

Computer Algebra and Material Design

Akihito Kikuchi

*Canon Inc, Tokyo, Japan**

Abstract

This article is intended to an introductory lecture in material physics, in which the modern computational group theory and the electronic structure calculation are in collaboration. The effort of mathematicians in field of the group theory, have ripened as a new trend, called “computer algebra”, outcomes of which now can be available as handy computational packages, and would also be useful to physicists with practical purposes. This article, in the former part, explains how to use the computer algebra for the applications in the solid-state simulation, by means of one of the computer algebra package, the GAP system. The computer algebra enables us to obtain various group theoretical properties with ease, such as the representations, the character tables, the subgroups, etc. Furthermore it would grant us a new perspective of material design, which could be executed in mathematically rigorous and systematic way. Some technical details and some computations which require the knowledge of a little higher mathematics (but computable easily by the computer algebra) are also given. The selected topics will provide the reader with some insights toward the dominating role of the symmetry in crystal, or, the “mathematical first principles” in it. In the latter part of the article, we analyze the relation between the structural symmetry and the electronic structure in C_{60} (as an example to the system without periodicity). The principal object of the study is to illustrate the hierarchical change of the quantum-physical properties of the molecule, in accordance with the reduction of the symmetry (as it descends down in the ladder of subgroups). As an application, this article also presents the computation of the vibrational modes of the C_{60} by means of the computer algebra. In order to serve the common interest of the researchers, the details of the computations (the required initial data and the small programs developed for the purpose) are explained as minutely as possible.

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I. INTRODUCTION

In the history of physics, the cooperation of physicists and mathematicians has yielded great harvest in the first half of the twentieth century, as the installation of group theory in quantum mechanics.¹ One of the main applications is realized in the field of solid-state physics.²⁻⁴ In subsequent years, however, such productive relationship between physics and mathematics became enfeebled, as physicists and mathematicians were pursuing their own interests separately. In material science, the typical tool of study has turned into “first principle electronic structure computation”, in which rapid computers are intensively used so that the quantitative

simulation could be achieved. In contrast, the group theoretical view in the quantum physics is rather a qualitative one, which could explain the likeness in similar material structures, but could not illuminate the origin of subtle but distinct differences. The standpoints of group theoretical analysis, and of first principles simulation, are located at cross-purposes. This is one of the reasons which brought about the breaking-off between the group theory and the first principles electronic structure computation. There is another hardship which hinders the collaboration of mathematics and physics. The computation of the “representation” in group theory,⁵⁻⁹ useful in physical applications, requires special arts, which are recondite to non-experts. Thus, for the purpose of general use, the character tables are listed up in literature and textbooks (recently, moreover in databases). Traditionally we are obliged to consult with the non-electric data, which is prone to troublesome errors. Such a circumstance has little affinity to the modern style of computational physics, where necessary data should easily be accessible in the computer or computed anew on one’s own responsibility. Nevertheless, it must be stressed here that such a cumbersome situation has already become surmountable. The development of the effective computer architectures and the program packages for computational group theory in recent decades have benefited mathematicians so well that they could actually obtain definite symbolic or numeric solutions to the problems of their own, not only in proving the existence of the solution.^{10,11} These computational tools are not restricted to mathematicians, but available to every scientific researcher. Powerful outcomes by mathematicians, also, will confer a modernized viewpoint to the material science, so that the conventional computational tools could be assisted and improved, although, in the present state, most of material scientists seem to be content in having old-fashioned knowledge of mathematics. This article takes several examples in the group theoretical analysis in the electronic structure calculation, and presents the details of the computation so that the readers would know how to

use modern mathematical packages of computational group theory. The necessary group theoretical data are computed by the desk-top computer, without references to other resources, and are applicable to the analysis of the quantum physics in materials which is principally governed by the symmetry of the system. The article furthermore expounds the possible style of the systematic material design, by which the electronic structure might be controlled artificially from the view point of the structural symmetry. From these topics, the potentiality of the cooperation of computer algebra and first-principles electronic structure (which are legitimate heirs of group theory and quantum mechanics) may be observed.

II. COMPUTATION OF GROUP THEORETICAL PROPERTIES USING “GAP”

The computational discrete algebra package GAP is one of powerful tools for the computation in the group theory.¹² It can be applied to the determination of the group theoretical properties which are necessary for solid-state electronic structure computation. For this purpose, the point group of the crystal must be determined. The group operations are to be listed up; the multiplication table is to be prepared; through which the character table is computed.

At first, the concept of the character of the group is explained here. Let us consider an equilateral triangle as in Fig. 1. There are operations in the plane, such as, the rotation by 60 degrees at the center of mass, and the reflection at an axis which connects the center of mass and one of the vertexes. These operations exchange vertexes among themselves, but fix the triangle unmoved. In the mathematical terminology, these operations consist a group C_{3v} . These operations are the permutation of the vertexes, numbered as 1,2,and 3 in clockwise direction.

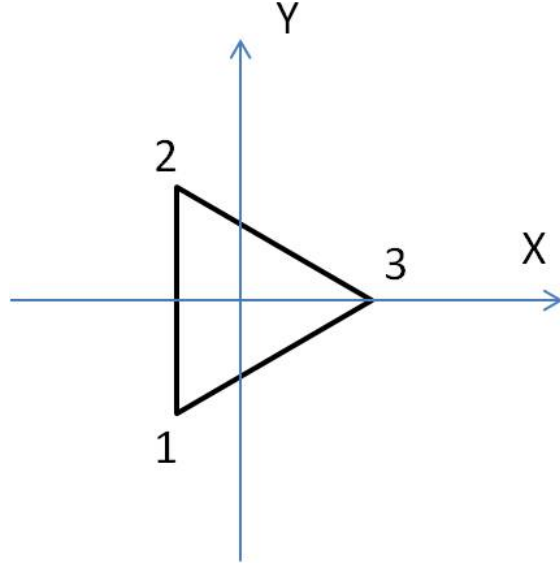


FIG. 1. A triangle.

They are expressed as

$$\begin{aligned}
 E &= \begin{pmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \end{pmatrix}, A = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix}, \\
 B &= \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \end{pmatrix}, C = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix}, \\
 D &= \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix}, F = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}.
 \end{aligned}$$

In the above the top and the bottom low denote the initial and the final arrangements of the vertexes respectively.

These operations can also be expressed by six rotation matrices in the x-y plane:

$$E = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, A = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$B = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}, C = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix},$$

$$D = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, F = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}.$$

The multiplication table among these elements is written in table I.

	E	A	B	C	D	F
E	E	A	B	C	D	F
A	A	E	D	F	B	C
B	B	F	E	D	C	A
C	C	D	F	E	A	B
D	D	C	A	B	F	E
F	F	B	C	A	E	D

TABLE I. The multiplication table.

Let us examine these maps:

$$\Gamma_1 : E, A, B, C, D, F \rightarrow 1$$

$$\Gamma_{1'} : E, D, F \rightarrow 1; A, B, C \rightarrow -1 \text{ (Determinant of matrices)}$$

$$\Gamma_2 : E, A, B, C, D, F \rightarrow E, A, B, C, D, F \text{ (Identity map as matrices)}$$

(1)

One can see that the multiplication table is kept unaltered by these maps with the replacement of the six symbols to corresponding targets. The geometrical operations in the triangle, forming a group, are represented by these maps, even if not always

faithfully; the viewpoint can be switched from geometrical one to numerical one. This is an example of the representation of the group; all elements in the group are represented by proxies of scalars or matrices; the multiplications among them are subject to the same rule as the original group elements. The trace of the matrix representation, such as Γ_2 , is called “character”, having certain properties favorable to the application in quantum physics, as will be seen later. The character table of C_{3v} is given in table II.

	E	A	B	C	D	F
Γ_1	1	1	1	1	1	1
$\Gamma_{1'}$	1	-1	-1	-1	1	1
Γ_2	2	0	0	0	-1	-1

TABLE II. The character table of C_{3v} .

As can be seen in the multiplication table, the group elements are divided into subsets such as

$$\text{Cl}(a) = \{g \in G \mid \text{there exists } x \in G \text{ such as } g = xax^{-1}\}. \quad (2)$$

These subsets are called conjugacy classes. The elements in the same conjugacy class have a common value of the character; it is customary for character tables to be labeled by conjugacy classes, not by each group elements. The conjugacy classes for C_{3v} are given by three subsets: $\{E\}$, $\{A, B, C\}$ and $\{D, F\}$.

The gap computation for this example proceeds as follows. The group is defined by the minimal set of generators including a rotation and a reflection:

```
gap> G:=Group((1,2,3),(1,2));
Group([ (1,2,3), (1,2) ])
```

The program returns the results in the shorthand notation preferred by mathematicians.

```

gap> Elements(G);
[ (), (2,3), (1,2), (1,2,3), (1,3,2), (1,3) ]
gap> M:=MultiplicationTable(G);
[ [ 1, 2, 3, 4, 5, 6 ], [ 2, 1, 4, 3, 6, 5 ], [ 3, 5, 1, 6, 2, 4 ],
  [ 4, 6, 2, 5, 1, 3 ], [ 5, 3, 6, 1, 4, 2 ], [ 6, 4, 5, 2, 3, 1 ] ]

```

The multiplication table is given by a matrix, which is represented by a doubly nested list; each of the inner lists should be read as one of the rows in the matrix. The entry M_{ij} shows the result of the multiplication $g_i \cdot g_j$ between elements g_i and g_j .

Subgroups and generators are computed by:

```

gap> AllSubgroups(G);
[ Group(()), Group([ (2,3) ]), Group([ (1,2) ]), Group([ (1,3) ]),
  Group([ (1,2,3) ]), Group([ (1,2,3), (2,3) ]) ]
gap> GeneratorsOfGroup(G);
[ (1,2,3), (1,2) ]
gap> G.1;
(1,2,3)
gap> G.2;
(1,2)
gap> S:=Subgroup(G, [(1,2)]);
Subgroup(G, [(1,2)]);
gap> Elements(S);
[ (), (1,2) ]
gap> A:=Group((1,2,3));
Group([ (1,2,3) ])
gap> IsSubgroup(G,A);

```

```

true
gap> IsSubgroup(A,G);
false
gap> A:=Group((1,2,3,4));
Group([ (1,2,3,4) ])
gap> IsSubgroup(G,A);
false

```

The group can also be defined from the multiplication table as

```

gap> G2:=GroupByMultiplicationTable(M);
<group of size 6 with 6 generators>
gap> Elements(G2);
[ m1, m2, m3, m4, m5, m6 ]

```

The elements in the group constructed from the multiplication tables are represented by abstract symbols $m_1, m_2, \dots, m_6$.

In order to construct the group from the rotation in the Euclidean space, the generating set of the rotation matrices should be given.

```

gap> M1:=[[ -1/2, ER(3)/2 ], [ -ER(3)/2, -1/2 ]];
[ [ -1/2, -1/2*E(12)^7+1/2*E(12)^11 ],
  [ 1/2*E(12)^7-1/2*E(12)^11, -1/2 ] ]
gap> M2:=[[1,0],[0,-1]];
[ [ 1, 0 ], [ 0, -1 ] ]
gap> G3:=Group(M1,M2);
Group(
[
  [ [ -1/2, -1/2*E(12)^7+1/2*E(12)^11 ],

```

```

[ 1/2*E(12)^7-1/2*E(12)^11, -1/2 ] ], [ [ 1, 0 ], [ 0, -1 ] ]
])

```

Here $ER(n)$ is $\sqrt{n}$ and $E(n)$ is the primitive n -th root of unity $\exp(2\pi i/n)$.

Let us inquire of the GAP package whether the three different definitions should generate equivalent groups.

```

gap> G=G;
true
gap> G2=G;
false
gap> G3=G;
false

```

The GAP program decides that the three groups are not identical in the strict sense, because they are composed from different resources, i.e. permutations, abstract symbols, and matrices. However, we can construct isomorphisms among them. The following GAP command returns the isomorphism on the generators of the groups.

```

gap> IsomorphismGroups(G,G);
[ (1,2,3), (1,2) ] -> [ (1,2,3), (1,2) ]
gap> IsomorphismGroups(G2,G);
[ m1, m2, m3, m4, m5, m6 ] -> [ (), (2,3), (1,2), (1,2,3), (1,3,2),
(1,3) ]
gap> IsomorphismGroups(G,G2);
[ (1,2,3), (1,2) ] -> [ m4, m3 ]
gap> G4:=Group((1,2,3,4))
gap> IsomorphismGroups(G,G4);
fail

```

The existence of the isomorphism between G and G_3 can also be verified in this way.

The conjugacy classes are computed by this command:

```
gap> ConjugacyClasses(G);
[ ()^G, (2,3)^G, (1,2,3)^G ]
```

To access entries in the conjugacy classes, a special method is needed. The following cannot work well:

```
gap> Elements(ConjugacyClasses(G));
[ ()^G, (2,3)^G, (1,2,3)^G ]
```

Instead, using “List” command and anonymous functions in λ calculus, we can access each entry in the list:

```
gap> List(Elements(G), x->x);
[ (), (2,3), (1,2), (1,2,3), (1,3,2), (1,3) ]
gap> List(Elements(G), x->x^-1);
[ (), (2,3), (1,2), (1,3,2), (1,2,3), (1,3) ]
gap> List(ConjugacyClasses(G), Elements);
[ [ () ], [ (2,3), (1,2), (1,3) ], [ (1,2,3), (1,3,2) ] ]
gap> List(ConjugacyClasses(G), Representative);
[ (), (2,3), (1,2,3) ]
```

The character table is computed by this command:

```
gap> irr:=Irr(G);
[ Character( CharacterTable( Sym( [ 1 .. 3 ] ) ), [ 1, 1, 1 ] ),
  Character( CharacterTable( Sym( [ 1 .. 3 ] ) ), [ 1, -1, 1 ] ),
  Character( CharacterTable( Sym( [ 1 .. 3 ] ) ), [ 2, 0, -1 ] ) ]
```

The character table can be accessible as a numeral list, or as a map on the group elements:

```
gap> List([1,2,3],y->List([1,2,3],x->irrg[y][x]));
[ [ 1, 1, 1 ], [ 1, -1, 1 ], [ 2, 0, -1 ] ]
gap> List([1,2,3],y->List(Elements(G),x->x^irrg[y]));
[ [ 1, 1, 1, 1, 1, 1 ], [ 1, -1, -1, 1, 1, -1 ],
  [ 2, 0, 0, -1, -1, 0 ] ]
```

The irreducible representation is computed by

```
gap> rep:=IrreducibleRepresentations(G);
[ Pcgs([ (2,3), (1,2,3) ]) -> [ [ [ 1 ] ], [ [ 1 ] ] ],
  Pcgs([ (2,3), (1,2,3) ]) -> [ [ [ -1 ] ], [ [ 1 ] ] ],
  Pcgs([ (2,3), (1,2,3) ]) ->
    [ [ [ 0, 1 ], [ 1, 0 ] ], [ [ E(3), 0 ], [ 0, E(3)^2 ] ] ] ]
gap> List(Elements(G),x->x^rep[3]);
[ [ [ 1, 0 ], [ 0, 1 ] ], [ [ 0, 1 ], [ 1, 0 ] ],
  [ [ 0, E(3)^2 ], [ E(3), 0 ] ], [ [ E(3), 0 ], [ 0, E(3)^2 ] ],
  [ [ E(3)^2, 0 ], [ 0, E(3) ] ], [ [ 0, E(3) ], [ E(3)^2, 0 ] ] ]
```

This command returns the irreducible representations, giving the relations between the generators of the group and the matrix representation. The characters are computed by taking traces of the matrix representation.

