INVARIANT THEORY IN CRYSTAL SYMMETRY

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The concepts of orbit, stratum, stabilizer, integrity basis of invariant polynomials, have important applications in physics. They are associated with compact transformation groups. We give a brief overview on these subjects. We show how we obtained the ring of invariant real functions on the Brillouin zone. Our results will find important applications in condensed matter physics.

1 Invariant Theory

1.1 Group actions

An action of a group G on a mathematical structure M is defined by a homomorphism $G \xrightarrow{\rho} \mathrm{Aut}M$ into the group of automorphisms of M. For instance if M is a vector space V, then Aut $M = GL(V)$, the linear group on V, and ρ is a linear representation.

The two actions $G \xrightarrow{\rho_i} \mathrm{Aut}M_i$ are equivalent if there exists an isomorphism: $M_1 \xrightarrow{\theta} M_2$ which is equivariant, i.e. it commutes with the two actions:

$$\forall g \in G : \theta \circ \rho_1(g) = \rho_2(g) \circ \theta \Leftrightarrow \rho_2(g) = \theta \circ \rho_1(g) \circ \theta^{-1} \tag{1}$$

Let us use a shorhand $g \cdot m$ for a unique action of G on M $\rho(g)(m)$. The set of transforms of m by G, denoted by $G \cdot m$, is the orbit of m. M is a disjoint union of its orbits. The set of orbits is called the orbit space and is denoted by $M|G$. In our applications the orbit space can be a manifold, called the orbifold, i.e. a manifold with singular points or sub-manifolds.

The set $G_m = \{g \in G, g \cdot m = m\}$ of elements of G which leave m fixed, is the stabilizer of m which is a subgroup of G. Mathematicians call it the isotropy group and physicists call it sometimes a little group or a local symmetry group. In general, one can easily prove that $G_{g \cdot m} = gG_m g^{-1}$. Thus the set of stabilizers of the elements of an orbit is a conjugacy class $[H]_G$ of subgroups of G (H is one of the stabilizers).

Let us denote $G : H$ for the type of a G-orbit whose stabilizers are the G-subgroups conjugate to H. When G is finite, the number of elements of an orbit of type $G : H$ is $|G : H| = |G|/|H|$.

In a group action a stratum is the union of orbits of the same type. Equivalently two points belong to the same stratum if and only if their stabilizers are conjugate. The set of strata is called the stratum space and is denoted by $M||G$. The unique stratum consisting of orbit types $G : 1$ is called the principal stratum.

Let us give a concrete example. We consider the actions of O_h on the carrier space $\vec{v} = (x, y, z)$ of the 3-dimensional vector representation. The group O_h contains three families of rotation axes which are respectively made of 3 axes of rotations by $\pi/2$, 4 axes of rotations by $2\pi/3$, 6 axes of rotations by π. Hence there exist seven strata:

- the generic 3-dimensional stratum contains all points which do not belong to a symmetry plane: stabilizer $C_1 = 1$. Each orbit includes 48 points. $\vec{v} = (x, y, z)$

- the two 2-dimensional strata whose stabilizers are $[C_s]_{O_h} = Pm$ and $[C_s']_{O_h} = Cm$ respectively: they contain all points belonging to a unique symmetry plane, P_i and P_j' respectively. Each orbit consists of 24 points. $\vec{v} = (x, y, 0)$ for C_s and $\vec{v} = (x, x, z)$ for C_s'.

- the stratum of stabilizers $[C_{3v}]_{O_h} = R3m$, it contains all points which are at the intersection of only three symmetry planes of type P_j'. Each orbit includes 8 points. $\vec{v} = (x, x, x)$

- the stratum of stabilizers $[C_{2v}]_{O_h} = Amm2$, it contains all points which are at the intersection of only four symmetry planes, one of type P_i and the other of type P_j'. Each orbit consists of 12 points. $\vec{v} = (x, x, 0)$

- the stratum of stabilizers $[C_{4v}]_{O_h} = P4mm$, it contains all points which are at the intersection of only four symmetry planes, two of type P_i and the other two of type P_j'. Each orbit consists of 6 points. $\vec{v} = (x, 0, 0)$

- the maximal stratum contains only one point, fixed by $O_h = Pm\bar{3}m$. The orbit is the origin. $\vec{v} = (0, 0, 0)$

