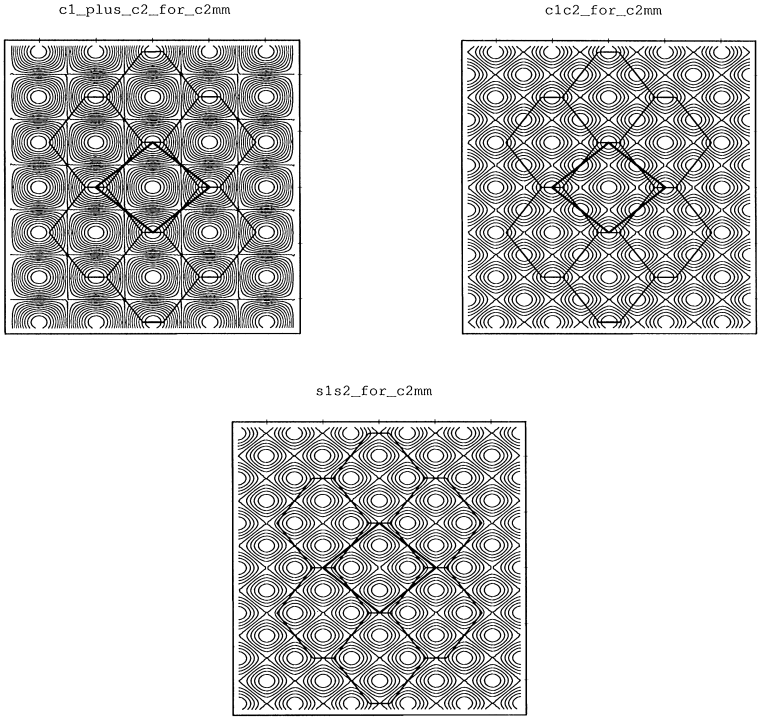

Fig. 1. Level lines for denominator and numerator invariants for *c2mm* class: upper left – $\theta_1 = c_1 + c_2$; upper right – $\theta_2 = c_1 c_2$, center – $\varphi = s_1 s_2$.

We recall that the most general polynomial in c_i, s_i on *BZ*, invariant by *c2mm* is of the form

$$f = p(\theta_1, \theta_2) + q(\theta_1, \theta_2) s_1 s_2 \quad \text{with } \theta_1 = c_1 + c_2, \quad \theta_2 = c_1 c_2 , \tag{77}$$

where p, q are arbitrary polynomials in two variables. It is not very difficult to discuss such a function when the degrees of p, q are low.

From the relations

$$\varphi^2 = (\theta_2 - \theta_1 + 1)(\theta_2 + \theta_1 + 1) \geq 0 ,$$
$$(c_1 - c_2)^2 = \theta_1^2 - 4\theta_2 \geq 0, \quad \theta_2 + 1 \geq 0 , \tag{78}$$

we can build the orbit space $BZ|c2mm$ of the action of *c2mm* on *BZ* in the space of basic (denominator) invariants θ_i. The coordinates of the critical orbits in this space can be obtained from the (k_1, k_2) coordinates of the corresponding points in *BZ*: $O = (0,0)$, $R = (\pi, \pi)$, $A = (\pi, 0)$, $B = (0, \pi)$. So

$$\text{coordinates } (\theta_1, \theta_2): \quad O = (2,1),\ R = (-2,1),\ A = B = (0,-1) . \tag{79}$$

The orbit space $BZ|c2mm$ shown in Fig. 2 is built from the three inequalities of (78); the first one gives the two straight lines $R - (AB)$ and $(AB) - O$, the second one gives the parabola tangent to the two straight lines at R and O, the third one limits the domain to that between the parabola and

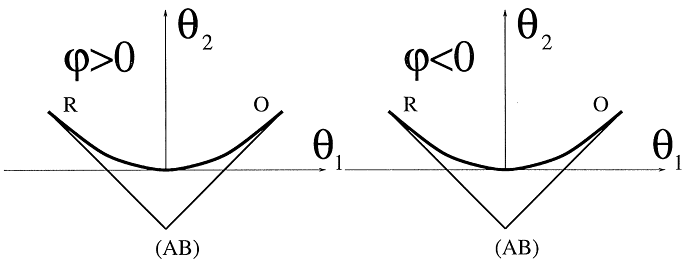

Fig. 2. Orbifold for *c2mm* class.