The character table is also computed by

```
gap> tbl:=CharacterTable(G);
CharacterTable( Sym( [ 1 .. 3 ] ) )
gap> Display(tbl);
CT1
```

```

2  1  1  .
3  1  .  1

```

```

1a 2a 3a
2P 1a 1a 3a
3P 1a 2a 1a

```

```

X.1    1  1  1
X.2    1 -1  1
X.3    2   . -1

```

To make use of the character table computed in this way, various subsidiary commands are prepared in GAP system. (N.B. The orderings of representations or characters by these commands do not always coincide with each other.)

```

gap> ConjugacyClasses(tbl);
[ ()^G, (2,3)^G, (1,2,3)^G ]
gap> Irr(tbl);
[ Character( CharacterTable( Sym( [ 1 .. 3 ] ) ), [ 1, -1, 1 ] ),
  Character( CharacterTable( Sym( [ 1 .. 3 ] ) ), [ 2, 0, -1 ] ),
  Character( CharacterTable( Sym( [ 1 .. 3 ] ) ), [ 1, 1, 1 ] ) ]

```

III. SOME PRELIMINARIES

A. Projection operator

Once the characters of the group are obtained, “projection operators” are constructed and assigned to each of the irreducible representation. The definition is as

follows:

$$P^{(p)} = \frac{l_p}{|G|} \sum_{T \in G} \chi_T^{(p)*} \cdot O_T, \quad (3)$$

where l_p is the dimension of the irreducible representation, $|G|$ is the order of the group, and $\chi_T^{(p)}$ is the character of the group element T , which is allowed to be complex-valued. O_T is the operator allotted to each T in the space in which the group action is defined. This operator acts on functions in the Euclidean space as follows:

$$O_T f(r) = f(T^{-1}(r)). \quad (4)$$

By this construction, we can distinguish whether a function belongs to the corresponding irreducible representation or not. If the projector is applied to the basis functions of the corresponding irreducible representations, these functions are invariant as a set: on the other hand, the projector is applied to the basis functions of different irreducible representations, the result of the projection goes to zero. (The epithet “invariant” should be understood in the following way: in many cases, plural basis functions belong to one irreducible representation. Through the group operations, these basis functions are interchanged with each other or re-expressed as the linear combination of them; moreover, they are never transformed into functions belonging to other representations. In a word, they are invariant as a subspace; if the subspace corresponding to a representation is minimal, no more being divisible, it is called irreducible. Whole of representations and characters of the arbitrary finite group could be computed exactly, without omission, by the principle of the group theory.)

If we know the explicit forms of the irreducible matrix representation $D_{ij}^{(p)}(R)$,

the projection operator of the following form is useful:

$$P_{kl}^{(p)} = \frac{l_p}{|G|} \sum_{T \in G} D_{kl}^{(p)*}(O_T) \cdot O_T. \quad (5)$$

Owing to the definition of the partner functions

$$O_T |p; l\rangle = \sum_j |p; j\rangle D_{jl}^{(p)}(T) \quad (6)$$

and the orthogonality theorem of the representation

$$\sum_T D_{ik}^{(p)*}(T) D_{lm}^{(q)}(T) = \frac{|G|}{l_p} \delta_{pq} \delta_{il} \delta_{km} \quad (7)$$

this projector transforms one basis vector into another basis in one irreducible representation:

$$P_{kl}^{(p)} |p; l\rangle = |p; k\rangle. \quad (8)$$

Moreover it can project out k-th partner function of the irreducible representation from an arbitrary function $F = \sum_q \sum_j f_j^{(q)} |q; j\rangle$ as

$$P_{kk}^{(p)} F = f_k^{(p)} |p; k\rangle. \quad (9)$$

At this junction, the connection between the group theory and the energy spectrum of the Schrodinger equations arises. Let the potential term be invariant under some symmetry operations. With this potential term, certain eigenfunctions should exist. When the symmetry operations are applied to the Schrodinger equation, the Laplacian, the potential and the energy spectrum are invariant: the changeable is only the wavefunction, which are expressed by the basis functions in the irreducible representation. If the irreducible representation is one-dimensional, the wavefunction

will be invariant up to a certain phase factor by the symmetry operation: on the other-hand, if the representation is multi-dimensional, the symmetry operation may generate different wave-functions which are other solutions to the same equation with the same eigenvalue. Such circumstances lead to the degeneracy of the energy spectrum. The identification of each wavefunction to its proper irreducible representation enables us to clarify the relation between the energy spectrum and the symmetry in the system, which is helpful in the analysis of the electronic properties of materials.

B. Space group

An n -dimensional space group S is a discrete subgroup in a group of Euclidean motions in $\mathbb{R}^n$, such that the subgroup T in S , composed of pure translations (without rotations or reflections) is a free Abelian subgroup of rank n , having finite index in S . Thus an exact sequence of groups exists as

$$0 \rightarrow T \rightarrow S \rightarrow P \rightarrow 1, \quad (10)$$

in which S acts on T by means of the conjugation action $t \rightarrow s \cdot t \cdot s^{-1}$, which represents the action of the point group P , defined as a factor group S/T , on the lattice translations.

In a more intuitive expression, the space group S is the set of symmetry operations in a periodic system; it is composed of rotations and reflections which fix components in the unit cell, combined with parallel movements along crystal axes; therefore S is of infinite order; the parallel movements, by themselves, compose the discrete subgroup T of infinite order, in which the direction and the stride of the movements are determined by the primitive lattice vectors. Meanwhile the point group P is the set of remainder of operations in S , taken modulo of the crystalline periodicity, i.e.

with the parallel movements in T being nullified; it is a finite group and may include fractional translations, which are represented by linear combinations of fractions of primitive lattice vectors.

C. Crystallographic group

In the case of crystallographic group, the symmetry operation is the affine mapping, composed of the linear parts R_T , including the reflection, rotation, and inversion, and the translation parts τ_T .¹³ The definition is

$$O_T = \{R_T|\tau_T\} : r \rightarrow R_T \cdot r + \tau_T, \quad (11)$$

$$O_T \cdot O_S = \{R_T \cdot R_S|\tau_T + R_T \cdot \tau_S\}, \quad (12)$$

$$O_T^{-1} = \{R_T^{-1}|-R_T^{-1} \cdot \tau_T\}. \quad (13)$$

The operation on the plane wave is

$$O_T \exp(ikr) = \exp(ik(R_T^{-1}r - R_T^{-1}\tau)) = \exp(i(R_T \cdot k)(r - \tau)). \quad (14)$$

The affine mapping gives rise to the phase factor $\exp(-i(R_T \cdot k)\tau)$, which is not unity at a general k -point. On the other hand, the matrix representation of the affine mapping is subject to the following relation:

$$D^{(p,k)}(\{R_k|f_{R_k} + \tau_n\}) = e^{-ik \cdot \tau_n} D^{(p,k)}(\{R_k|f_R\}) \quad (15)$$

The trace of the matrix $D^{(p,k)}$ is the character: therefore the phase-factors in the character and the wave-number part in the Bloch-type wavefunction (e^{ikr} in $e^{ikr}u_k(r)$) are canceled with each other as complex conjugates; in the general k -point, the phase

shift in the character can actually be negligible in the projection operator. (Indeed there are textbooks or lectures omitting these terms.) However, if the Bloch-type wavefunction is expressed by plane-wave expansion $\sum C_G e^{i(k+G)r}$, one should be cautious. The phase shift in the periodic part is $e^{iR_k(G)\tau_n}$, which remains without cancellation in the projection operation.

D. Theoretical set-up for Wyckoff positions

The mathematical definition of the Wyckoff positions is stated as follows.

Let G be a space group, T be its translation lattice, K be its point group, t_g be fractional translations. Each element in G has a form of $\{k|t_k + t\}$ for $k \in K$ and $t \in T$, and acts on a vector v in $V = \mathbb{R}^n$ as

$$\{k|t_k + y\}(v) = k \cdot v + t_k + t. \quad (16)$$

The stabilizer of $v \in V$ under this action is denoted as $\text{Stab}_G(v) = \{g \in G | g(v) = v\}$. Let $v \in V$. An equivalence relations $\sim$ is set up if $\text{Stab}_G(v)$ is conjugate to $\text{Stab}_G(w)$, i.e. $\text{Stab}_G(w) = \text{Stab}_G(g(v)) = g \text{Stab}_G(v) g^{-1}$ for some $g \in G$. This equivalence classes of $\sim$ is called the Wyckoff positions of G .

This definition, given in the mathematicians' terminology, is a little recondite for physicists. For a more intuitive understanding, it can be restated as:

The Wyckoff positions are a set of coordinate points, composed from two subsets:

[Type 1] The coordinate points which may be fixed by a certain symmetry operation of the point group. They are regarded as generators of the Wyckoff positions.

[Type 2] The coordinate points generated from those in Type 1 subset by all of the symmetry operations.

The command in GAP “WyckoffPositions(S)” returns the type 1 set for a space group S; the equivalent coordinate points to a generator “W” in type 1 set by the symmetry operations are computed from another command “WyckoffOrbit(W)”.

E. Units in the computation

Throughout the computations of quantum physics in this article, we use atomic units, abbreviated as a.u. if necessary; for the length, the Bohr radius($a_0 \cong 5.292 \times 10^{-11}\text{m}$); for the energy, the Hartree unit($E_h \cong 27.211\text{eV}$).

IV. APPLICATION 1: IDENTIFICATION OF WAVEFUNCTIONS TO IRREDUCIBLE REPRESENTATIONS

The application in this section is the classical example in group theory in quantum physics.

A. The simplest case: at Γ point

In this section, the group theoretical analysis of the wavefunction is exemplified. The wavefunctions at Γ point in the diamond crystal are classified to corresponding irreducible representations. The treatment for the general k -point ($k \neq 0$) shall be discussed later.(The knowledge on the distinction between symmorphic or non-symmorphic crystal is necessary; the existence of these two types of crystal makes the discussion not a little complicated.)

At first, the character table should be computed. The symmetric operations in the diamond structure, whose unit cell is minimal one, including two carbon atoms, are given in the appendix, as well as the multiplication table of these operations.

When one uses the GAP packages, there are several options for the preparation of the point group; of which three types are usable.

First: the symmetry operations are given as a set of three dimensional matrix.

```
gap> MT[ 1]:=[[ 1, 0, 0],[ 0, 1, 0],[ 0, 0, 1]];;
gap> MT[ 2]:=[[ 1, 0, 0],[ 0, -1, 0],[ 0, 0, -1]];;
.....
gap> MT[ 48]:=[[ 0, 0, 1],[ 0, 1, 0],[ -1, 0, 0]];;
gap> G:=Group(MT);
```

Second: the multiplication table in the group is supplied.

```
gap> M:=[[1,2,3,...,48],[...],...,[...]];;
gap> G:=GroupByMultiplicationTable(M);
gap> Elements(G);
[ m1, m2, m3, m4,.....,m45, m46, m47, m48 ]
```

In this case, the group elements are denoted by symbolical way, m1,m2,...,m48.

Actually, all of group elements are not necessarily provided to define a group: it is enough to give the smallest generating set, from which other elements are constructed. The group should be remade by means of the smallest generating set. (In the present implementation of GAP, especially when the multiplication table is supplied, the following tendency in the computation is observed: the computations for groups, constructed from the minimal generating set, are much quicker than those for groups where the all elements are stored as generators.) For the case of the diamond, the computation goes as:

```

GS:=SmallGeneratingSet(G);
[ m36, m48 ]
G:=Group(GS);
<group with 2 generators>

```

The command “SmallGeneratingSet()” yields a reasonably small generating set. In the cases of finite solvable groups (a typical example of this is the crystal point group) and of finitely generated nilpotent groups, “MinimalGeneratingSet()” command is also available to get minimal generators, but the computation is time-consuming. In addition, each element “elm” in the group “G” can be expressed by generators, by means of Factorization(G,elm):

```

gap> List(Elements(G),x->Factorization(G,x));
[ <identity ...>, x2^-1*x1*x2*x1, x2^2, (x2*x1)^2, x2^2*x1^2,
  x1*x2^2*x1, x1^2, x2^-1*x1^-1*x2^-1*x1, x1^-1*x2^-1*x1*x2,
  x2^-1*x1^2*x2, x2^-1*x1*x2*x1^-1, x1^-2, x2^-1*x1, x1^-1*x2^-1,
  x2*x1, x2*x1*x2^2, x2^2*x1*x2, x2*x1^-1, x1*x2, x2^-1*x1^-1,
  x1^-1*x2^-1*x1^2, x2^-1*x1^3, x2*x1*x2^2*x1^2, x2*x1^3, x1^3,
  x2^-1*x1^-1*x2^-1*x1^2, x2^2*x1^3, x1*x2^2*x1^2, x2^2*x1^-1,
  x2*x1*x2, x1^-1, x2^-1*x1*x2, x1*x2^2, x2^2*x1, x2^-1*x1^-1*x2^-1,
  x1, x1^2*x2, x1*x2*x1^-1, x2*x1^-2, x1*x2^2*x1*x2, x2*x1*x2^2*x1,
  x2*x1^2, x1^-1*x2^-1*x1, x2^-1*x1^2, x1*x2*x1, x2^-1,
  x2*(x2*x1)^2, x2 ]

```

Third: the crystallographic groups are defined by four dimensional augmented matrices, in which both of the point group operations and the translations are inscribed. The notations for the augmented can be given in the following form

$$\begin{pmatrix} A & v \\ 0 & 1 \end{pmatrix} \quad (17)$$

acting on column vectors $(x, 1)$ from the right or, alternatively,

$$\begin{pmatrix} A^T & 0 \\ v & 1 \end{pmatrix} \quad (18)$$

acting on row vectors $(x, 1)$ from the left, which represent the affine mapping $x \rightarrow A \cdot x + v$. (Crystallographers prefer the later notation.)

Once the crystallographic group is defined, the point group can easily be deduced. The definition of the crystallographic group may require more business; but it will be of use in the later applications, to which a certain idea of the crystallographic group are essential.

As for the diamond case, in the GAP computation, the crystallographic group is defined as follows. (The minimal generating set is used for simplicity.)

```
gap> M1:=[[0,0,1,0],[1,0,0,0],[0,-1,0,0],[1/4,1/4,1/4,1]];;
gap> M2:=[[0,0,-1,0],[0,-1,0,0],[1,0,0,0],[0,0,0,1]];;
gap> S:=AffineCrystGroup([M1,M2]);
<matrix group with 2 generators>
gap> P:=PointGroup(S);
Group([ [ [ 0, 0, 1 ], [ 1, 0, 0 ], [ 0, -1, 0 ] ],
        [ [ 0, 0, -1 ], [ 0, -1, 0 ], [ 1, 0, 0 ] ] ])
```

By these preparations the conjugacy classes and the character table of the diamond crystal are computed as tables III and IV. (The group elements for the symmetry operation are given in a table in the appendix. The entries in the conjugacy classes

are given by the numbering of the table of the group elements.)