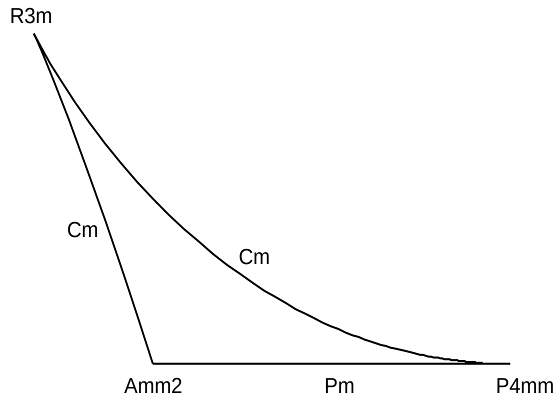

Figure 1. The orbifold of the vector representation of O_h.

1.2 Smooth Actions of a Compact Group

As we saw in the previous example groups actions on the carrier space reveal sophisticated structures. One can visualize the structure of strata through Fig. 1, which will be explained later. The manifold of orbits "orbifold" has a hierachical structure. In the example there are three isolated cusps which are buried in the two curves which enclose the area. The stabilizers of the cusps are supergroups of those of the curves. The stabilizer of the generic stratum corresponding to the area is the common subgroup of the stabilizers of the curves.

We quote some theorems concerning the structure of strata. A serious reader may consult Refs. [3,4,5]. A theorem due to Montgomery & Yang [6] states on the hierachical structure of the orbifold.

> *Theorem 1:* In the smooth action of a compact group G on a finite dimensional manifold M, the set of strata is finite. There exists a unique stratum with minimal symmetry that is open dense in M. The maximal strata are closed. More generally the union of a stratum S and all the strata $> S$ is a closed set.

Given a smooth action of G on the manifold, the stabilizer G_m acts linearly on the tangent hyperplane $T_m(M)$ of M at m. A G-invariant vector field $\vec{v}(m)$ on M has to be a fixed vector of G_m. Thus we have

Lemma 1: In the smooth action of a compact group G on a finite dimensional manifold M, a G-invariant vector field on M must be tangent to the closure of the stratum of m, i.e. $v(m) \in T_m(S(m))$.

Michel [7] derived a theorem on the critical strata that have been widely used in the minimization of Higgs-Landau potentials [8,9]:

Theorem 2: In the smooth action of a compact group G on a finite dimensional manifold M, the gradient of every G-invariant functions vanishes on the orbits which are isolated in their strata. These orbits are called critical.

1.3 Rings of G-invariant Functions

Polynomial Ring and Molien Function

Let us recall some results on the action of G on $\mathcal{P}_n$, the ring of polynomials on the carrier space V_n. Let us denote by $\mathcal{P}_n^{(m)}$ the subspace of homogeneous polynomials of degree m. Then we have

$$\mathcal{P}_n = \oplus_{m=0}^{\infty} \mathcal{P}_n^{(m)}, \quad \dim(\mathcal{P}_n^{(m)}) = \binom{m+n-1}{m}. \tag{2}$$

Let $\vec{v} \in V_n$ and $p \in \mathcal{P}_n$. The action of G on $\mathcal{P}_n$ is defined by

$$g \cdot p(\vec{v}) = p(g^{-1} \cdot \vec{v}). \tag{3}$$

To obtain an invariant polynomial one simply sums all polynomials of a G-orbit: $q(\vec{v}) = \sum_{g \in G} g \cdot p(\vec{v})$. It is trivial to verify that $g \cdot q(\vec{v}) = q(\vec{v})$ for any $g \in G$.

We remark that the action defined in Eq. (3) transforms $\mathcal{P}_n^{(m)}$ into themselves and that $\mathcal{P}_n^{(m)}$ form a reducible carrier space. The character $\chi^{(m)}(g)$ of the linear representation of G on $\mathcal{P}_n^{(m)}$ was first given by Molien [10] through the generating function,

$$\sum_{m=0}^{\infty} \chi^{(m)}(g) \lambda^m = \det(I_n - \lambda g)^{-1} \tag{4}$$

where λ is a dummy variable. Let us label by an index α the different equivalent classes of irreducible representations of the compact or finite group G and denote by $\chi_\alpha(g)$ the corresponding character. Let $c_\alpha^{(m)}$ the multiplicity of the irreducible representation α which appears in the G representation on

$\mathcal{P}_n^{(m)}$. From Eq. (4) we can derive, for finite G,

$$M_\alpha(\lambda) \equiv \sum_{m=0}^{\infty} c_\alpha^{(m)} \lambda^m = |G|^{-1} \sum_{g \in G} \bar{\chi}_\alpha(g) \det(I_n - \lambda g)^{-1} \tag{5}$$

Chevalley [11] proved two important theorems on the invariant polynomials.