its two tangents at R, O. The two basic invariants θ_1 and θ_2 do not specify completely the orbit. If the auxiliary invariant $\varphi \neq 0$, there are two orbits with the same values of θ_1 and θ_2 and opposite values for φ. So we represent in Fig. 2 the space of orbits as a two-piece puzzle with corresponding points on the boundary having $\varphi = 0$ glued together: i.e. glue together the two parts $\varphi > 0$ and < 0 along the common boundary $R-(AB)-O$. The two boundaries $R-O$ stay distinct since they correspond to opposite signs of $\varphi \neq 0$. A schematic representation of the orbit space for *c2mm* is a disk with the critical orbit (AB) in the interior and the two critical orbits R and O on the boundary.

The geometrical form of the orbifold depends on the choice of integrity basis polynomials. This choice is ambiguous as we remarked several times. For example, we can use instead of θ_2 the combination $a\theta_2 + \theta_1^2$ with an arbitrary parameter $a \neq 0$. The choice $a = -4$ gives in particular the $\theta'_2 = (c_1 - c_2)^2$ as a basic polynomial. In coordinates (θ_1, θ'_2) the space of orbits would have the geometrical form with $R-O$ boundary being straight line and both $R-(AB)$ and $(AB)-O$ boundaries being parabola. More generally one should remark that the geometry of space of orbits changes with changing the basic polynomials but the type of singularity at vertices remains the same: the two critical orbits O, R are represented by cusp points and the critical orbit AB by the crossing of two lines at an angle $\neq 0$.

Using the same Fig. 2 we can explain the orbit space for the *p*4 arithmetic class. The two basic invariants for *p*4 are the same as for *c2mm* but the numerator invariant φ_{p4} is different. Its square is a product of the three factors:

$$\varphi_{p4}^2 = (\theta_2 - \theta_1 + 1)(\theta_2 + \theta_1 + 1)(\theta_1^2 - 4\theta_2) \geq 0 , \tag{80}$$

so $\varphi_{p4} = 0$ on the whole boundary $O-(AB)-R-O$. This means that to represent the space of orbits for *p*4 we should glue together the two sub-orbifolds $\varphi > 0$ and < 0 through the whole boundary. The result is the topological S_2 sphere with three marked points corresponding to critical orbits.

The space of orbits for *p4mm* class is finally just one part of the *c2mm* or *p*4 orbifold. We can fulfill on this orbifold the same topological analysis of the level sets of a simple function written in terms of θ_1 and θ_2 as that realized in Chapter I for the O_h group (see Section 5.4 of Chapter I).

To see the location of stationary points for an arbitrary functions $f(\theta_1, \theta_2)$ it is sufficient to consider the parallels $f(\theta_1, \theta_2) = \text{constant}$ on the orbifold. In particular, for the θ_1 function the topology of the level $\theta_1 = \text{const}$ changes only when this level passes through the critical orbits, i.e. for $\theta_1 = -2, 0, 2$.

For the θ_2 function, the level lines $\theta_2 = \text{const}$ which pass through the critical orbits have the isolated values $\theta_2 = -1, 1$. Besides that, there is another exceptional level line $\theta_2 = 0$' which is tangent to the boundary $R - O$ at $\theta_1 = 0$, $\theta_2 = 0$. This means that for the θ_2 function two orbits $(0,0)$ on both parts ($\varphi > 0$ and $\varphi < 0$) of the *c2mm* orbifold are orbits of stationary points (four saddle points), but they are not critical points. In fact θ_1 and θ_2 functions are invariant with respect to *p*4*mm* class and for these four points form one orbit for the *p*4*mm* class.