Class	Group Elements
C.1	1 (The identity)
C.2	2 , 3 , 4
C.3	5 , 6 , 7 , 8 , 9 , 10 , 11 , 12
C.4	13 , 16 , 17 , 18 , 21 , 23
C.5	14 , 15 , 19 , 20 , 22 , 24
C.6	25
C.7	26 , 27 , 28
C.8	29 , 30 , 31 , 32 , 33 , 34 , 35 , 36
C.9	37 , 40 , 41 , 42 , 45 , 47
C.10	38 , 39 , 43 , 44 , 46 , 48

TABLE III. Conjugacy classes of the point group in the diamond structure. The elements are indexed in the same way as the table of the symmetry operations.)

	C.1	C.2	C.3	C.4	C.5	C.6	C.7	C.8	C.9	C.10
x.1	1	1	1	1	1	1	1	1	1	1
x.2	1	1	1	-1	-1	-1	-1	-1	1	1
x.3	1	1	1	-1	-1	1	1	1	-1	-1
x.4	1	1	1	1	1	-1	-1	-1	-1	-1
x.5	2	2	-1	0	0	-2	-2	1	0	0
x.6	2	2	-1	0	0	2	2	-1	0	0
x.7	3	-1	0	-1	1	-3	1	0	1	-1
x.8	3	-1	0	-1	1	3	-1	0	-1	1
x.9	3	-1	0	1	-1	-3	1	0	-1	1
x.10	3	-1	0	1	-1	3	-1	0	1	-1

TABLE IV. The character table of the basic diamond structure at Γ point.

We can apportion the wavefunctions at Γ point to each irreducible representations by applying the projection operator. (It is enough to check whether the numerical result of the projection remains almost as it is, or it nearly vanishes to zero.) The identification in the example of the diamond is given in table V. In the numerical expansion coefficients of the wavefunctions, we can imagine the existence of a hidden mechanism, as is suggested by the successions of zeros, or the interchanges of specific

values with the alteration of signs. The hierarchy and the symmetry in them can be unraveled and classified by the group theoretical analysis.

	k_1	k_2	k_3	$\ G\ ^2$	1	2	3	4	5	6	7	8
1	0	0	0	0	-0.9765	0	0	0	0	0	0	0
2	-1	-1	-1	1.6243	0.0742	0.3519	-0.0007	0.2934	-0.3562	-0.1637	-0.3913	-0.3212
3	1	1	1	1.6243	0.0742	0.3519	-0.0007	0.2934	0.3562	0.1637	0.3913	0.3212
4	0	-1	0	1.6243	-0.0742	-0.1488	0.1173	0.4172	-0.0785	0.5376	0.1078	-0.3212
5	0	1	0	1.6243	-0.0742	-0.1488	0.1173	0.4172	0.0785	-0.5376	-0.1078	0.3212
6	0	0	1	1.6243	-0.0742	0.3159	0.301	-0.1397	0.084	0.295	-0.4612	0.3212
7	0	0	-1	1.6243	-0.0742	0.3159	0.301	-0.1397	-0.084	-0.295	0.4612	-0.3212
8	1	0	0	1.6243	-0.0742	0.1848	-0.419	0.0159	-0.5186	0.0788	0.1777	0.3212
9	-1	0	0	1.6243	-0.0742	0.1848	-0.419	0.0159	0.5186	-0.0788	-0.1777	-0.3212
10	-1	-1	0	1.8756	0	0.0285	-0.2391	0.3432	0	0	0	-0.1671
11	1	1	0	1.8756	0	0.0285	-0.2391	0.3432	0	0	0	0.1671
12	0	-1	-1	1.8756	0	0.1325	0.3315	0.2199	0	0	0	-0.1671
13	0	1	1	1.8756	0	0.1325	0.3315	0.2199	0	0	0	0.1671
14	1	0	1	1.8756	0	0.3968	-0.0935	-0.0981	0	0	0	0.1671
15	-1	0	-1	1.8756	0	0.3968	-0.0935	-0.0981	0	0	0	-0.1671
Ene.					-2.1091	19.5799	19.5799	19.5799	25.1394	25.1394	25.1394	33.1443
Rep.					x.1	x.10	x.10	x.10	x.7	x.7	x.7	x.2

TABLE V. The identification between the irreducible representation and the wavefunctions in diamond crystal at Γ point. Wavefunctions are expressed by coefficients (C_i, k_1, k_2, k_3) in the plane wave expansion $C_i \exp(iGr)$; $G = k_1 G_1 + k_2 G_2 + k_3 G_3$, where G_1, G_2, G_3 are reciprocal vectors. The left columns (from the second to the fifth) indicate ($k_1, k_2, k_3, |G|^2$) and the remaining parts give the coefficients C_i . The energies and the irreducible representations are given in last two columns indicated by “Ene.” and “Rep.”, respectively. The carbon atoms are placed at $\pm(1/8 \cdot a_1 + 1/8 \cdot a_2 + 1/8 \cdot a_3)$ so that the coefficients of the wavefunctions in the plane wave expansion are real-valued.

B. Character table computation in super-cell

It is a standard way to use the minimal unit cell. In the diamond structure, the minimal primitive cell is chosen to be the same as the face-centered one, in which two carbon atoms are located with the point-group $G(I \times O, C_2 \times S_4)$. Meanwhile, one can

choose the cubic unit cell; the volume of which is four times as large as the minimal cell, because the cubic cell is constructed from four of the simplest unit cell stuck together obliquely. The unit cell enlarged in the similar way, (if possible, in which extra atoms are embedded) is called super-cell. The point groups of the super-cells are inevitably altered by the presence of extra fractional translations. The group theoretical computations for such super-cells will be difficult for bare human powers, since the point group becomes larger and more complicated. Nevertheless, if one can use the computer algebra system, the character tables are easily computed. We should note that it is more advisable to compute characters of groups by ourselves if we can. Although the possible super-cells are infinite, the character tables available in textbooks and databases are limited, possibly only for the minimal unit cell.

For the super-cell, actually, the point group of the minimal crystal can be extended by the semidirect product with a finite Abelian group, by which extra fractional translations in the enlarged cell are represented. (The construction of the semidirect product will be stated elsewhere in the following section of this article.) The easiest and straight way for this is to remake the multiplication table. This can be done in the following way: first, apply possible fractional translations to group elements in symmetry operations of the minimal cell, so that all symmetry operations in the super-cell are prepared in the following form:

$$\{E|\tau_i\}\{R_j|\sigma_j\}. \quad (19)$$

By means of these new set of operations, we must construct the multiplication table in the super-cell:

$$\{R_j|\sigma_j + \tau_i\}\{R_k|\sigma_k + \tau_l\} = \{R_p|\sigma_p + \tau_q\}. \quad (20)$$

In the evaluation, we can make use of the multiplication table in the minimal cell:

$$\{R_j|\sigma_j\}\{R_k|\sigma_k\} = \{R_j \cdot R_k|\sigma_j + R_j\sigma_k\} \equiv \{R_p|\sigma_p\} \quad (21)$$

There is a relation:

$$\{R_j|\sigma_j + \tau_i\}\{R_k|\sigma_k + \tau_l\} = \{R_j \cdot R_k|\sigma_j + \tau_i + R_j\sigma_k + R_j\tau_l\} = \{R_p|\sigma_p + \tau_q\}. \quad (22)$$

From the equations (21) and (22), it leads that

$$\tau_q \equiv \sigma_j + \tau_i + R_j\sigma_k + R_j\tau_l - \sigma_p \text{ (modulo translational vectors)} \quad (23)$$

Using this τ_q , the extended multiplication table can be constructed with ease.

The exemplar calculation for the diamond structure shall be executed in this section. The basic unit cell in the diamond structure is the face-centered one, including two atoms, The lattice vectors are defined as

$$a_1 = (0, 1/2, 1/2), a_2 = (1/2, 0, 1/2), a_3 = (1/2, 1/2, 0) \quad (24)$$

This basic unit cell could be extended four-fold, in which atomic coordinates are given by translations such as $x \rightarrow x + \tau_i$ ($i = 0, 1, 2, 3$). The vectors τ_i are defined as:

$$\tau_0 = (0, 0, 0), \tau_1 = (0, 1/2, 1/2), \tau_2 = (1/2, 0, 1/2), \tau_3 = (1/2, 1/2, 0) \quad (25)$$

The extended unit cell is the cubic one, including eight atoms, to which the lattice vectors are defined as:

$$a'_1 = (1, 0, 0), a'_2 = (0, 1, 0), a'_3 = (0, 0, 1) \quad (26)$$

Let F be the group composed of the four fractional translation vectors τ_i ($i = 0, 1, 2, 3$). And let T be the group of primitive lattice translations, composed of a'_1, a'_2, a'_3 and the zero vector. The factor group $N(=F/T)$ is a finite group, whose generators $\hat{\tau}$ are given by the projection of τ_i onto N . This factor group is the Klein four group, or $Z_2 \oplus Z_2$. The generators satisfy the following relations.

$$\begin{aligned} 2 \cdot \hat{\tau}_i &= \hat{\tau}_0 \\ \hat{\tau}_1 + \hat{\tau}_2 + \hat{\tau}_3 &= \hat{\tau}_0 \end{aligned} \tag{27}$$

The point-group G' in the cubic unit cell is the semidirect product $N \rtimes G$, between the group of the fractional translations N and the point-group G in the basic unit cell. The new group includes 192 ($= 48 \times 4$) elements. The textbooks or databases, however, only show the point group of the basic, minimal unit cells, but not those of the extended super-cells. In the latter cases, the point group is of the semidirect product; one can compute its character tables by straightforwardly constructing the multiplication table, or, in a more complicated and elegant way, i.e. by making use of the induced representation of the group, when the group N is Abelian. The computation of the induced representation will be explained in the appendix.

The group elements in the extended group are renumbered as follows:

$$\{E|\tau_i\}\{R_j|s_j\} \rightarrow (i \times 48 + j)\text{th element of the extended group} \tag{28}$$

The conjugacy classes and the character tables for the extended group are given in table VI and VII.

Class	Group Elements
$\hat{C}.1$	$[0,1]$

$\hat{C}.2$	$[0,2],[0,3],[0,4],[1,2],[2,3],[3,4]$
$\hat{C}.3$	$[0,5],[0,6],[0,7],[0,8],[0,9],[0,10],[0,11],[0,12],$ $[1,5],[1,6],[1,7],[1,8],[1,9],[1,10],[1,11],[1,12],$ $[2,5],[2,6],[2,7],[2,8],[2,9],[2,10],[2,11],[2,12],$ $[3,5],[3,6],[3,7],[3,8],[3,9],[3,10],[3,11],[3,12]$
$\hat{C}.4$	$[0,13],[0,17],[0,21],[1,16],[1,17],[1,23],$ $[2,16],[2,18],[2,21],[3,13],[3,18],[3,23]$
$\hat{C}.5$	$[0,14],[0,15],[0,19],[0,20],[0,22],[0,24],$ $[1,14],[1,15],[1,19],[1,20],[1,22],[1,24],$ $[2,14],[2,15],[2,19],[2,20],[2,22],[2,24],$ $[3,14],[3,15],[3,19],[3,20],[3,22],[3,24]$
$\hat{C}.6$	$[0,16],[0,18],[0,23],[1,13],[1,18],[1,21],$ $[2,13],[2,17],[2,23],[3,16],[3,17],[3,21]$
$\hat{C}.7$	$[0,25],[1,25],[2,25],[3,25]$
$\hat{C}.8$	$[0,26],[0,27],[0,28],[1,26],[1,27],[1,28],$ $[2,26],[2,27],[2,28],[3,26],[3,27],[3,28]$
$\hat{C}.9$	$[0,29],[0,30],[0,31],[0,32],[0,33],[0,34],[0,35],[0,36],$ $[1,29],[1,30],[1,31],[1,32],[1,33],[1,34],[1,35],[1,36],$ $[2,29],[2,30],[2,31],[2,32],[2,33],[2,34],[2,35],[2,36],$ $[3,29],[3,30],[3,31],[3,32],[3,33],[3,34],[3,35],[3,36]$
$\hat{C}.10$	$[0,37],[0,40],[0,41],[0,42],[0,45],[0,47],$ $[1,41],[1,42],[2,45],[2,47],[3,37],[3,40]$
$\hat{C}.11$	$[0,38],[0,39],[0,43],[0,44],[0,46],[0,48],$ $[1,38],[1,39],[1,43],[1,44],[1,46],[1,48],$ $[2,38],[2,39],[2,43],[2,44],[2,46],[2,48],$

	[3,38],[3,39],[3,43],[3,44],[3,46],[3,48]
$\hat{C}.12$	[1,1],[2,1],[3,1]
$\hat{C}.13$	[1,3],[1,4],[2,2],[2,4],[3,2],[3,3]
$\hat{C}.14$	[1,37],[1,40],[1,45],[1,47],[2,37],[2,40],[2,41],[2,42], [3,41],[3,42],[3,45],[3,47]

TABLE VI: Conjugacy classes for the cubic diamond structure. The element $\{1|\tau_j\}\{R_i|\sigma_j\}$ is denoted as [j,i].

	$\hat{C}.1$	$\hat{C}.2$	$\hat{C}.3$	$\hat{C}.4$	$\hat{C}.5$	$\hat{C}.6$	$\hat{C}.7$	$\hat{C}.8$	$\hat{C}.9$	$\hat{C}.10$	$\hat{C}.11$	$\hat{C}.12$	$\hat{C}.13$	$\hat{C}.14$
y.1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
y.2	1	1	1	-1	-1	-1	-1	-1	-1	1	1	1	1	1
y.3	1	1	1	-1	-1	-1	1	1	1	-1	-1	1	1	-1
y.4	1	1	1	1	1	1	-1	-1	-1	-1	-1	1	1	-1
y.5	2	2	-1	0	0	0	-2	-2	1	0	0	2	2	0
y.6	2	2	-1	0	0	0	2	2	-1	0	0	2	2	0
y.7	3	-1	0	-1	1	-1	-3	1	0	1	-1	3	-1	1
y.8	3	-1	0	-1	1	-1	3	-1	0	-1	1	3	-1	-1
y.9	3	-1	0	1	-1	1	-3	1	0	-1	1	3	-1	-1
y.10	3	-1	0	1	-1	1	3	-1	0	1	-1	3	-1	1
y.11	6	-2	0	-2	0	2	0	0	0	0	0	-2	2	0
y.12	6	-2	0	2	0	-2	0	0	0	0	0	-2	2	0
y.13	6	2	0	0	0	0	0	0	0	-2	0	-2	-2	2
y.14	6	2	0	0	0	0	0	0	0	2	0	-2	-2	-2

TABLE VII. The character table of the cubic diamond unit cell at Γ point.

The eight lowest eigenvalues in energy spectra in the minimal and cubic diamond cell are shown in table VIII. There are two sets of threefold degeneracy in the former case. On the other hand, in the latter, there is one sixfold degeneracy, which is attributable to the overlap of the spectra at the three X points in the Brillouin zone of the minimal unit cell. However, the character tables of Γ point in the minimal diamond cell could not assign them in suitable representation; the character tables

rebuilt for the cubic cell can do this.

Minimal	-2.11	19.58	19.58	19.58	25.14	25.14	25.14	33.14
Representation	x.1	x.10	x.10	x.10	x.7	x.7	x.7	x.2
Cubic	-2.11	6.74	6.74	6.74	6.74	6.74	6.74	13.03
Representation	y.1	y.14	y.14	y.14	y.14	y.14	y.14	y.12

TABLE VIII. The energy spectra at Γ point in the minimal and cubic diamond unit cell. The assigned irreducible representations are also shown.