Theorem 3: The ring $\mathcal{P}^G$ of invariant polynomials of a finite reflection group G acting on the orthogonal carrier space V_n is an n-variable polynomial ring.

Theorem 4: For a finite reflection group G, the ring $\mathcal{P}$ of the polynomials on V_n is a free module on the ring $\mathcal{P}^G$ of invariant polynomials. Its dimension is $|G|$ and it carries the regular representation of G.

More explicitly, $\mathcal{P}^G$ is the ring of all n variable polynomials whose variables are n algebraically independent polynomials θ_k, $1 \leq k \leq n$. The degree d_k of the θ_k are obtained from the Molien function of the form:

$$M(\lambda) = \frac{N(\lambda)}{D(\lambda)}, \quad D = \prod_{k=0}^{n} (1 - \lambda^{d_k}) \tag{6}$$

The numerator $N(\lambda)$ is a polynomial with positive coefficients,

$$N(\lambda) = \sum_\delta \nu_\delta \lambda^\delta; \quad \nu_\delta > 0, \ \nu_0 = 1. \tag{7}$$

For finite groups generated by reflections $N(\lambda) = 1$. For each power δ in Eq. (7) there exist ν_δ G-invariant linearly independent homogeneous polynomials φ_α of degree δ. However, the numerator invariants φ_α are algebraic functions of the n denominator invariants θ_k. The ring $\mathcal{P}^G$ is a free module and the $N(1)$ polynomials φ_α form its basis. In other words any G-invariant polynomials are written uniquely as a linear combination of the φ_α's:

$$P = \sum_{\alpha=0} p_\alpha(\theta_k(v_j))\varphi_\alpha(v_j) \quad \text{with } \varphi_0 = 1, \tag{8}$$

where the coefficients p_α are n variable polynomials θ_k.

Integrity basis, syzygy

We will use the term "integrity basis" for the basis formed by denominator and numerator invariants. It was used initially by Weyl [12]. We shall write this structure of module as,

$$\mathcal{P}^G = P[\theta_1, \theta_2, ..., \theta_n] \bullet (1, \varphi_1, ..., \varphi_k). \tag{9}$$

Eq. (9) describes a structure of algebra module of ring with scalars $P[\theta_1, \theta_2, ..., \theta_n]$ and basis φ_α. There exist syzygies between φ's in the form,

$$\varphi_\alpha \varphi_\beta = \sum_\gamma c_{\alpha\beta}^\gamma \varphi_\gamma, \quad \text{with } \varphi_0 = 1. \tag{10}$$

Let us give a simple example: $O = 432$ acting on the vector representation. The Molien function is $M(\lambda) = (1+\lambda^9)/(1-\lambda^2)(1-\lambda^4)(1-\lambda^6)$. There are three denominator invariants, $\theta_k = \sum_{i=1}^3 x_i^{2k}$, and one numerator invariant, $\varphi = x_1 x_2 x_3 (x_1^2 - x_2^2)(x_2^2 - x_3^2)(x_3^2 - x_1^2)$. There is one syzygy,

$$\varphi^2 = \theta_3 (\frac{1}{2}\theta_2^3 - 27\theta_3^2 - 9\theta_1\theta_2\theta_3 - \frac{5}{4}\theta_1^2\theta_2^2 + 5\theta_3\theta_1^3 + \theta_2\theta_1^4 - \frac{1}{4}\theta_1^6). \tag{11}$$

Given a ring $\mathcal{P}^G$, it can be represented by different modules. For example the obvious equivalence

$$\begin{aligned} \mathcal{P}^G &= P[\theta_1, \theta_2, ..., \theta_n] \bullet (1, \varphi_1, ..., \varphi_k) \\ &= P[\theta_1, \theta_2, ..., \theta_n^2] \bullet (1, \varphi_1, ..., \varphi_k)(1, \theta_n) \end{aligned} \tag{12}$$

enables one to change the system of denominator invariants (to go from θ_n to θ_n^2) with simultaneous doubling of the number of numerator invariants. It will be useful when one wants to impose constraints on θ_n^2 rather than on θ_n.