On the reciprocal space, the patterns of level lines of θ_2 and φ are identical, with alternate (vertical or horizontal) bands of maxima and minima. Indeed, by a translation $(\pi/2, \pi/2)$ on *BZ* the translated function $\tilde{\theta}_2$ coincides with φ:

$$\tilde{\theta}_2 = \cos(k_1 - \pi/2)\cos(k_2 - \pi/2) = \sin(k_1)\sin(k_2) = \varphi \ . \tag{81}$$

Moreover, by a dilation of one period one makes the two periods equal and one obtains the θ_i functions of *p*4*mm*.

As indicated by Table 17, for the symmetry *p*4*mm* or *p*4 the points *O* (center of the square *BZ* cell) and *R* (the four vertices) must be maximum or minimum of *any invariant Morse function*. From Fig. 1 after scaling transformation which makes the lattice quadratic one can show that it is true for the perfect Morse functions θ_i (see Table 7). At the same time the auxiliary invariant function φ_{p4} is not a Morse function since its Hessian vanishes identically at *O* and *R*. This function shown in Fig. 3 has two non-degenerate saddle points on the orbit *AB*. It has also one *p*4-orbit of 4 maxima and one of four minima; these extrema are on a circle of *BZ* centered at *O* and the *M*'s and *m*'s are alternate: indeed φ_{p4} is *p*4 invariant and not *p*4*mm* invariant. The complete list of stationary points of the φ_{p4} function finally includes four maxima, four minima, two non-degenerate saddle points and two degenerate saddle points. Slight perturbation of φ_{p4} by a Morse-type function removes two degenerate saddle points producing the non-degenerate maxima (or minima) at *O* and *R* and four saddle points near *O* and near *R*.

An interesting relation between functions θ_1 and θ_2 can be seen from Figs. 1. This relation has a very simple form for the *p*4*mm* class. To go from one function to another one needs to make a rotation by $\pi/4$ and to scale with factor $\sqrt{2}$. A corresponding transformation of the k_1, k_2 variables can be written with the matrix

$$\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \tag{82}$$

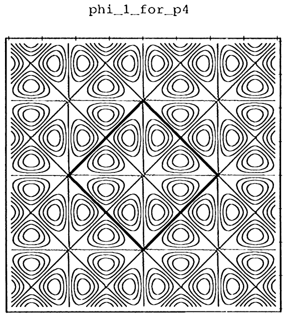

Fig. 3. Level lines for the numerator invariant polynomial φ_{p4}.

whose determinant is 2. The corresponding relation between θ_1 and θ_2 has the form

$$\theta_2(k_1,k_2) = \tfrac{1}{2}\theta_1(k_1 + k_2, k_1 - k_2)\ . \tag{83}$$

The factor 1/2 is unimportant because invariant polynomials are defined up to a scalar factor. The correspondence in Eq. (83) is the reflection of the identity

$$2\cos(A)\cos(B) = \cos(A+B) + \cos(A-B)\ . \tag{84}$$

7.1. Invariant functions for 2-D hexagonal classes

Let us analyze first the invariant functions $\theta_1^{p6mm} = c_1 + c_2 + c_1c_2 - s_1s_2$ and $\theta_2^{p6mm} = c_1c_2(c_1c_2 - s_1s_2)$ (where the superscripts relate to the arithmetic class *p*6*mm* in Table 7), which are the basic invariant polynomials for all hexagonal arithmetic classes *p*3, *p*6, *p*31*m*, *p*3*m*1 and *p*6*mm*.

These two invariant functions are represented in Fig. 4. There is a simple relation between these two functions:

$$\theta_2(k_1,k_2) = \tfrac{1}{4}(1 + \theta_1(2k_1, 2k_2))\ . \tag{85}$$

This relation follows from the explicit form of these functions taking into account the trigonometric identity

$$4\cos(A)\cos(B)\cos(C) = \cos(A+B+C) + \cos(A+B-C) + \cos(B+C-A) + \cos(C+A-B)\ , \tag{86}$$

with $C = A + B$.