V. APPLICATION 2: A SYSTEMATIC WAY OF THE MATERIAL DESIGNING

A. How to manage quantum-dynamics in crystal?

The group theoretical view will be able to bring about a systematic way of material design. In this section, although in the level of table-top exercise, a practicable form of material design is presented. In a nutshell, through the systematic reduction of the crystal symmetry, the band-structure could tactically be modulated; the degeneracy of the energy spectrum can be artificially split into different levels and the new energy-gap can be opened. Toward the systematic reduction of the crystal symmetry, the crystallographic concept, called Wyckoff positions, is utilized.^{13,15} This mathematical idea is not an abstract one, but actually computable by means of the computer algebra.

One should note this: the degeneracy of the energy spectrum is governed by the symmetry of the crystal. From the mathematical viewpoint, the point group of the crystal system is the manifestation of the symmetry; the subgroups of the point group describe the possible style with the reduced symmetry. (It is well known that a material has general tendency to reduce its own symmetry in order to release itself

from the energetically unstable situation owing to the existence of the degeneracy of occupied energy levels.) By tracing the tree structure of the inclusion relations of the subgroup of the finite groups, one can enumerate every possibility of reduced symmetry. For each of reduced symmetries one can compute group representations. The comparison of the character tables in the subgroups and the parent groups (by means of analyzing compatibility relations) one can rummage the possibility of the breaking-down of the energy spectrum degeneracy. The opening of the energy-gaps in the reduced symmetry will be speculated, sorted and classified with their group theoretical origins. This plan, therefore, will lead into a kind of systematic way of material design. It must be admitted that such a tactic still lacks in sufficiently quantitative argument, since the only possible existence of energy-gap, together with their relationship with crystal symmetry reduction, is discussed. In order to evaluate the stability of the reduced structure, or the actual possibly of its existence, one must employ massive first-principles computation. However, the group theoretical inspection has its own merit; it can be achieved by a light and quick computation, frugal in hardware usage; maybe simple computations in the level of elementary perturbation theory will do. Hence it can be applied to screening purposes for picking up candidates before serious massive first-principles computation.

As an example, consider the crystallographic group of cube, including following operations.

- Three rotations along x, y, or z axes by 90 degrees.
- Exchange of x, y, and z axes (Rotations along the diagonal in the cube by 120 degrees).
- The inversion and reflections are omitted for simplicity.

These rotations generate 24 operations in the cubic lattice to construct the point

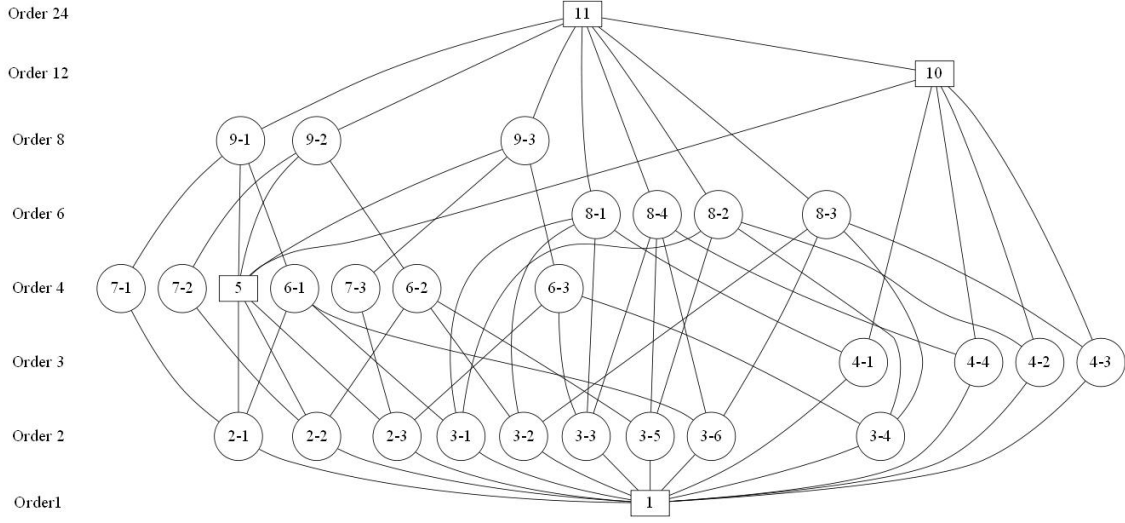


FIG. 2. The paradigm of the crystal symmetry, or the subgroup lattice.

group. Using GAP, The relationship of the inclusion in subgroups (the lattice subgroup) can be inquired and visualized(Fig.2). The point group of the cubic lattice is located at the topmost node of the tree. We can trace the subgroups of lower symmetries in descending along the branches and finally arrive at the trivial group (the identity group), which is located at the root of the tree. This means that we can explore and predict the alternation of the band structure (viz, the splitting of the degenerated energy levels, or the opening of new band gaps) systematically, by consulting with the “paradigm” of the crystal symmetry.

Now there arise following questions.

Question 1. *How to make up actual crystal structures in correspondence with the subgroups of lower symmetries?*

Answer 1. The reduction of the symmetry may be occasioned, for example, by the presence of alien atoms, or the occurrence of point defects in the perfect crystal. The change in the electronic structure will be investigated by simple perturbation theory

with sufficient accuracy.

Question 2. *In what positions alien atoms or point defects can be located? It is easy to cause the great change the symmetry, or, to abolish it completely. However, for the case with the small change in the symmetry, for example, that between neighboring connected entries in the subgroup lattice, can we set up favorable atomic dispositions?*

Answer 2. Choose an arbitrary point. Apply all of the operations of the subgroup in consideration to this coordinate. The number of the generated points is equal to the order of the subgroup. The set of these points is invariant with respect to the operation of the subgroup. By disposing alien atoms or defects in this set of points, we can reduce the symmetry of the crystal, and, continuing this way, descend through the subgroup lattice.

Question 3. *It is impossible for us to dispose alien atoms at arbitrary points in the crystal. With the view of the material design, a certain restriction should be imposed on the number of alien atoms. We would like to know the set of atomic sites, with a limitation in number, and invariant by the subgroup operation.*

Answer 3. Make use of the concept of the Wyckoff position.

The mathematical definition is given in the appendix. In a familiar word of material sciences, the Wyckoff positions are the set of equivalent points in the unit cell, which are transformed among themselves by symmetry operations. In general, the total number of such points is the same as that of the symmetry operations (the order of the point group). However, if the generating point of the Wyckoff position remains fixed by certain operations of the point group, the total number of Wyckoff positions will be fewer, which will be a factor of the order of the point group. In mathematical word, it is equal to the order of some factor group. In GAP program, the Wyckoff position is easily computed from a “Cryst” package.

In this example of the cubic lattice, the Wyckoff positions are classified as follows:

- A discrete point $(0,0,0)$.
- A discrete point $(1/2,1/2,1/2)$.
- The centers of the edges of the cube: $(1/2,0,0), (0,1/2,0), (0,0,1/2)$.
- The centers of the faces: $(1/2,1/2,0), (1/2,0,1/2), (0,1/2,1/2)$
- A segment $(x,0,0)$ ($0 < x < 1$), invariant by 90-degrees rotation along the x axis.
- A segment $(0,y,0)$ ($0 < y < 1$), invariant by 90-degrees rotation along the y axis.
- A segment $(0,0,z)$ ($0 < z < 1$), invariant by 90-degrees rotation along the z axis.
- A segment $(x,1/2,1/2)$ ($0 < x < 1$), invariant by 90-degrees rotation along the x axis.
- A segment $(1/2,y,1/2)$ ($0 < y < 1$), invariant by 90-degrees rotation along the y axis.
- A segment $(1/2,1/2,z)$ ($0 < z < 1$), invariant 90-degrees rotation along the z axis.
- A segment (t,t,t) , invariant 120-degrees rotations which exchange three axes. (In the similar way, all of diagonal lines of the cube belong to this type.)
- Several segments (not discrete points), connected to the vertexes, the centers of the edges.
- Arbitrary points in the unit cell.

In table IX, the Wyckoff positions of the group of full symmetry of the cubic cell and those of one of the subgroups are compared. These two groups have common

generators of the Wyckoff positions. However, in some of them, the number of equivalent positions differs. By making use of such positions and stationing atoms in them, we can switch the crystal symmetry. For example, take the Wyckoff positions given in the 7-th low. They are in the orbit of the generating point $(t, 0, 1/2)$. The group of No.11 and No.10 are isomorphic to the symmetric group S_4 and the alternative group A_4 respectively. In the full symmetry, given by the group of No.11, the orbit is composed of 12 points. On the other hand, in the reduced symmetry of the group No.10, these 12 points is split into two orbits, each of which includes 6 points. If atoms (say, of type W) are positioned in all of 12 points in the cubic lattice, the crystal symmetry remains unaltered as that of the group of No.11. However, if, in the half part of them, at the Wyckoff positions of the Group No.10, the atoms are replaced by those of type B, the crystal symmetry is reduced to the group of No.10. Those Wyckoff positions are illustrated in Fig. 3, where two split orbits are shown in B(black) and W(white) atoms.

Group NO.11 (#G=24)	Size	Group NO.10 (#G=12)	Size
$[0,0,0]$	1	$[0,0,0]$	1
$[1/2,1/2,1/2]$	1	$[1/2,1/2,1/2]$	1
$[0,1/2,1/2]$	3	$[0,1/2,1/2]$	3
$[1/2,0,0]$	3	$[1/2,0,0]$	3
$[t,0,0]$	6	$[t,0,0]$	6
$[t,1/2,1/2]$	6	$[t,1/2,1/2]$	6
$[t,0,1/2]$	12	$[0,t,1/2]$	6
		$[1/2,t,0]$	6
		(Split in two)	
$[t,t,0]$	12	not existent	0
$[t,t,1/2]$	12	not existent	0
$[t,t,t]$	8	$[t,t,t]$	4
$[t1,t2,t3]$	24	$[t1,t2,t3]$	12

TABLE IX. The Wyckoff positions in the cubic lattice. The left three columns gives the generators and the right two show the number of equivalent points.

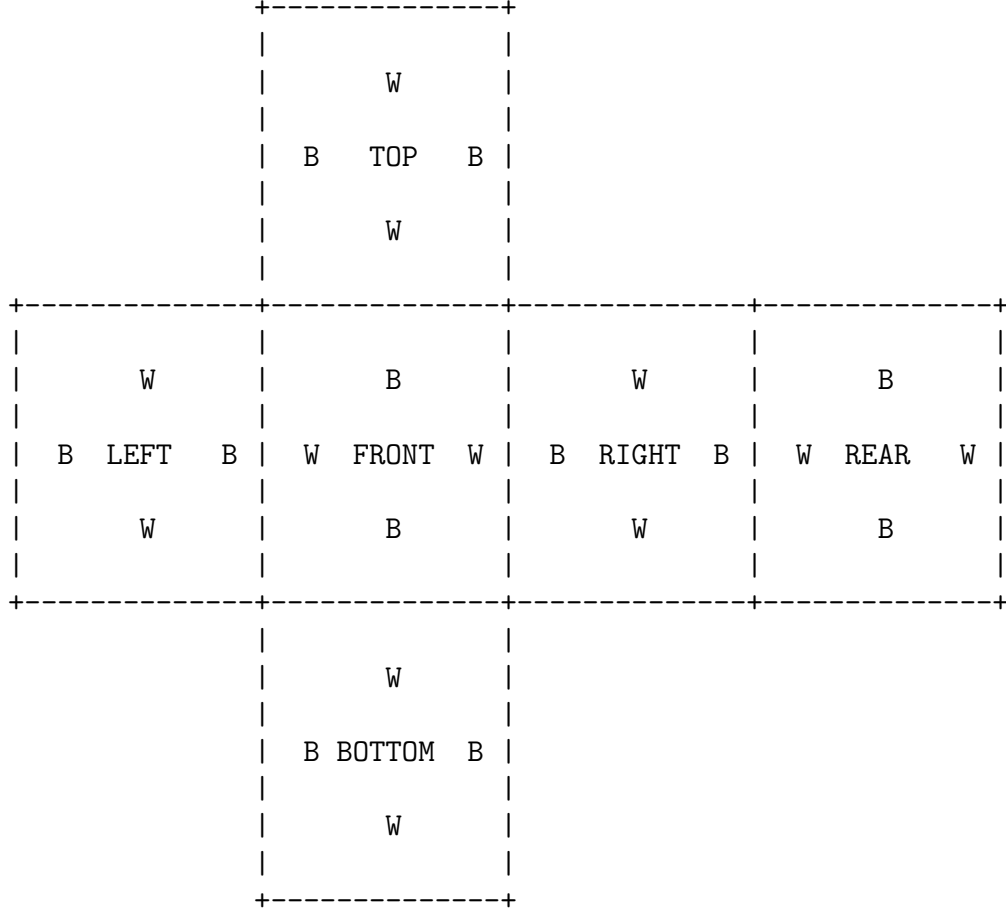


FIG. 3. An illustration of split Wyckoff Orbit in the six faces of the cube.

B. Control of band gaps by means of the Wyckoff positions

In this section, the example of the material design discussed in the previous section is presented; in which ab-initio electronic structure calculations are executed, where the symmetry of the crystal is artificially altered and the band gaps are controlled.

The exemplar calculation goes in the following way: in order to alter the crystal symmetry, certain coordinate points are chosen; and at these localities we put impu-

rities, which interact to electrons with short-ranged potentials; these impurities are assumed to be neutral; therefore they do not alter the net charge. The change in the symmetry of the crystal will be caused by the presence of impurities, the effects of which are expressed by model potentials with adjustable parameters. We use the following form of the scattering potential. It is given in the real space as

$$V(r) = C \exp \left(-\frac{1}{2} \left(\frac{r}{r_{loc}} \right)^2 \right) \quad (29)$$

where Ω is the volume. We use two parameters, i.e. $Z = C\sqrt{(2\pi)^3}(r_{loc}^3)$ (strength) and r_{loc} (range). The reciprocal space representation is

$$V(K) = \frac{1}{\Omega} Z \exp \left(-\frac{1}{2} (r_{loc} K)^2 \right), \quad (30)$$

where Ω is the volume, required in the normalization of the plane wave $\frac{1}{\sqrt{\Omega}} \exp(iKr)$.

A simple example is taken from diamond band structure. The coordinate of the carbon atoms are

$$\begin{aligned} & (0 \cdot V_1 + 0 \cdot V_2 + 0 \cdot V_3) \\ & (1/4 \cdot V_1 + 1/4 \cdot V_2 + 1/4 \cdot V_3). \end{aligned} \quad (31)$$

The lattice vectors are

$$\begin{aligned} V_1 &= \left(\frac{a}{2}, \frac{a}{2}, 0 \right), \\ V_2 &= \left(\frac{a}{2}, 0, \frac{a}{2} \right), \\ V_3 &= \left(0, \frac{a}{2}, \frac{a}{2} \right). \end{aligned} \quad (32)$$

In this structure, the lowest eight eigenvalues at Γ point are shown in table X.

There are two set of threefold degeneracy above and below the band gap, the energy

Γ	-2.11	19.58	19.58	19.58	25.14	25.14	25.14	33.14
Representation	x.1	x.10	x.10	x.10	x.7	x.7	x.7	x.2

TABLE X. The lowest eight eigenvalues at Γ point in the diamond structure.

levels of which are at 19.58 a.u. and 25.14 a.u.. (The irreducible representations to them are x.10 and x.7 respectively, as given in the previous section.)