Hilbert [13] did not distinguish two kinds of invariants. He used all generators of the ring of invariants as denominator invariants. The number of generators is finite but larger than the number of algebraically independent polynomials. In such a case the generating function for invariant polynomials can be of the form,

$$M(\lambda) = \frac{1 - \sum \lambda^{f_i} + \sum \lambda^{g_i} - \cdots}{\prod(1-\lambda^{d_i})}. \tag{13}$$

It means that there are s generators of degrees $d_1, d_2, \cdots, d_s$. The generators are algebraically dependent and there are t polynomial relations (syzygies of the first kind) between these generators which are of degree $f_1, f_2, \cdots, f_t$ with respect to initial variables. Furthermore there exist some relations (syzygies of the second kind) among syzygies of the first kind characterized by degrees $g_1, g_2, \cdots, g_u$.

The integrity basis is very useful to describe the space of orbits. The idea is to use invariant polynomials as coordinates in the space of orbits. By definition an invariant polynomial is constant along the orbit. Given two orbits, there is at least one polynomial of $\mathcal{P}^G$ which takes different values on them [8]. One can use the integrity basis to label the points of the orbit space $V|G$. The number n of different θ_k is equal to the dimension of the orbit space. In fact Fig. 1 was obtained from the invariants: $\theta_1 = x^2 + y^2 + z^2$, $\xi_x = (x^4 + y^4 + z^4)/\theta_1^2$, $\xi_y = (x^2y^2z^2)/\theta_1^3$. Fig. 1 is the slice of the orbit space at $\theta_1 = 1$. It actually represents the stratum space. Thus it has been used in many applications [9,14,15,16].

2 The Ring of Invariant Real Functions on the Brillouin Zone

2.1 Geometric and Arithmetic Classes, Brillouin Zone

There are 17 space groups in dimension $d = 2$ and 230 in $d = 3$. Their invariant subgroup of translation L acts trivially on the reciprocal space and the Brillouin zone. So the space group G acts effectively through the quotient group $G/L = P$ which is a finite point group ($G \stackrel{\theta}{\to} G/L = P^z$). We label the image of P by P^z. There are 10, 32 geometric classes (equivalent in $O(d)$, called point group) and 13, 73 arithmetic classes (equivalent in $GL(d, Z)$, called symmorphic group), respectively in $d = 2, 3$.

Let us consider two AC's: $p2mm$ and $c2mm$. $c2mm$ is obtained from $p2mm$ by adding the rectangle centers as lattice points (called centring). Their common GC is $2mm = c_{2v}$ and they are generated by

$$p2mm : \pm\sigma_3 = \pm \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad c2mm : \pm\sigma_1 = \pm \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{14}$$

They are equivalent in $O(2)$ but not so in $GL(2, Z)$.

Let us consider 2 one-dimensional space groups: $G_0 = Z$ and $G_1 = Z \rtimes Z_2(-I)$. The point group P for G_1 is generated by $-I$. A unirrep (unitary irreducible representation) of $L = Z$ is of the form $Z \ni n \mapsto \exp(ink)$. Since n is an integer, the representation label k is defined a real number modulo 2π only. On the other hand the set of unirreps of L form a group ($k \mapsto g_k = \exp(ink)$, with the law of addition modulo 2π) which is called the dual group $\hat{L}$ or BZ (Brillouin Zone). This group BZ is isomorphic to U_1. Its topology is that of a circle. The action of the point group P on BZ is defined by $(-I) \cdot k = -k$. Note that this action, which is the linear representation σ on the reciprocal space (the set of real numbers k), is not linear on BZ. It has two fixed points $k = 0$ and $k = \pi$.