It is easy to see that function θ_1^{p6mm} is a Morse-type function with a minimal (compatible with symmetry) number of stationary points. All stationary points of θ_1 are on critical orbits of *p*6*mm* class. θ_1 possesses one maximum, two minima, and three saddle points. (Naturally, if we change the sign of the function, the minima and maxima are interchanged.) If we consider the hexagonal cell, one critical orbit (orbit O in the notation of Table 17) lies in the center (one-point orbit); another critical orbit (CC') corresponds to vertices of the hexagon. It is a two-point orbit; due to k_1, k_2 periodicity three vertices correspond to the same point on the torus whereas one point of this orbit can be transformed into another by a geometrical operation (rotation by $\pi/3$). At last, the third

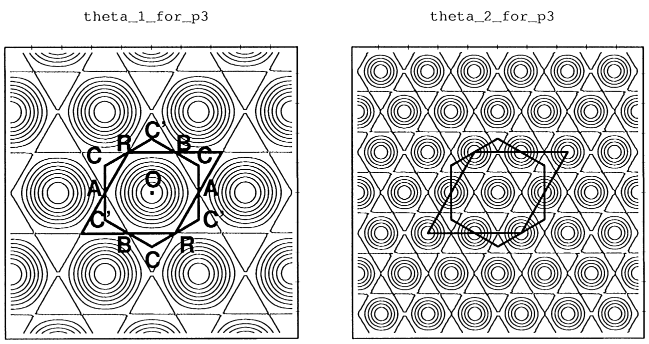

Fig. 4. θ_1^{p6mm} (left) and θ_2^{p6mm} (right) invariant functions for *p*6*mm* (or *p*3, *p*6, *p*31*m*, *p*3*m*1) class.

critical orbit (RAB) corresponds to the middle of the edges. Opposite points on the BZ should be identified (they correspond to the same point on the torus) and thus we have a three-point orbit.

The same system of stationary points can be easily seen on k_1, k_2 rhombohedral representation of the torus. Three stationary points are inside the rhomb. One point O (center of rhomb) forms itself the orbit, two others (CC') are related through a geometric operation and form one two-point orbit. Four vertices of the rhomb correspond to one point R of the torus. Four middle points of the edges correspond in fact to two points (A, B) of the torus. Vertices and middle-edges are related by geometrical operations and form one three-point orbit (RAB) on the torus.

We just remind that the minimal number of stationary points of a Morse-type function on torus (without symmetry) is four (one minimum, one maximum and two saddle points). Number of stationary points lying on critical orbits in the presence of $p6mm$ symmetry is six. Thus θ_1 is a Morse-type function with the minimal possible number of stationary points compatible with $p6mm$ symmetry.

The function θ_2 is also a Morse-type function. But the number of its stationary points is much larger than the minimal number required by critical orbits. Besides the critical orbits it has three other orbits of stationary points. Each of these three orbits includes six points related by geometrical symmetry operations. The total number of stationary points is 24 (eight minima, four maxima, and 12 saddle points). In fact, the symmetry of θ_2 function is higher than the symmetry of θ_1 due to the translational symmetry on a half of period. The reflection of this fact is the equivalence between stationary points forming different orbits (for example, one-point orbit of the center and three-point orbit of the middle edges become equivalent by half of the translation of the lattice).

To understand better the correspondence between an arbitrary invariant function and its system of stationary points we turn again to the representation of level lines for different functions directly on the space of orbits drawn in terms of invariant polynomials. The space of orbits for $p6mm$ is shown in Fig. 5.

To find the admissible values of θ_1 and θ_2 we take into account restrictions imposed on θ_i by natural inequalities $\phi_1^2 \geq 0$ and $\phi_2^2 \geq 0$. As soon as $\phi_1 = s_1 + s_2 - (c_1 s_2 + c_2 s_1)$ and $\phi_2 = s_1 - s_2 + c_1 s_2 - c_2 s_1 + 2(c_1 - c_2)(c_1 s_2 + c_2 s_1)$ are invariants of $p3m1$ and $p31m$, respectively, ϕ_1 and ϕ_2 are pseudoinvariants of $p6mm$ (invariants of subgroup of index two) and their squares are polynomials in θ_1 and θ_2. Thus the equations for the boundary of the orbifold of $p6mm$ can be written as

$$(RAB) - E - O\colon \quad \theta_2 = \tfrac{1}{4}(\theta_1 - 1)^2, \; -1 \leq \theta_1 \leq 3\,, \tag{87}$$