The band gap (in exact terms, the degeneracy of the eigenvalues) is modified by the insertion of a single impurity in the crystal. Its position is chosen at $(1/8 \cdot V_1 + 1/8 \cdot V_3 + 1/8 \cdot V_3)$. The point group of the genuine diamond structure (of the order of 48) is reduced to its subgroup (of the order of 12.) The symmetry operations of the subgroup are shown in table XI.

TABLE XI. The symmetry operations with the presence of an impurity.

	R11	R12	R13	R21	R22	R23	R31	R32	R33	T1	T2	T3
1	1	0	0	0	1	0	0	0	1	0	0	0
2	0	1	0	0	0	1	1	0	0	0	0	0
3	0	0	1	1	0	0	0	1	0	0	0	0
4	0	-1	0	-1	0	0	0	0	-1	1/4	1/4	1/4
5	-1	0	0	0	0	-1	0	-1	0	1/4	1/4	1/4
6	0	0	-1	0	-1	0	-1	0	0	1/4	1/4	1/4
7	-1	0	0	0	-1	0	0	0	-1	1/4	1/4	1/4
8	0	-1	0	0	0	-1	-1	0	0	1/4	1/4	1/4
9	0	0	-1	-1	0	0	0	-1	0	1/4	1/4	1/4
10	0	1	0	1	0	0	0	0	1	0	0	0
11	1	0	0	0	0	1	0	1	0	0	0	0
12	0	0	1	0	1	0	1	0	0	0	0	0

The character table of this subgroup is given in table XII. The rows S1,...,S6 show the character values of the subgroup, and the rows G7 and G10 shows those of the group of the full diamond symmetry (without impurity).

TABLE XII. The character table of the diamond structure with an impurity. The characters for each operation are shown here.

	1	2	3	4	5	6	7	8	9	10	11	12
S.1	1	1	1	1	1	1	1	1	1	1	1	1
S.2	1	1	1	-1	-1	-1	-1	-1	-1	1	1	1
S.3	1	1	1	-1	-1	-1	1	1	1	-1	-1	-1
S.4	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1
S.5	2	-1	-1	0	0	0	-2	1	1	0	0	0
S.6	2	-1	-1	0	0	0	2	-1	-1	0	0	0
x.7	3	0	0	-1	-1	-1	-3	0	0	1	1	1
x.10	3	0	0	1	1	1	3	0	0	1	1	1

In the rows of the table, there are two relations : $x.7=S.2+S.5$ and $x.10=S.1+S.6$; which are called matching relations.(In some mathematical context, they are referred as branching rules.) These relations indicate the threefold degeneracy in the energy levels in the full diamond symmetry split into two irreducible representations S.2 and S.5, or S.1 and S.6 with the presence of an impurity. The character values of the identity element, shown in the second columns from the left, are the degeneracy of the energy levels; so we can predict the threefold-degeneracy split into two different levels, viz. twofold and single levels.

To inspect this, the actual computation is executed; where the impurity potential is set to be a weak Gaussian form. For example, set the parameters in eq.30 as $Z = -0.1, r_{loc} = 0.1$. The lowest eight eigenvalues are given in table XIII. The prediction by group theory is realized there.

Γ	-2.18	18.86	19.67	19.67	25.04	25.18	25.18	33.13
----------	-------	-------	-------	-------	-------	-------	-------	-------

TABLE XIII. The lowest eight eigenvalues at Γ point in the diamond structure with an impurity.

In the practice of the artificial material design, for example, the following demand

will arise:

Demand: How to substantiate the situation, in which the band gap is altered, but the degeneracy of the energy levels is unaffected?

Let us proceed with the example of diamond. In the diamond structure, there are plural possible Wyckoff positions. (The computation can be done by GAP.) For example, chose the position of $(1/8V_1 + 1/8V_2 + 1/8V_3)$. By the symmetry operations it is transformed in three other points such as: $(5/8V_1 + 1/8V_2 + 1/8V_3)$, $(1/8V_1 + 5/8V_2 + 1/8V_3)$, $(1/8V_1 + 1/8V_2 + 5/8V_3)$. If impurities are stationed at these four points, there is no change in the point group; thus the degeneracy of the energy spectrum remains unchanged. The computed energy spectrum is given in table XIV, which guarantees the validity of the group theory. The band dispersions along $\Gamma(0,0,0) - X(2\pi/a,0,0)$ are shown in Fig. 4, in which that of the basic diamond structure, and that with single impurity, and that with four impurities are compared.

Γ	-2.41	18.83	18.83	18.83	25.11	25.11	25.11	33.07
----------	-------	-------	-------	-------	-------	-------	-------	-------

TABLE XIV. The lowest eight eigenvalues at Γ point in the diamond structure with four impurities.

There is a certain noteworthy point in these two cases (of the single impurity , and of the four impurities). In the former, the single impurity is located at $(1/8V_1 + 1/8V_2 + 1/8V_3)$; this point is one of the Wyckoff positions in the point group of the crystal with the deteriorated symmetry; it remains fixed by any symmetry operation and not transformed into other positions; however, this point also belongs to the Wyckoff position of the perfect diamond crystal and there transformed to four points. We can interpret this circumstance as follows: the former example corresponds to a situation, where the only one of the four Wyckoff position in the latter case is

chosen, so that the symmetry of the crystal could be reduced. In a similar way, (but in a more general and liberal way, by inserting extra atoms or excavating vacancy site) we can reduce the crystal symmetry for the purpose of controlling the band structure; by doing this we can cleave into the degeneracy of the energy spectra and open extra energy gaps.

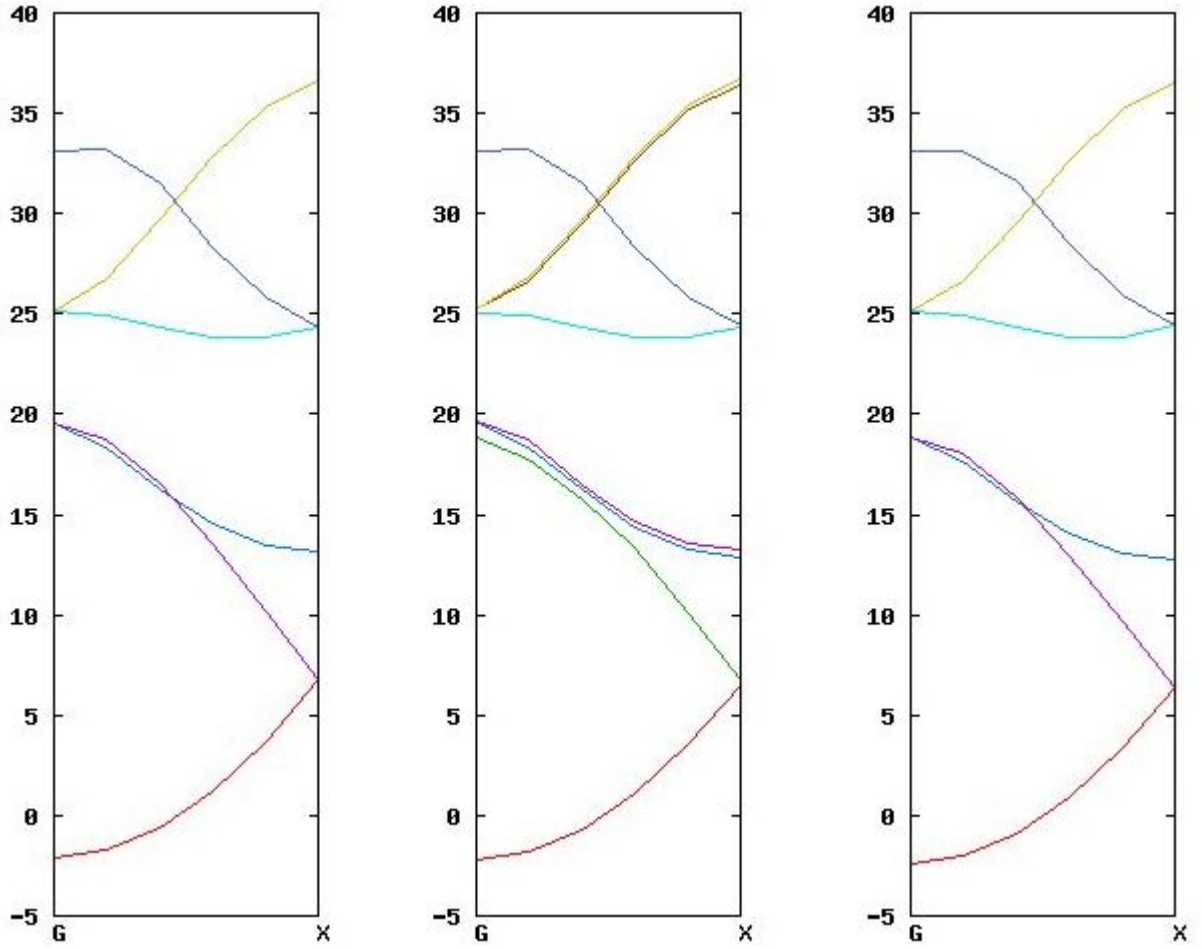


FIG. 4. The band dispersions in diamond structures altered by the presence of impurities, along Γ -L direction. The left figure is that without impurity: the center, with a single impurity: the right, with four impurities.

C. A possible plan of material design in the super-cell

Now we have seen that the band structure is controllable by the presence of impurities or defects, although the presented example is of instructive purpose, and not realistic, as an only model case for the sake of illustrating possible form of theoretical material design. The diamond structure is compressed in such a compact cell that the supernumerary atoms could not be actually stationed at arbitrary places, such as at Wyckoff positions. Meanwhile, in recent decades, crystalline materials which has a large unit cell such as In_3O_2 have been put into practical use. At a glance, In_3O_2 seems to have a huge complex structure. However, actually, it is a super-cell composed from the stacking of body-centered lattice of In-O, with oxygen vacancies. The band dispersion is almost free-electron like; its behavior under the presence of doped Sn, viz. impurities in the cell, can be understood by the group theoretical view.¹⁶ Furthermore the modern material composing technologies, such as epitaxial growth, or micro atom-scale probes, may enable us to realize such microscopic disposition of atoms in super-cell structure, which will lead to actual phase of material design. In the super-cell, there is a more broad freedom in atomic arrangement, in which certain atoms could be replaced or removed so that the periodical arrangement of impurities or defects should be permitted.

Now a principle of material design based on group theoretical view can be proposed.

- 1 Chose a certain crystal as a starting point: this crystal should have small and simple unit cells.
- 2 Consider an enlarged cell, composed of the stacking of the minimal unit cell. (The crystal axes may be cut anew and a super-cell should be created.)
- 3 We can determine the band structure and the band gap of the enlarged cell,

simply by folding the band structure of the minimal cell. (The folding of the band structure is to re-distribute k-points of the old Brillouin zone to the new one in accordance with the new periodicity and to redraw the band dispersion by means of new k-points.)

- 4 Suppose a situation where the symmetry is reduced by the formation of super-cell with atomic displacements. Check the possibility of the opening of the extra band gaps (or the splitting of the degeneracy) at k-points with high symmetries, such as at Γ points and the boundary of the Brillouin zone. The group theoretical view, such as the character theory, the compatible relation, the subgroup lattices, or the Wyckoff positions, should be fully made use of. The change in the band structure may be quantitatively evaluated by simple perturbation theory. These sorts of trial-and-errors, by tracing the sequence of crystal symmetry, will help us to search crystal structures with more desirable band structure.

VI. TECHNICAL DETAILS

In the preceding sections of the article, the basics for the usage of computer algebra, concerning with the computation of group theoretical properties, are explained and applied to the analysis of the wave-functions. Moreover, the possible scheme for controlling band gaps, by means of tracing the sequence of subgroups, which corresponds to the reduction of crystal symmetry, is suggested through simple electronic structure computations. Meanwhile, in this part, the topics are rather promiscuous and technical, such as the computation of characters of the group of the super cell by means of “semi-direct product” which is an effective way to extend groups, or the special treatment for non-symmorphic crystal, and so on. Moreover, “mathematical

first principle” of crystal formation is demonstrated based on the cohomology theory, which shall explain us how specific types of crystals, finite in number, can exist in accordance with the actions of certain point groups. The topics might arrive at somewhat higher mathematics, that may be not well-known to physicists. However, with the aid of computer algebra, one can conquer such hardships so that he might actually execute necessary computations. As for the fundamental knowledge of the group theory and its application, the reader should consult with standard references, such as Refs. 1, 2, 3, 4, 5, 6 for the group theory, such as Refs. 7, 8, 9 for the representation theory, such as Refs. 10, 11 for the algorithm in the computer algebra. We make use of the computer algebra package GAP,¹² as well as in the previous sections.

A. Determination of crystal symmetry

It is essential for us to determine the crystal symmetry in order to execute the group theoretical analysis. The symmetry operations which fix the crystal axes and atomic coordinates must be listed to construct the point group. The determination algorithm of the point group is composed of the following two stages.

Stage 1. *Determination of the point group of the lattice.*

Let $A = (A_1, A_2, A_3)$ be the lattice vectors. There are two large categories of the crystal system; the one of which is hexagonal, and the other is cubic. In the former, rotations along the crystal axis by 60 degrees are allowed; in the latter, the rotations of this kind are composed of those by 90 degrees. The point group of arbitrary crystal system is given as a subgroup which is reduced from the full hexagonal or cubic symmetries. The full set of the symmetry operations (i.e. rotation matrices) for the hexagonal or cubic symmetry should be prepared, and from which

admissible operations are extracted.

For each operation R of the full symmetry group, compute the rotation of the lattice vectors:

$$R \cdot A_i (i = 1, 2, 3). \quad (33)$$

If the vector $R \cdot A_i$ protrudes out of the unit cell, it must be pulled back according to the crystal periodicity. Hereafter the pulling back of a vector x into the unit cell is denoted as $P(x)$. For example, $R \cdot A_i = l \cdot A_1 + m \cdot A_2 + n \cdot A_3$ for integers l, m, n , then exactly $P(R \cdot A_i) = 0$.

Then store the operation R such as

$$\|P(R \cdot A_i)\| \leq \epsilon$$

for all $A_i (=1,2,3)$, with a threshold value ϵ (This is an attention needed only in the floating-point computation.) From the stored set of admissible operations $\{R\}_C$, the point group of the crystal system is determined; in this stage, however, the symmetry preservation in the atomic positions is not yet checked.

Stage 2. *Determination of the point group of the crystal.*

The symmetry operations which fix atomic coordinates should be extracted now. The atom transformation table, the fractional translations associated to each rotation, and the multiplication table should be provided at the same time. Let X and Y be entries in the set of atomic positions $\{X\}$, and let $T(X)$ and $T(Y)$ be the corresponding type of atoms.

For each $R \in \{R\}_L$, and for each $X \in \{X\}$, compute $R \cdot X$; and chose

every $Y \in \{X\}$ such as $T(X) = T(Y)$. Now the vector $\tau_c = P(R \cdot X - Y)$ is a candidate for the fractional translation associated to R . If τ_c is the admissible fractional translation to R , the following conditions should be satisfied.

Condition: for all X_1 in the atomic coordinates, there exist a Y_1 such that

$$\|\tau_c - P(R \cdot X_1 - Y_1)\| \leq \epsilon,$$

and

$$T(X_1) = T(Y_1).$$

If this condition is satisfied, store R and τ_c as a symmetry operation $\{R|\tau_c\}$ in the point group of the crystal.