Let $\{\vec{b}_i\}$ be the basis vectors of a Bravais lattice L. The basis $\{\vec{b}_i^*\}$ of its dual lattice L^* is defined by $(\vec{b}_i^*, \vec{b}_j) = \delta_{ij}$. If the Bravais group P_L^z of L is represented by the matrices g, then its dual group is represented by

$$g \in P_L^z \leftrightarrow \tilde{g} \stackrel{def}{=} (g^\top)^{-1} = (g^{-1})^\top \in P_{L^*}^z. \tag{15}$$

In other words, the Bravais group of L acts on BZ through its contragradient representation $\tilde{P_L^z} =: ((P_L^z)^{-1})^\top$. We will be dealing with the contragradient representations throughout this work.

2.2 Linearization, Orthogonalization and Modularization

We will need three techniques to obtain rings of modules of invariant functions on the Brillouin zone for all AC's. To illustrate the methods we take one-dimensional space groups for example. In dealing with periodic functions in BZ, it is handy to work with $\cos k$ and $\sin k$ instead of k. Indeed physicists actually measure Fourier components of physical observables.

We can linearize the action of $P \in G_1/L$ on BZ by extending the linear representation σ to one acting on a 2-dimensional orthogonal space V_2 with orthogonal coordinates $c = \cos k$ and $s = \sin k$. 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

$$\rho(-I) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \equiv \sigma(-I) \oplus \gamma(-I), \tag{16}$$

where γ is the trivial representation. $\rho(-I)$ represents a reflection in the 2-dimensional space. It leaves c invariant and changes the sign of s. Thus the ring of its invariant polynomials is the ring of 2 variable polynomials $P[c, s^2]$. The BZ equation defines an ideal of this polynomial ring. The quotient is the polynomial ring $P[c]$.

The representation matrices of some AC's are not orthogonal. One can extend the k space dimension artificially with constraints. In the extra dimensional space the matrices become orthogonal and much easier to handle. However, we should impose the constraints at the end.

For the space group G_0, the ring of invariant polynomials is $P[c, s]$. We can replace this ring by the module of basis $(1, s)$ on the ring $P[c]$ that we denote by $P[c] \bullet (1, s)$. We shall need this operation on and on.

2.3 2D Examples: hexagonal system, $p3$

Its σ representation is generated by $\widetilde{(p3)} = ((-1,-1),(1,0))$ which transforms the k vector, $\vec{k} = k_1 \vec{b}_1^* + k_2 \vec{b}_2^*$, according to

$$\widetilde{(p3)} \begin{pmatrix} k_1 \\ k_2 \end{pmatrix} = \begin{pmatrix} -1 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} k_1 \\ k_2 \end{pmatrix} = \begin{pmatrix} -k_1 - k_2 \\ k_1 \end{pmatrix}. \tag{17}$$

Let us define k_0 by the relation

$$k_0 + k_1 + k_2 \equiv 0 \bmod 2\pi. \tag{18}$$

The matrix $(\widetilde{p3})$ acts on the 'basis' (k_0, k_1, k_2) like an orthogonal matrix, $(R3) = ((0,0,1),(1,0,0),(0,1,0))$ which is the generator of the arithmetic class $R3$ in $d = 3$. From $(\widetilde{p3})$ we can generate all 3 matrices of $p3$. We linearize the actions using Eq. (16) and then use Eq. (5) to obtain the Molien function,

$$M(t) = \frac{1 + 2t^2 + 6t^3 + 2t^4 + t^6}{(1-t)^2(1-t^2)^2(1-t^3)^2}. \tag{19}$$

We get invariants like $c_1 + c_2 + c_0$, $s_1 + s_2 + s_0$, $c_1^2 + c_2^2 + c_0^2$, $s_1^2 + s_2^2 + s_0^2$, $c_1c_2c_0$, $s_1s_2s_0$ for denominator invariants and 11 numerator invariants! We have to impose the condition Eq. (18) to eliminate c_0 and s_0. It takes ingenius and complicated algebra to obtain the integrity basis. We list basic invariants without derivation. We refer the reader to Ref. [1] for further details.

denominator invariants:

$$\theta_1 = c_1 + c_2 + (c_1c_2 - s_1s_2), \quad \theta_2 = c_1c_2(c_1c_2 - s_1s_2), \tag{20}$$

numerator invariants:

$$\begin{aligned} \varphi_1 &= s_1 + s_2 - (c_1s_2 + c_2s_1), \\ \varphi_2 &= s_1 - s_2 + c_1s_2 - c_2s_1 + 2(c_1 - c_2)(c_1s_2 + c_2s_1), \end{aligned} \tag{21}$$

syzygies:

$$\begin{aligned} \varphi_1^2 &= 1 - 2\theta_1 + \theta_1^2 - 4\theta_2, \\ \varphi_2^2 &= 2 + 4\theta_1 + \theta_1^2 + 20\theta_2 - 2\theta_1^3 + 20\theta_1\theta_2 - \theta_1^4 + 4\theta_1^2\theta_2 - 4\theta_2^2. \end{aligned} \tag{22}$$