$(CC') - D - F - O$:

$$\theta_2 = \tfrac{1}{2}\theta_1^2 + \tfrac{5}{2}\theta_1 + \tfrac{5}{2} - \tfrac{1}{2}(2\theta_1 + 3)^{3/2}, \; -\tfrac{3}{2} \leq \theta_1 \leq 3\,, \tag{88}$$

$(CC') - (RAB)$:

$$\theta_2 = \tfrac{1}{2}\theta_1^2 + \tfrac{5}{2}\theta_1 + \tfrac{5}{2} + \tfrac{1}{2}(2\theta_1 + 3)^{3/2}, \; -\tfrac{3}{2} \leq \theta_1 \leq -1\,. \tag{89}$$

In Fig. 5 the boundary $(RAB) - E - O$ corresponds to $\phi_1^2 = 0$ whereas the boundary $(RAB) - (CC')$ and $(CC') - D - F - O$ corresponds to $\phi_2^2 = 0$.

The geometrical form of the orbifold is rather complicated but as soon as it is known we can use simple geometrical construction to find the system of stationary points of functions just by

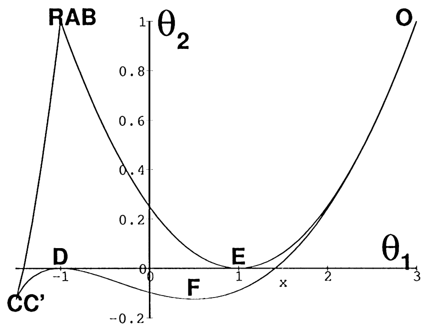

Fig. 5. Orbifold for *p6mm* class in θ_1^{p6mm}, θ_2^{p6mm} variables.

analyzing the constant levels of the functions on the orbifold. Let us take the θ_1 function. $\theta_1 = const$ levels are simple vertical lines in Fig. 5. Exceptional sections of the orbifold correspond to orbit O (maximum of θ_1), to orbit (RAB) (saddle point) and to orbit (CC') (minimum). All these three orbits are critical and they are clearly seen in Fig. 4.

Let us now take the θ_2 function. Its levels correspond to horizontal lines in Fig. 5. Section $\theta_2 = 1$ is exceptional. It corresponds to two different orbits: O and (RAB). Both these orbits are maxima. Next, exceptional section corresponds to $\theta_2 = 0$. We have again two independent by symmetry orbits D and E. These two orbits are saddles. At last the section $\theta_2 = -\frac{1}{8}$ is again an exceptional section with two independent orbits CC' and F. All these stationary points are clearly seen on the contour plot of θ_2 function shown in Eucleadean space in Fig. 4. We can analyze equally for example, what will be the system of stationary points for a linear combination $\theta_2 + \tan(\alpha)\theta_1$ with $\alpha \neq 0$. The level set of this function is represented by a set of parallel lines forming with axis θ_1 an angle α. This function has generically no additional symmetry and on each critical level there is typically only one orbit of critical points. Positions of stationary points can be graphically found as points where constant level functions are tangent to the border of the orbifold.

An interesting example is given by the function $\theta_1 - \theta_2$. Levels $\theta_1 - \theta_2 = const$ are tangent to orbifold at points O and (CC'). Remark that two boundaries of the orbifold are tangent at these points. Consequently, the orbits O and (CC') are degenerate points of the function. Orbit O is a degenerate maximum and orbit (CC') is a degenerate saddle. Fig. 6 confirms this system of stationary points. The apparent number of stationary points on the BZ hexagonal (or rhombohedral) cell for this function is six. These points cannot be non-degenerate because they do not satisfy the Morse inequalities. In fact there are one maximum in the center O, two degenerate saddles (CC') (vertices of hexagon), and three non-degenerate minima (RAB) at the middle of edges of the hexagon.