This algorithm works well if the unit cell is minimal, in the sense that the fractional translation is uniquely determined; i.e. with respect to one symmetry operation of $\{R|t\}$, other operations, such as $\{E|s\}\{R|t\} = \{R|t+s\}$, do not coexist in the point group operations. If the unit cell is not minimal, in other words, if it is a super-cell (the accumulation of the minimal unit cell), the existence of plural τ for one R cannot be negligible. The readers will be able to find and utilize subroutines or functions purposed for the identification of the crystal symmetry (possibly with more efficacy than the algorithm in this section) in the band calculation packages of one's own.

B. Symmetry operations in the reciprocal space

As for the plane wave, the symmetry operation in the real-space is given as

$$\{R_T|\tau_T\} \exp(ikr) = \exp\left(ik\left(R_T^{-1}r - R_T^{-1}\tau_T\right)\right) = \exp\left(i(R_T \cdot k) \cdot (r - \tau_T)\right). \quad (34)$$

Consequently, it is more convenient to give operations with respect to reciprocal lattice vectors in the wave number space. If the wave-number-vector k is expressed as $k_1 \cdot G_1 + k_2 \cdot G_2 + k_3 \cdot G_3$, the rotation matrix for coefficients in the rotated vector $R_T \cdot k$ is given as

$$\begin{pmatrix} R'_{11} & R'_{12} & R'_{13} \\ R'_{21} & R'_{22} & R'_{23} \\ R'_{31} & R'_{32} & R'_{33} \end{pmatrix} \begin{pmatrix} k_1 \\ k_2 \\ k_3 \end{pmatrix}. \quad (35)$$

Thus the rotation matrix for the coefficients is computed from that in the Euclidean space as:

$$R' := \left((a_1, a_2, a_3)^{-1} R^T (a_1, a_2, a_3) \right)^T \quad (36)$$

where a_1, a_2, a_3 are primitive lattice vectors.

For the case of the face-centered unit cell, the gap computation is done as:

```
gap> A:=[ [ 0, 1/2, 1/2 ], [ 1/2, 0, 1/2 ], [ 1/2, 1/2, 0 ] ];;
gap> RM:=[ [ 1, 0, 0 ], [ 0, -1, 0 ], [ 0, 0, -1 ] ];;
gap> TransposedMat(A^-1*TransposedMat(RM)*A);
[ [ -1, 0, 0 ], [ -1, 0, 1 ], [ -1, 1, 0 ] ]
```

The rotation matrices in the reciprocal space, as well as those in the real space, are given in the appendix for cubic and hexagonal symmetries.

C. The computation of the compatibility relation

The irreducible representation of the diamond structure shows branching if the k -point moves from Γ point to non-zero k -point. The situation of the branching (the compatibility relation) can be checked by GAP. For this purpose, the computation goes as follows:

- Compute the character table for the small group. Then, for each representation, evaluate the characters of elements in the small group, and store them in the lists $S_1, S_2, \dots, S_N$. (Let N be the number of the representations of the Small group.)
- Compute character values of elements in the small group, using the irreducible representation at Γ point, and store them in the lists $G_1, G_2, \dots, G_M$. (Let M be the number of the representations of the point group.)
- If the j -th irreducible representation (G_j) branches into the composition of those in the small (S_i) as follows

$$G_j = \sum_{i=1}^N C_i^j \times S_i \quad (37)$$

the coefficients are computed by the inner product of the lists as

$$C_i^j = G_j \cdot S_i / |\#K| \quad (38)$$

where $|\#K|$ is the order of the small group.

For this purpose, this function can be used:

```
GetCompati:=function(A,B)
local repA,repB,AV,BV,CV;
repA:=Irr(A);
repB:=Irr(B);
if ( false=IsSubgroup(A,B) ) then
Print("A < B ; Inverse A and B."); return;
fi;
```

```

AV:=List(repA,y->List(Elements(B),x->x^y));
BV:=List(repB,y->List(Elements(B),x->x^y));
CV:=AV*TransposedMat(BV)/Size(B);
return CV;
end;

```

Symmetry operations defined in wave-number space are used here. These matrices are three dimensional ones given in Table XLV.(They are stored as “MT[]” in the following.) The coordinate of the K point along $\Gamma - X$ point is given, as the coefficients to reciprocal lattice vectors.

```

gap> kx:=[0,1,1];
[ 0, 1, 1 ]

```

The symmetry operations which fix the k-point are extracted, and from them the small group is generated.

```

gap> FL:=Filtered(MT,i->i*kx=kx);
[ [ [ 1, 0, 0 ], [ 0, 1, 0 ], [ 0, 0, 1 ] ],
  [ [ -1, 0, 0 ], [ -1, 0, 1 ], [ -1, 1, 0 ] ],
  [ [ 0, -1, 1 ], [ 0, 0, 1 ], [ -1, 0, 1 ] ],
  [ [ 0, 1, -1 ], [ -1, 1, 0 ], [ 0, 1, 0 ] ],
  [ [ 0, 1, -1 ], [ 0, 1, 0 ], [ -1, 1, 0 ] ],
  [ [ 0, -1, 1 ], [ -1, 0, 1 ], [ 0, 0, 1 ] ],
  [ [ 1, 0, 0 ], [ 0, 0, 1 ], [ 0, 1, 0 ] ],
  [ [ -1, 0, 0 ], [ -1, 1, 0 ], [ -1, 0, 1 ] ] ]

```

We can directly construct the small group from the above list of the output. For the purpose of the comparison of the representations, however, the point group and

the small group must be expressed by common abstract symbols such as “m1,m2,...”, which are employed to make up the multiplication table.(There is an alternative: the point group could be constructed from the 48 matrices of symmetry operations in wave-number space.)

```
gap> FL:=List(FL,i->Position(MT,i));
[ 1, 2, 19, 20, 27, 28, 41, 42 ]
gap> FL:=List(FL,i->Elements(G)[i]);
[ m1, m2, m19, m20, m27, m28, m41, m42 ]
gap> GS:=Group(FL);
<group with 8 generators>
```

The character table of the full point group GN is given as:

```
gap> ConjugacyClasses(GN);
[ m1^G, m2^G, m5^G, m13^G, m14^G, m25^G, m26^G, m29^G,
m37^G, m38^G ]
gap> Display(Irr(GN));
[ [ 1, 1, 1, 1, 1, 1, 1, 1, 1, 1 ],
[ 1, 1, 1, -1, -1, -1, -1, -1, 1, 1 ],
[ 1, 1, 1, -1, -1, 1, 1, 1, -1, -1 ],
[ 1, 1, 1, 1, 1, -1, -1, -1, -1, -1 ],
[ 2, 2, -1, 0, 0, -2, -2, 1, 0, 0 ],
[ 2, 2, -1, 0, 0, 2, 2, -1, 0, 0 ],
[ 3, -1, 0, -1, 1, -3, 1, 0, 1, -1 ],
[ 3, -1, 0, -1, 1, 3, -1, 0, -1, 1 ],
[ 3, -1, 0, 1, -1, -3, 1, 0, -1, 1 ],
[ 3, -1, 0, 1, -1, 3, -1, 0, 1, -1 ] ]
```

The character table of the small group is as follows:

```
gap> List(ConjugacyClasses(GS),Elements);
[ [ m1 ], [ m2 ], [ m19, m20 ], [ m27, m28 ], [ m41, m42 ] ]
gap> Display(Irr(GS));
[ [ 1, 1, 1, 1, 1 ],
  [ 1, 1, -1, -1, 1 ],
  [ 1, 1, -1, 1, -1 ],
  [ 1, 1, 1, -1, -1 ],
  [ 2, -2, 0, 0, 0 ] ]
```

The branching relations are computed now:

```
gap> Display(GetCompati(GN,GS));
[ [ 1, 0, 0, 0, 0 ],
  [ 0, 1, 0, 0, 0 ],
  [ 0, 0, 1, 0, 0 ],
  [ 0, 0, 0, 1, 0 ],
  [ 0, 1, 0, 1, 0 ],
  [ 1, 0, 1, 0, 0 ],
  [ 1, 0, 0, 0, 1 ],
  [ 0, 0, 0, 1, 1 ],
  [ 0, 0, 1, 0, 1 ],
  [ 0, 1, 0, 0, 1 ] ]
```

This output list should be read as the indication of the following branching relation:

POINT GROUP	SMALL GROUP
G.1	-> S.1
G.2	-> S.2

G.3	->	S.3
G.4	->	S.4
G.5	->	S.2 + S.4
G.6	->	S.1 + S.3
G.7	->	S.1 + S.5
G.8	->	S.4 + S.5
G.9	->	S.3 + S.5
G.10	->	S.2 + S.5

D. The character table at the boundary of the Brillouin zone

1. The necessity of the special treatment for the non-symmorphic crystal

In general non-zero k-points, the wave-functions are apportioned to representations different to that of Γ point. The new representations are deduced from subgroups of the point group; the subgroup admissible to each k-point must be composed of operations which fix that k-point. The invariance on the k-point by symmetry operations should be kept up to the periodicity of the wave-space. Thus at the boundary of the Brillouin zone, different but equivalent k-points are mingled together in the representation. In general, it is sufficient to chose the subgroup which connects equivalent k-points and compute the representation in the same way as in Γ point. However, in special cases, this naive approach inevitably fails owing to the existence of two-different kind of crystal structures, i.e. the distinction between the symmorphic and non-symmorphic ones. Let us review this troublesome situation.

The matrix representation could be written as

$$D^k(\{\alpha|\tau\}) = \exp(-ik \cdot \tau)\Gamma(\alpha). \quad (39)$$

Then the product is

$$D^k(\{\alpha_1|\tau_1\})D^k(\{\alpha_2|\tau_2\}) = \exp(-ik \cdot (\tau_1 + \tau_2))\Gamma(\alpha_1)\Gamma(\alpha_2) = \exp(-ik \cdot (\tau_1 + \tau_2))\Gamma(\alpha_1\alpha_2). \quad (40)$$

The product should be equal to this:

$$D^k(\{\alpha_1 \cdot \alpha_2 | \alpha_1 \cdot \tau_2 + \tau_1\}) = \exp(-ik \cdot (\alpha_1 \cdot \tau_2 + \tau_1))\Gamma(\alpha_1\alpha_2). \quad (41)$$

These equations lead to the relation:

$$\exp(i(\alpha_1^{-1} \cdot k - k) \cdot \tau_2) = 1. \quad (42)$$

Certain conditions are required so that the above relation should be valid:

- 1 The k point is inside the Brillouin zone; α_1^{-1} does not move k (i.e. $\alpha_1 \cdot k = k$).
At Γ point, this condition is always satisfied.
- 2 The k point is located at the boundary of the Brillouin zone: the vector $\alpha_1 \cdot k - k$ may coincide with a certain reciprocal vector due to the periodicity on the wave space. The subgroups of the operations of these kind are called small groups. In addition the τ_2 should be zero or a lattice translation vector in the real space.

The crystal structure, in which the second condition always holds, is said to be symmmorphic. In certain types of crystals, however, there exist affine mappings with non zero τ_2 , which are fractions of some lattice translational vectors. This type of the crystal is called non-symmorphic. Indeed, the diamond structure is non-symmorphic one, as can be seen in the symmetry operations for this crystal. For the non-symmorphic case, therefore, the relation to be satisfied with respect to the

product of the matrix representation does not hold at the boundary of the Brillouin zone. Thus it is necessary to employ special methods to treat this case. One of these treatments was proposed by Herring.¹⁴ The intuitive interpretation of this method could be given in the following way. One should bear in mind these two points: First, at Γ point, there is no problem in the representation even in the non-symmorphic case. Secondly, the k-point at the boundary of the Brillouin zone can be pull back at Γ point, if the unit cell is extended. For example, in a one-dimensional crystal with the lattice constant of a , the k-point $k = \pi/a$ is at the boundary of the Brillouin zone. However, when the doubled unit cell (with the lattice constant $2a$) is assumed, the k-point $k = \pi/a$ agrees with the new primitive reciprocal lattice vector; hence it is equivalent to the Γ point. The irreducible representation at π/a in the small original cell can be deduced from that at Γ point in the enlarged cell. Thus the difficulty in non-symmorphic representation can be eluded. We shall examine the actual computation of this method in the next section.

2. Herring Method: An example

Assume a double array of atoms, as in the Fig. 5. This figure shows two types of one-dimensional periodic lattice, consisted by double lines of atoms. In case I, two rows forms one dimensional periodic system of squares. In case II, the two lows are shifted by half of the lattice constants. The latter is of non-symmorphic type. The symmetry operations which fix the k-point at $k = \pi/a$ for the latter case is given as

$$e = \{E|0\} \tag{43}$$

$$c = \{C_2|0\} \text{ A rotation by 180 degrees along the origin}$$

$$m = \{\sigma_x|a/2\} \text{ A reflection over x axis}$$

$$g = \{\sigma_y|a/2\} \text{ A reflection over y axis}$$

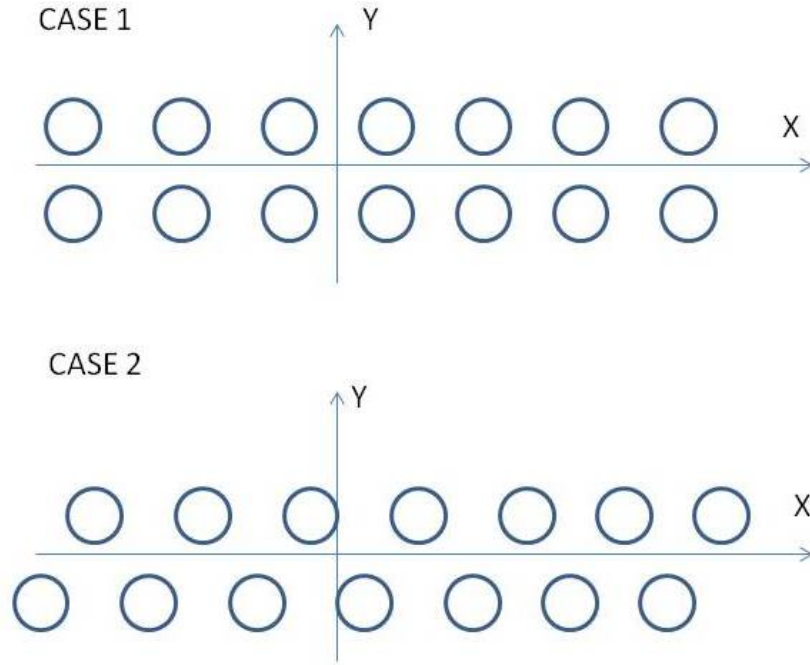


FIG. 5. Symmorphic and non-symmorphic one-dimensional crystals.

From the aforementioned reasons, the irreducible representation of this group is not the proper one to represent the small group at $k = \pi/a$.