Thus $p3$ has the ring of module of invariant polynomials,

$$\mathcal{R}^{p3} = P[\theta_1, \theta_2] \bullet (1, \varphi_1)(1, \varphi_2). \tag{23}$$

2.4 3D Examples

$\boxed{P, C, A, R \text{ Arithmetic Classes}}$

There are only 4 different γ representations in this category;

$$\begin{aligned} \mathcal{R}^{P1} &= P[c_1, c_2, c_3], \quad \mathcal{R}^{Cm} = P[c_1 + c_2, c_1c_2, c_3], \\ \mathcal{R}^{R3m} &= P[c_1 + c_2 + c_3, c_1^2 + c_2^2 + c_3^2, c_1c_2c_3], \\ \mathcal{R}^{P3} &= P[c_1 + c_2 + (c_1c_2 - s_1s_2), c_1c_2(c_1c_2 - s_1s_2), c_3]. \end{aligned} \tag{24}$$

- *Pmmm classes*

The eight groups $P1$, $P\bar{1}$, $P2$, Pm, $P2/m$, $P222$, $Pmm2$, $Pmmm$ are in this class. We start with the largest module, that of $P1$. The modules of its supergroups are its submodules. The module of $P1$ is

$$\mathcal{R}^{P1} = P[c_1, c_2, c_3] \bullet (1, s_1)(1, s_2)(1, s_3). \tag{25}$$

$P\bar{1}$ has a reflection through the origin and thus changes $s_i \to -s_i$ simultaneously. Eliminating odd degree terms in s_i from Eq. (25) we obtain its module, $\mathcal{R}^{P\bar{1}} = P[c_1, c_2, c_3] \bullet (1, s_1 s_2, s_2 s_3, s_3 s_1)$.

Pm has a reflection through $z = 0$ plane and odd degree terms in s_3 must be absent from its module, $\mathcal{R}^{Pm} = P[c_1, c_2, c_3] \bullet (1, s_1)(1, s_2)$.

- *$Cmmm$, $P4/mmm$ classes*

There are 7 AC's in the $Cmmm$ class and 8 in the $P4/mmm$ class. We rewrite Eq. (25) into a form

$$\mathcal{R}^{P1} = P[c_1 + c_2, c_1 c_2, c_3] \bullet (1, c_1 - c_2)(1, s_1)(1, s_2)(1, s_3). \tag{26}$$

$C2/m$ is generated by two reflections $\pm j3 = \pm((0,1,0),(1,0,0),(0,0,1))$ which permute indices $(1 \leftrightarrow 2)$ and/or change $s_i \to -s_i$ simultaneously. Keeping the combination of terms in Eq. (26) that respect these symmetries we obtain its module, $\mathcal{R}^{C2/m} = P[c_1 + c_2, c_1 c_2, c_3] \bullet (1, s_1 s_2, (s_1 + s_2)s_3, (c_1 - c_2)(s_1 - s_2)s_3)$.

$P4$ is generated by a reflection $(P4) = ((0,-1,0),(1,0,0),(0,0,1))$ which permute indices $(1 \leftrightarrow 2)$ with simultaneous change $s_1 \to -s_1$. Keeping symmetry preserving terms in Eq. (26) we obtain its module, $\mathcal{R}^{P4} = P[c_1 + c_2, c_1 c_2, c_3] \bullet (1, s_3, (c_1 - c_2)s_1 s_2)$.

- *$R\bar{3}m$, $Pm\bar{3}m$ classes*

There are 5 AC's in the $R\bar{3}m$ class and 5 in the $Pm\bar{3}m$ class. Their common ring is $P[c_1 + c_2 + c_3, c_1^2 + c_2^2 + c_3^2, c_1 c_2 c_3]$. Their module structures are too complicated to list them here. (eg., the dimension of the $R3$ module is 16.) We refer the reader to Ref. [1].