Invariant functions for such subgroups as *p*6, *p*31*m*, *p*3*m*1, and *p*3 can be represented as well on the same hexagonal Brillouin cell but the symmetry of the function is naturally lower. Auxiliary invariant polynomials ϕ_1, ϕ_2, and ϕ_3 are plotted in Fig. 7.

First of all remark that all three functions ϕ_1, ϕ_2, and ϕ_3 are of non-Morse type. Each has a degenerate stationary point at the center O of the hexagonal cell. The point O is a critical orbit with the symmetry at least *p*3. This means that this point should be stable (maximum or minimum) for a Morse-type function.

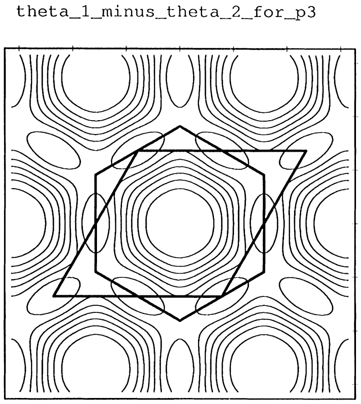

Fig. 6. $\theta_1^{p6mm} - \theta_2^{p6mm}$ invariant function for *p6mm* (or for any another hexagonal) class.

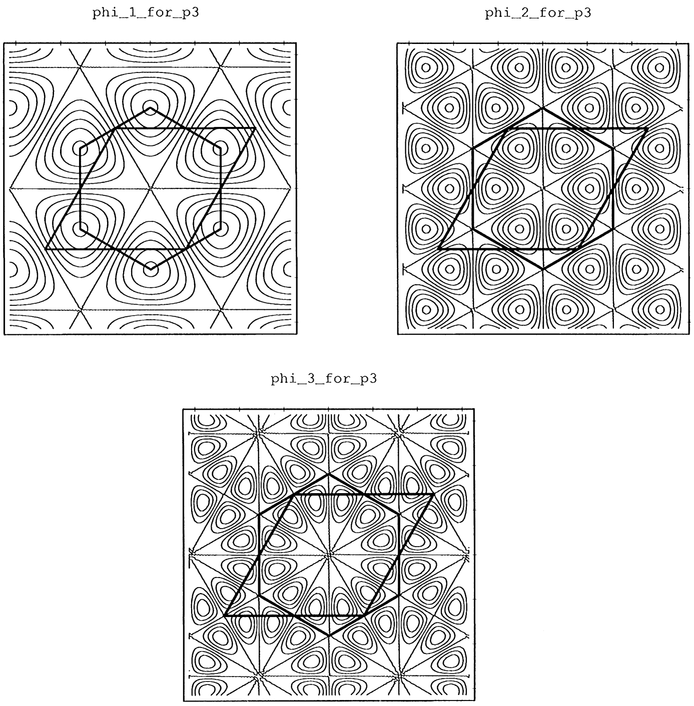

Fig. 7. Graphical representation for auxiliary invariant polynomials for *p*3 class: upper left – ϕ_1^{-+} invariant function for *p*3*m*1 class; upper right – ϕ_2^{--} invariant function for *p*31*m* class; center – ϕ_3^{+-} invariant function for *p*6 class.

The number of stationary points on the torus for ϕ_1 is three (one degenerate saddle in the center of hexagonal cell, one maximum and one minimum on the vertices of the hexagon). This number is less than the number four required by Morse theory for a minimal number of non-degenerate stationary points of the function on a torus. The minimal number of stationary points of a smooth function on a manifold is given by Lusternik–Schnirelman category of the manifold (Lusternik and Schnirelmann, 1930; Lusternik and Schnirelmann, 1934; Fomenko and Fuks, 1989). The category for d-torus is equal to $d+1$. Thus the minimal possible number of stationary points on the 2-torus is three and the function ϕ_1 supplies the example of a function with the minimal possible number of stationary points on the torus.