According to the Herring method, instead of this, a factor group G/I should be

made use of, where G is a group of infinite order, composed of

$$\begin{aligned}
e' &= \{E|2na\}, \\
c' &= \{C_2|2na\}, \\
m' &= \{\sigma_x|a/2 + 2na\}, \\
g' &= \{\sigma_y|a/2 + 2na\}, \\
\bar{e}' &= \{E|a + 2na\}, \\
\bar{c}' &= \{C_2|a + 2na\}, \\
\bar{m}' &= \{\sigma_x|3a/2 + 2na\}, \\
\bar{g}' &= \{\sigma_y|3a/2 + 2na\},
\end{aligned} \tag{44}$$

and I is the normal subgroup composed of

$$e' = \{E|2na\}. \tag{45}$$

This factor group is the point group in the unit cell extended twofold in x direction. By extending the unit cell, the k -points at the boundary of the original Brillouin zone are pulled back at Γ point in the new Brillouin zone. As the newly allotted Γ -point is of the zero vector, the mathematical difficulty in the representation can be avoided. This situation should rather be interpreted as follows: the wavefunction at $k = \pi/a$ has the periodicity of $2a$, that is two times as large as the original lattice width. On the other hand, the wavefunction at $k = 0$ in the original Brillouin zone also matches into the periodicity of $2a$. (Because originally it has periodicity of a) In the representation at the new Γ point, those in the old Γ point and the old boundary point are mingled with each other. These two different contributions, however, can be distinguishable. Let us check the character of the elements of following types $E|\tau$, viz. of the simple fractional translations in the extended cell, in which the

linear operation is the identity. With respect to the representation of the boundary of the Brillouin zone of the original smaller cell, the representation matrix should be represented as $D^{k=\pi/a}(\{E|a\}) = \exp(-i\frac{\pi}{a}a)I^d = -I^d$; character of which is equal to $-d$ (d is the dimensionality of the representation). From Table XVI we can see the proper irreducible representation at $k = \pi/a$ is given by Γ_5 alone.

	e'	$\bar{e}'$	c'	$\bar{c}'$	m'	$\bar{m}'$	g'	$\bar{g}'$
e'	e'	$\bar{e}'$	c'	$\bar{c}'$	m'	$\bar{m}'$	g'	$\bar{g}'$
$\bar{e}'$	$\bar{e}'$	e'	$\bar{c}'$	c'	$\bar{m}'$	m'	$\bar{g}'$	g'
c'	c'	$\bar{c}'$	e'	$\bar{e}'$	$\bar{g}'$	g'	$\bar{m}'$	m'
$\bar{c}'$	$\bar{c}'$	c'	$\bar{e}'$	e'	g'	$\bar{g}'$	m'	$\bar{m}'$
m'	m'	$\bar{m}'$	g'	$\bar{g}'$	$\bar{e}'$	e'	$\bar{c}'$	c'
$\bar{m}'$	$\bar{m}'$	m'	$\bar{g}'$	g'	e'	$\bar{e}'$	c'	$\bar{c}'$
g'	g'	$\bar{g}'$	m'	$\bar{m}'$	c'	$\bar{c}'$	e'	$\bar{e}'$
$\bar{g}'$	$\bar{g}'$	g'	$\bar{m}'$	m'	$\bar{c}'$	c'	$\bar{e}'$	e'

TABLE XV. The Multiplication table.

	e'	$\bar{e}'$	$[c', \bar{c}']$	$[m', \bar{m}']$	$[g', \bar{g}']$
Γ_1	1	1	1	1	1
Γ_2	1	1	1	-1	-1
Γ_3	1	1	-1	1	-1
Γ_4	1	1	-1	-1	-1
Γ_5	2	-2	0	0	0

TABLE XVI. The character table.

The prediction by the character table can be verified. The electronic structure calculation is executed to the mismatched double alloy of Na atoms: The two atoms are placed at $\pm(1/4a_x + 1/8a_y)$ in the unit cell with $a_x = (a, 0, 0)$, $a_y = (0, 4a, 0)$, $a_z = (0, 0, 5a)$ and $a = 8.1\text{au}$. This computation affirms that every pair of eigenvalues at the boundary of the Brillouin zone shows the double-fold degeneracy.

The above example is a simple one-dimensional model. For a non-symmorphic three dimensional crystal, the irreducible representation for the k-point at the boundary of the Brillouin zone can be computed in the similar way. For this purpose we

k=0	-2.775	-2.124	-0.506	-0.479	0.139	0.753	0.780	1.054
k= π/a	-0.717	-0.717	-0.072	-0.072	1.501	1.501	1.528	1.528

TABLE XVII. Energy spectrum at $k=0$ and π/a in the mismatched double alloy of Na atoms.

should set up a super-cell structure, the periodicity of which should be equal to that of the wavefunction at the boundary k -point in consideration; the symmetry operations to be taken into account of must be confined to ones which fix the boundary k -point up to the periodicity of the old Brillouin zone of the small cell. (To consider the full symmetry of the new super-cell may be superfluous); the irreducible representation at Γ point in the super-cell is mixture of the wavefunctions at Γ point and the k -point in consideration, but we can distinguish them by the comparison of the character of the pure fractional translation. The example of the three dimensional case is the irreducible representation of diamond structure in the face-centered cell at X point $k_X = [0, 2\pi/a, 0](= 1/2G_2 + 1/2G_3)$. The necessary super-cell is the cubic unit cell. We can check this: the primitive lattice vectors in the cubic cell is expressed by those in the face-centered cell as $\hat{a}_1 = a_1 + a_2 - a_3$, $\hat{a}_2 = a_1 - a_2 + a_3$ and $\hat{a}_3 = a_1 + a_2 - a_3$; so there are relations as $\hat{a}_1 \cdot k_X = 0$, $\hat{a}_3 \cdot k_X = 0$ and $\hat{a}_2 \cdot k_X = 2\pi$. These relations indicate that the wavefunction at k_X in the face-centered cell fits itself into the cubic super-cell, in the sense that the translations by the primitive lattice vector in the cubic cell causes no phase shift in the wavefunction. The symmetry operations for the small group at k_X are constructed from those which fix k_X ($k_X \rightarrow k_X$) and those which invert k_X ($k_X \rightarrow -k_X$), due to the periodicity in the wave-number space. In contrast, the full symmetry operations in the cubic cell couples six wavefunctions at $[\pm 2\pi/a, 0, 0], [0, \pm 2\pi/a, 0],$ and $[0, 0, \pm 2\pi/a]$. As the wave-vector k_X cannot be fixed, the corresponding irreducible representation for the full symmetry is not adequate for the small group at k_X . (Elsewhere in this article, the point group of the full

symmetry operations in the cubic unit cell is computed; from which the small group at k_X can be derived as a subgroup.)

E. The semidirect product and the induced representation

In the previous section of this article, concerning with the computation of the character tables for the super-cell structures, we have to remake the multiplication table of the extended group by the presence of the fractional translation. However, if we make use of the mathematical idea of the semi-direct product, we can treat such a problem more effectively. In this section, this concept is explained and the possible computation GAP is presented.

The semidirect product $A \ltimes G$ is obtained by extending a group G by an another group A in the following way. The elements in the new group are given as the Cartesian product of each group:

$$\{(a, g); a \in A, g \in G\}. \quad (46)$$

The multiplication is defined as

$$(a_1, g_1) \cdot (a_2, g_2) = (a_1 g_1(a_2), g_1 g_2), \quad (47)$$

in which the notation $g_1(a_2)$ means the automorphism in A acting on a_2 , induced by g_1 in G . The typical example of this is the affine mapping in crystallographic group. The definition is given as follows:

$$O_T = \{R_T | \tau_T\} : r \rightarrow R_T \cdot r + \tau_T \text{ (Affine mapping)}, \quad (48)$$

$$O_T \cdot O_S = \{R_T \cdot R_S | \tau_T + R_T \cdot \tau_S\}. \quad (49)$$

If the group A is Abelian, the representation of the semidirect product is given by

$$\chi_V(a, g) = \frac{1}{|G_x|} \sum_{h \in G; hgh^{-1} \in G_x} x(h(a)) \chi_U(hgh^{-1}). \quad (50)$$

Here G_x is the set of elements in G , such that the character x in A is fixed by the automorphism induced by elements in G_x . All of the irreducible representations of the semidirect product are exhausted by this formula through possible combinations of the character x in A and the irreducible representation χ_U of G_x . (For the theoretical background, consult references of pure mathematics.^{8,17})

One of the simplest example is $C_{3v} = \text{Group}((1, 2, 3), (1, 2)) \equiv S_3$. One can check the validity of this formula, taking $C_3 = \text{Group}((1, 2, 3))$ as A and $I = \text{Group}((1, 2))$ as G . Let us follow this computation.

The character tables of those three groups are given as

	$[(\)]$	$[(1,2),(2,3),(3,1)]$	$[(1,2,3),(1,3,2)]$
χ_1	1	1	1
χ_2	1	-1	1
χ_3	2	0	1

TABLE XVIII. The character table of C_{3v} .

	$[e_A=(\)]$	$[a_A=(1,2,3)]$	$[a_A^{-1}=(1,3,2)]$
x_1	1	1	1
x_2	1	ω	ω^2
x_3	1	ω^2	ω

TABLE XIX. The character table of C_3 , where $\omega = \exp(2\pi/3)$.

	$[e_G=()]$	$[g_G=(1,2)]$
y_1	1	1
y_2	1	-1

TABLE XX. The character table of I.

The automorphism on A by G is defined as:

$$\begin{aligned}
e_G(e_A) &= e_A, \\
e_G(a_A) &= a_A, \\
e_G(a_A^{-1}) &= a_A^{-1}, \\
g_G(e_A) &= e_A, \\
g_G(a_A) &= a_A^{-1}, \\
g_G(a_A^{-1}) &= a_A.
\end{aligned} \tag{51}$$

As a trivial case, take x_1 . Since $G_{x_1} = G$, y_1 can be chosen as χ_U . Since G is Abelian, i.e. $hgh^{-1} = g$, the formula is

$$\begin{aligned}
\chi_V(a, g) &= \frac{1}{|G_{x_1}|} \sum_{h \in G; hgh^{-1} \in G} x_1(h(a)) y_1(hgh^{-1}) \\
&= \frac{1}{2} \sum_{h \in G; hgh^{-1} \in G_{y_1}} x_1(h(a)) y_1(g) = \frac{1}{2}(1 + 1) = 1,
\end{aligned} \tag{52}$$

for all elements in the semidirect product.

Again take x_1 . Since $G_{x_1} = G$, y_2 can also be chosen as χ_U . The formula is

$$\chi_V(a, g) = \frac{1}{2} \sum_{h \in G; hgh^{-1} \in G_{x_1}} x_1(h(a)) y_2(hgh^{-1}). \tag{53}$$

It gives

$$\begin{aligned}
\chi_V(e_A, e_G) &= \frac{1}{2}(1+1) = 1, \\
\chi_V(a_A, e_G) &= \chi_V(a_A^{-1}, e_G) = \frac{1}{2}(1+1) = 1, \\
\chi_V(e_A, g_G) &= \frac{1}{2}(-1-1) = -1, \\
\chi_V(a_A, g_G) &= \chi_V(a_A^{-1}, g_G) = \frac{1}{2}(-1-1) = -1.
\end{aligned} \tag{54}$$

Take x_2 . Since $G_{x_2} = \langle \text{Id} \rangle$ (the trivial group of the identity), it must be $\chi_U = 1$. The formula is

$$\begin{aligned}
\chi_V(a, g) &= \sum_{h \in G; hgh^{-1} \in G_{x_2}} x_2(h(a)) \chi_U(hgh^{-1}) \\
&= \sum_{h \in G; hgh^{-1} \in G_{x_2}} x_2(h(a)) \cdot 1.
\end{aligned} \tag{55}$$

It gives

$$\begin{aligned}
\chi_V(e_A, e_G) &= (1+1) = 2, \\
\chi_V(a_A, e_G) &= \chi_V(a_A^{-1}, e_G) = (\omega + \omega^2) = -1, \\
\chi_V(e_A, g_G) &= 0, \\
\chi_V(a_A, g_G) &= \chi_V(a_A^{-1}, g_G) = 0.
\end{aligned} \tag{56}$$

The last two characters are zero, since for any h , $hgh^{-1} = g \notin \langle \text{Id} \rangle$, no terms are summed up.

(N.B. When we take x_1 , it seems plausible that we could also choose $G_{x_1} =$

$\langle \text{Id} \rangle$. Then the formula is

$$\begin{aligned}\chi_V(a, g) &= \sum_{h \in G; hgh^{-1} \in G_{x_1}} x_1(h(a)) \chi_U(hgh^{-1}) \\ &= \sum_{h \in G; hgh^{-1} \in \langle \text{Id} \rangle} x_1(h(a)) \cdot 1.\end{aligned}\tag{57}$$

It gives

$$\begin{aligned}\chi_V(e_A, e_G) &= 2, \\ \chi_V(a_A, e_G) &= \chi_V(a_A^{-1}, e_G) = 2, \\ \chi_V(e_A, g_G) &= 0, \\ \chi_V(a_A, g_G) &= \chi_V(a_A^{-1}, g_G) = 0.\end{aligned}\tag{58}$$

However, this result is not irreducible. It is essential to use the maximal set of G_x .)

There are other combination of characters including x_3 of C_{3v}). However, they only produce the redundant results.

The aforementioned computations are tedious and complicated; a naive implementation by means of GAP programming language could be given as follows:

```
#The definition of the groups G and A.
#The irreducible representations and the lists of
#group elements are prepared.

G:=Group((1,2));
A:=Group((1,2,3));
repG:=Irr(G);
repA:=Irr(A);
Gmem:=Elements(G);
```

```

Amem:=Elements(A);

# The definition of the automorphism on A induced by G.
# The elements of G and A are indexed
#   G[1],G[2],...
#   and
#   A[1],A[2],....
# The elements in A are mapped as
#   A[i]^G[j]=A[au[i,j]];
#
au:=[[1,1],[2,3],[3,2]];
# This list means the following automorphism:
#   ^E_G  : E -> E, A -> A,    A^-1 -> A^-1
#   ^g_G  : E -> E, A -> A^-1, A^-1 -> A

GAction:=function(a,g,A,G)
# A function to compute the automorphism on an element "a" in A
# induced by an element "g" in G.
  local apos,gpos,ha;
  apos:=Position(Amem,a);
  gpos:=Position(Gmem,g);
  ha:=au[apos][gpos];
  return Amem[ha];
end;

ProSumma:=function(a,g,A,G,Gx,iA,iG)
# A subordinate function to compute the character

```

```

# of the elements (a,g),
# when the character in A (iA) and Gx are specified.
local k,sum,l1,l2,l3,l4,repGx;
l1:=List(Gmem,x->x*g*x^-1);
l2:=List(Gmem,x->GAction(a,x,A,G));
#Print("Action on A by g      :", l2,"\n");
l3:=List(l2,x->x^repA[iA]);
#Print("Their Characters in A :", l2,"\n");
#Print("Character h*g*h^-1    :", List(l1,x->x^repG[iG]),"\n");
repGx:=Irr(Gx);
sum:=0;
for k in [1..Size(l1)]
do
  if l1[k] in Gx then
    l4:=l1[k]^repGx[iG];
    sum:=sum+l3[k]*l4;
  fi;
od;
sum:=sum/Size(Gx);
return sum;
end;

```

```

InvarianceCHK:=function(iA,g,au,A,G)
local Gx,ol,tl;
Gx:=[];
ol:=List(Amem,x->x^repA[iA]);
tl:=List(Amem,x->Amem[au[Position(Amem,x)][Position(Gmem,g)]]);