- *Hexagonal classes*

There are 16 AC's in the hexagonal class. By adding c_3 and s_3 to the 2-dimensional case we can easily obtain the modules.

F, I Arithmetic Classes

8 F classes

We computed the Molien function for the ρ representation for $Fm\bar{3}m$ and obtained $N(1) = 6912$. It means that there are 6911 numerator invariants with the highest degree 25. We cannot use the same methods as used up to now.

- *3 F-orthorhombic classes*

We start with the $Pmmm$ lattice. A P-lattice vector have arbitrary integer coordinates μ_i in the orthogonal basis. But the coordinates of an F-lattice vector are restricted by the condition, $\sum_i \mu_i \in 2Z$. By duality the primitive lattice is transformed into itself and becomes a sublattice of $F^* = P^* \cup \vec{w} + P^*$ with $\vec{w} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. That is the "body centring". In passing to the reciprocal lattice of an F lattice a new period $2\pi\vec{w} = (\pi, \pi, \pi)$ must be introduced for the invariant functions. This condition changes the signs of c_i and s_i. We rewrite the module of invariants for $Pmmm$,

$$\mathcal{R}^{Pmmm} = P[c_1, c_2, c_3] \equiv P[c_1^2, c_2^2, c_3^2] \bullet (1, c_1)(1, c_2)(1, c_3). \quad (27)$$

Keeping only even degree polynomials in Eq. (27) we obtain the module for $Fmmm$, $\mathcal{R}^{Fmmm} = P[c_1^2, c_2^2, c_3^2] \bullet (1, c_1c_2, c_2c_3, c_3c_1)$.

- *5 F-cubic classes*

In the similar way we obtain the module for F-cubic arithmetic classes.

$$\mathcal{R}^{Fm\bar{3}m} = P[c_1^2+c_2^2+c_3^2, c_1c_2+c_2c_3+c_3c_1, c_1c_2c_3] \bullet (1, (c_1+c_2+c_3)c_1c_2c_3). \quad (28)$$

8 I classes

These lattices are obtained from P-lattices by adding three face centrings: $(\frac{1}{2}, \frac{1}{2}, 0)$, $(\frac{1}{2}, 0, \frac{1}{2})$,$(0, \frac{1}{2}, \frac{1}{2})$. To pass to the reciprocal lattices we add three periods: $(\pi, \pi, 0)$, $(\pi, 0, \pi)$, $(0, \pi, \pi)$. This introduces simultaneous changes of c_i and s_i for each pair of indices.

- *3 I-orthorhombic classes*

From Eq. (27) we keep only $c_1c_2c_3$ to obtain the module of $Immm$, $\mathcal{R}^{Immm} = P[c_1^2, c_2^2, c_3^2] \bullet (1, c_1c_2c_3)$.

- *5 I-cubic classes*

We rewrite the module of $Pm\bar{3}m$ as

$$\mathcal{R}^{Pm\bar{3}m} = P[c_1^2+c_2^2+c_3^2, c_1c_2c_3, c_1^4+c_2^4+c_3^4] \bullet (1, c)(1, c_1c_2+c_2c_3+c_3c_1). \quad (29)$$

where $c = c_1 + c_2 + c_3$. There are no terms to keep for $Im\bar{3}m$ and its module basis is 1.

8 I-tetragonal classes

These classes are self-dual except for $(I\bar{4}m2 \leftrightarrow I\bar{4}2m)$. In ITC they are presented as the primitive tetragonal ones with the centring $\vec{w} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. We can use this directly on the reciprocal lattice replacing $\vec{w}$ by $2\pi\vec{w}$. But one should beware that in the direct space our coordinates are not the ones used in ITC. With the centring $2\pi\vec{w}$ the invariant polynomials are homogeneous in c_i and s_i and of even degree.

We start with

$$\mathcal{R}^{P4/mmm} = P[c_1+c_2, c_1c_2, c_3] = P[c_1^2+c_2^2, c_1c_2, c_3^2]\bullet(1, c_1+c_2, c_3, (c_1+c_2)c_3). \tag{30}$$

Keeping only even degree terms in Eq. (30) we obtain the module for the largest group in this class, $\mathcal{R}^{I4/mmm} = P[c_1^2+c_2^2, c_1c_2, c_3^2]\bullet(1, (c_1+c_2)c_3)$.

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