Function ϕ_2 is related to ϕ_1 through a linear transformation of variables. This transformation is slightly more complicated than simple scaling between θ_1 and θ_2. Namely, we can remark that if we turn the image of ϕ_1 function by $\pi/6$ (or equivalently by $\pi/2 = \pi/6 + \pi/3$) and scale by a factor of $1/\sqrt{3}$ we will have ϕ_2. The exact transformation reads

$$\phi_2^{--}(k_1, k_2) = \tfrac{1}{2}\phi_1^{-+}(2k_1 + k_2, k_2 - k_1) . \tag{90}$$

Again the factor $\frac{1}{2}$ is unimportant whereas the determinant of the transformation in k_1, k_2 variables which is equal to 3 is important. This determinant characterizes the increase of the area of the cell which triples under this transformation. Consequently, the number of stationary points for ϕ_2 on the torus is three times the number of stationary points for ϕ_1. We see on BZ cell three degenerate saddles O, (CC') (one in the center and two in the vertices of hexagon) and three maxima and three minima inside the hexagon.

An auxiliary invariant function ϕ_3 is the product $\phi_1\phi_2$. It has three degenerate saddles O, (CC'), three non-degenerate saddles (RAB), and six minima and six maxima at two generic orbits.

To conclude our examples of the orbifold representation we remark that the space of orbits of index two subgroups of *p6mm* (namely of *p6*, *p31m*, *p3m1*) can be represented as two identical copies of *p6mm* orbifold glued together through the identification of boundary points corresponding to zero value of auxiliary (numerator) invariant of the subgroup. Thus to get the *p6* orbifold one must glue two copies of *p6mm* orbifold along the whole boundary. The function ϕ_3 which is a numerator invariant of *p6* vanishes along the whole boundary. For *p3m1* the identification should be done along $O-(RAB)$ and for *p31m* along $O-(CC')-(RAB)$. Finally the *p3* orbifold in $\theta_1^{p6mm}, \theta_2^{p6mm}$ variables can be represented as a four-body decomposition with certain identification of boundaries.

8. Conclusion

We have not only given a minimal set of generators for the ring of invariant polynomials on the Brillouin zone for each arithmetic class, but also we have given the (richer structure of the) free modules on a polynomial ring P: any invariant polynomial is a linear combination of the polynomials of the module basis with coefficients in P. The generators of P and the module basis are homogenuous polynomials except for the 2D hexagonal system. This mathematical structure has a meaning independent of the coordinate system; the choice of coordinates is necessary for writing explicitly the invariants. For each arithmetic class we have chosen one of the choices made by the international tables of crystallography (ITC, 1996). We recall that this choice of coordinates is not fixed. It is a family of bases depending on some arbitrary parameters (among the values of the elements $(\boldsymbol{b}_i, \boldsymbol{b}_j)$) of the Gram matrix), their number depending on the crystallographic system: 6 for triclinic, 4 for monoclinic, 3, 2 or 1 dilations of axes for the other systems; these variations of parameters preserve not only the symmetry, but also the integral matrices of the representation of the point group. The computation of invariants is based on these matrices.

The ring of invariants is evident in a few cases and in many other cases it is easy to construct one by one invariant polynomials. It is amazing that the complete set of generators for the 73 arithmetic classes can be written in a few short tables.

For each problem in solid state physics, physicists who have to solve it for studying a given material, know how to introduce the crystal symmetry; so their results satisfy all requirements of the symmetry. These methods (e.g. LAPW = linearized augmented plane wave) work well and are presently introduced in computer codes; with them specialists can make the symmetry preserving computations they need. Of course these computations always use an approximation method and it could be interesting to express the results in a development in the invariant polynomials.[9] These computations can help to think more about physics laws.

We offer these free modules of invariant polynomials for a different approach of thinking about the implications of crystal symmetry. For instance it is easy to form from the tables, the orbit spaces $BZ\,|\,P^z$. This has been done in Section 7, for 2D, on some examples. In the first three chapters we have shown many examples of the use of the orbit spaces. There has been some trend, in several domain of physics, to use them more; it may also be done in solid state physics.

We hope that the tool we give in this chapter can find many applications by their users.

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[9] Or equivalently, in trigonometric series, since there are well-known algebraic transformations of $\cos nx$ and $\sin nx$ into nth degree polynomials in $\cos x, \sin x$.