```

```

tl:=List(tl,x->x^repA[iA]);
return ol=tl;
end;

GetGx:=function(iA,au,A,G)
local cl,Gx;
cl:=List(G,g->InvarianceCHK(iA,g,au,A,G));
Gx:=Filtered(G,g->InvarianceCHK(iA,g,au,A,G));
return Group(Gx);
end;

# List of elements in the semidirect product [A,G]
# is given by the Cartesian products of sequential numbers.
Elist:=[[1,1],[1,2],[2,2],[3,2],[2,1],[3,1]];

ProChr:=function(au,A,G,iA)
local Gx,repGx,index,retTBL;
Gx:=GetGx(iA,au,A,G);
repGx:=Irr(Gx);
retTBL:=[];
for index in [1..Size(repGx)]
do;
Append(retTBL,
[ List(Elist,x->ProSumma(Amem[x[1]],Gmem[x[2]],A,G,Gx,iA,index))]
) ;
od;
return retTBL;

```

```
end;
```

```
gap> for iA in [1..Size(repA)]
do;
  Display(ProChr(au,A,G,iA));
od;
[ [ 1, 1, 1, 1, 1, 1 ],
  [ 1, -1, -1, -1, 1, 1 ] ]
[ [ 2, 0, 0, 0, -1, -1 ] ]
[ [ 2, 0, 0, 0, -1, -1 ] ]
```

In GAP, the semidirect product can be constructed by a built-in function.

```
gap> A=Group((1,2,3));
Alt( [ 1 .. 3 ] )
gap> G=Group((1,2));
Sym( [ 1 .. 2 ] )
```

The automorphism in A is evaluated as follows:

```
gap> au:=AutomorphismGroup(A);
<group of size 2 with 1 generators>
gap> auE:=Elements(au);
[ [ (1,2,3) ] -> [ (1,2,3) ], [ (1,2,3) ] -> [ (1,3,2) ] ]
gap> gens:=GeneratorsOfGroup(G);
[ (1,2) ]
```

The automorphism in A induced by G is defined as follows: (The generator (1,2) in G causes the automorphism in A as (1,2,3)->(1,3,2). Indeed (1,2,3)*(1,3,2)=1: this is the inversion.)

```

gap> hom:=GroupHomomorphismByImages(G,au,gens,[auE[2]]);
[ (1,2) ] -> [ [ (1,2,3) ] -> [ (1,3,2) ] ]
gap> p:=SemidirectProduct(G,hom,A);
Group([ (3,4,5), (1,2)(4,5) ])
gap> Irr(p);
[ Character( CharacterTable( Group([ (3,4,5), (1,2)(4,5) ]) ),
  [ 1, 1, 1 ] ), Character( CharacterTable( Group([ (3,4,5), (1,2)
(4,5) ]) ), [ 1, 1, -1 ] ), Character( CharacterTable( Group([ (3,
4,5), (1,2)(4,5) ]) ), [ 2, -1, 0 ] ) ]

```

F. The computation of the character table in the cubic diamond by GAP

In this section, the character table in the cubic diamond structure is computed by GAP command for semidirect product. The point group G of the basic diamond structure is extended by the Abelian group of fractional translations N .

The point group G is given in the table in the appendix of this article, as the set of 48 three dimensional matrices. (Although in the table accompanying fractional transformations are listed, the point group G is constructed solely from three-dimensional rotation matrices; the fractional translations are omitted in the point group construction; they are included in the Abelian group N .) The group N is the factor group F/T , where generators of F are

$$\tau_1 := (1/4, 1/4, 1/4), \tau_2 := (1/4, -1/4, -1/4), \tau_3 := (-1/4, -1/4, 1/4) \quad (59)$$

and those of T are

$$(1, 0, 0), (0, 1, 0), (0, 0, 1). \quad (60)$$

Using these generators, the group A and T are given as the vector space (or module)

over integers.

For the convenience, the group F/T can be expressed as another factor group A/B , where

$$A := \text{Group}((1, 2, 3, 4), (5, 6, 7, 8), (9, 10, 11, 12)); \quad (61)$$

and

$$\begin{aligned} B := & \text{Group}((1, 2, 3, 4)^2 * (5, 6, 7, 8)^2, (5, 6, 7, 8)^2 * (9, 10, 11, 12)^2, \\ & (9, 10, 11, 12)^2 * (1, 2, 3, 4)^2) \\ (= & \text{Group}((1, 3)(2, 4)(5, 7)(6, 8), (5, 7)(6, 8)(9, 11)(10, 12), (1, 3)(2, 4)(9, 11)(10, 12)); \end{aligned} \quad (62)$$

This definition corresponds to the relations of the fractional translations in F/I ;

$$4 * \bar{\tau}_i := (0, 0, 0) [\text{Identity}] \quad (63)$$

and

$$2 * (\bar{\tau}_1 + \bar{\tau}_2) = 2 * (\bar{\tau}_2 + \bar{\tau}_3) = 2 * (\bar{\tau}_3 + \bar{\tau}_1) \equiv (0, 0, 0) [\text{Identity}] \quad (64)$$

The gap computation goes as follows:

```
gap> A:=Group((1,2,3,4),(5,6,7,8),(9,10,11,12));
Group([ (1,2,3,4), (5,6,7,8), (9,10,11,12) ])
gap> B:=Group((1,2,3,4)^2*(5,6,7,8)^2,(5,6,7,8)^2*(9,10,11,12)^2,
(9,10,11,12)^2*(1,2,3,4)^2);
Group([ (1,3)(2,4)(5,7)(6,8), (5,7)(6,8)(9,11)(10,12), (1,3)(2,4)
(9,11)(10,12) ])
gap> N:=FactorGroup(A,B);
Group([ f1, f2, f3, f4 ])
gap> NaturalHomomorphismByNormalSubgroup(A,B);
```

```
[ (1,2,3,4), (5,6,7,8), (9,10,11,12) ] -> [ f3, f2, f1 ]
```

The last command returns the homomorphism from A to another group whose kernel is B : in other words, gives the mapping of A onto A/B . The tree generators $(1,2,3,4), (5,6,7,8), (9,10,11,12)$ in A are mapped to $f3, f2, f1$ in A/B .

```
gap> N.1;
f1
gap> N.2;
f2
gap> N.3;
f3
gap> N.4;
f4
```

There is a newcomer $f4$; we must identify it. For this purpose, it is enough to compute the multiplication table of for generators.

```
gap> NV:=[N.1,N.2,N.3,N.4];
[ f1, f2, f3, f4 ]
gap> TransposedMat([NV])*[NV];
[ [ f4, f1*f2, f1*f3, f1*f4 ], [ f1*f2, f4, f2*f3, f2*f4 ],
  [ f1*f3, f2*f3, f4, f3*f4 ],
  [ f1*f4, f2*f4, f3*f4, <identity> of ... ] ]
```

We can see the relation $f1*f1=f2*f2=f3*f3=f4$, which means that the element $f4$ corresponds to elements $(1,2,3,4)^2, (5,6,7,8)^2, (9,10,11,12)^2$, viz. the fractional transformation $(1/2, 1/2, 1/2)$.

The size of the fractional group is given as

```
gap> Size(C);
16
```

Concerning with this, the volume of the parallelepiped spanned by τ_i is

```
gap> AbsoluteValue(Determinant(A));
1/16
```

Thus, in the unit cubic cell, the translations by τ_i generates 16 discrete points, the number of which is equal to the order of F/I .

It is sufficient to define the automorphisms in N induced by G only for the generators of G : the candidates of which are two matrices, those of No.36 and No.48 in the list of symmetry operations.

$$M36 := \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}, M48 := \begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad (65)$$

Let us check the operations of these two matrices on τ_i .

```
gap> A:=[[1,1,1],[-1,-1,1],[-1,1,-1]]/4;
[ [ 1/4, 1/4, 1/4 ], [ -1/4, -1/4, 1/4 ], [ -1/4, 1/4, -1/4 ] ]
gap> A:=TransposedMat(A);
[ [ 1/4, -1/4, -1/4 ], [ 1/4, -1/4, 1/4 ], [ 1/4, 1/4, -1/4 ] ]
gap> M36:=[[0,0,1],[1,0,0],[0,-1,0]];
[ [ 0, 0, 1 ], [ 1, 0, 0 ], [ 0, -1, 0 ] ]
gap> M48:=[[0,0,-1],[0,-1,0],[1,0,0]];
[ [ 0, 0, -1 ], [ 0, -1, 0 ], [ 1, 0, 0 ] ]
```

The generators are set to be the transposed forms of above matrices.¹⁸

```

gap> TM36:=TransposedMat(M36);
[ [ 0, 1, 0 ], [ 0, 0, -1 ], [ 1, 0, 0 ] ]
gap> TM48:=TransposedMat(M48);
[ [ 0, 0, 1 ], [ 0, -1, 0 ], [ -1, 0, 0 ] ]
gap> (A*TM36*A^-1);
[ [ 0, -1, 0 ], [ 0, 0, -1 ], [ -1, 0, 0 ] ]
gap> (A*TM48*A^-1);
[ [ 0, 1, 0 ], [ 0, 0, 1 ], [ -1, -1, -1 ] ]

```

The operations by M36 and M48 are given as:

$$M36 \cdot \tau_1 = -\tau_2 \tag{66}$$

$$M36 \cdot \tau_2 = -\tau_3$$

$$M36 \cdot \tau_3 = -\tau_1$$

$$M48 \cdot \tau_1 = \tau_2$$

$$M48 \cdot \tau_2 = \tau_3$$

$$M48 \cdot \tau_3 = -\tau_1 - \tau_2 - \tau_3$$

We can identify τ_i to three permutations:

$$\tau_1 := (9, 10, 11, 12) \equiv f1 \tag{67}$$

$$\tau_2 := (5, 6, 7, 8) \equiv f2$$

$$\tau_3 := (1, 2, 3, 4) \equiv f3$$

Other identifications will do. But we use the identification consistent to the result of the “NaturalHomomorphismByNormalSubgroup” command.

It suffices that the automorphism in N induced by G is defined at generators of

groups.

```
gap> gens:=GeneratorsOfGroup(N);;
gap> CC1:=[gens[2]^-1,gens[3]^-1,gens[1]^-1,gens[4]];;
gap> CC2:=[gens[2],gens[3],(gens[1]*gens[2]*gens[3])^-1,gens[4]];;
gap> hom1:=GroupHomomorphismByImages(N,N,gens,CC1);;
gap> hom2:=GroupHomomorphismByImages(N,N,gens,CC2);;
```

The command “GroupHomomorphismByImage($G, H, \text{gens}, \text{imgs}$)” defines a homomorphism from the group G to the group H through the mapping of the list “gens” of the generators of G to the list “imgs” of the images in H . If the definition of the mapping is irrelevant, the program returns a “fail” message.

```
gap> CC3:=[gens[3]^-1,gens[1]*gens[3]^-1,gens[2]*gens[3]^-1];;
gap> hom3:=GroupHomomorphismByImages(N,N,[gens[1],gens[2],gens[3]],CC3);
fail
```

Let G be the point group of the minimal unit cell, generated from the matrices TM36 and TM48. By those preparations, we can make the semidirect product $G \ltimes N$.

```
gap> au:=AutomorphismGroup(N);;
gap> G:=Group(TM36,TM48);;
gap> GTON:=GroupHomomorphismByImages(G,au,GeneratorsOfGroup(G),[hom1,hom2]);;
gap> GPN:=SemidirectProduct(G,GTON,N);;
gap> irrep:=Irr(SemidirectProduct(G,GTON,N));;
```

Once the semidirect product $G \ltimes N$ is computed, the representation of the point group in the cubic diamond can be deduced from a suitable subgroup of this. For this purpose let us see the embedding of G and N into the semidirect product. The command “Embedding” creates the embedding from G and N into the semidirect

product, and the command “Projection” creates the projection from the semidirect product to G.

```
gap> embd1:=Embedding(GPN,1);
CompositionMapping( [ f1, f2, f3, f4, f5 ] -> [ f1, f2, f3, f4, f5 ],
  CompositionMapping( Pcgs([ (5,8)(6,7), (1,2)(3,5,7,4,6,8), (3,7,6)(4,8,5),
    (1,6)(2,5)(3,7)(4,8), (1,3)(2,4)(5,8)(6,7) ]) -> [ f1, f2, f3, f4, f5 ],
    <action isomorphism> ) )
gap> embd2:=Embedding(GPN,2);
[ f1, f2, f3, f4 ] -> [ f6, f7, f8, f9 ]
gap> GeneratorsOfGroup(G);
[ [ [ 0, 1, 0 ], [ 0, 0, -1 ], [ 1, 0, 0 ] ],
  [ [ 0, 0, 1 ], [ 0, -1, 0 ], [ -1, 0, 0 ] ] ]
gap> List(GeneratorsOfGroup(G),g->Image(embd1,g));
[ f2, f1*f3*f5 ]
gap> GeneratorsOfGroup(N);
[ f1, f2, f3, f4 ]
gap> List(GeneratorsOfGroup(N),g->Image(embd2,g));
[ f6, f7, f8, f9 ]
gap> Projection(GPN);
[ f1, f2, f3, f4, f5, f6, f7, f8, f9 ] ->
[ [ [ 1, 0, 0 ], [ 0, 0, 1 ], [ 0, 1, 0 ] ],
  [ [ 0, 1, 0 ], [ 0, 0, -1 ], [ 1, 0, 0 ] ],
  [ [ 0, 0, -1 ], [ -1, 0, 0 ], [ 0, 1, 0 ] ],
  [ [ -1, 0, 0 ], [ 0, 1, 0 ], [ 0, 0, -1 ] ],
  [ [ 1, 0, 0 ], [ 0, -1, 0 ], [ 0, 0, -1 ] ],
  [ [ 1, 0, 0 ], [ 0, 1, 0 ], [ 0, 0, 1 ] ],
```

$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix},$
 $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix},$
 $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \end{bmatrix}$

The correspondence of the generators is given in tableXXI.

Elements in G and N	Elements in $G \ltimes N$
TM36(in G)	f2
TM48(in G)	f1*f3*f5
f1(in N) (The image of (9,10,11,12))	f6
f2(in N) (The image of (5,6,7,8))	f7
f3(in N) (The image of (1,2,3,4))	f8
f4(in N) (The image of (1,3)(2,4) or (5,7)(6,8) or (1,3)(2,4))	f9

TABLE XXI. The correspondence of the generators in groups G, N and $G \ltimes N$.

The generators of the point group of the cubic diamond structure are these elements:

$$\begin{aligned}
 &\{m36|\tau_i\} \\
 &\{m48|0\}
 \end{aligned} \tag{68}$$

(τ_i can be any of three alternatives. The addition of pure fractional translations $\{E|\tau_i\}$ is superfluous in this case.)

The corresponding subgroup can be constructed in this way:

Subgroup(GPN, [GPN.2*GPN.6, GPN.1*GPN.3*GPN.5])

or

Subgroup(GPN, [GPN.2*GPN.7, GPN.1*GPN.3*GPN.5])

or

Subgroup(GPN, [GPN.2*GPN.8, GPN.1*GPN.3*GPN.5])

These three definitions generate the same group so that any choice can be used.

G. Crystal lattice and Cohomology

1. A brief introduction to group cohomology

In the modern style, the crystal group can be described by the theory of the cohomology, which is actually computable by the computer algebra.

At first, we construct the one-cohomology. Let $K \in GL(n, \mathbb{Z})$ and define $V := \mathbb{R}^n / \mathbb{Z}^n$. The one-cocycle is defined as

$$Z^1(K, V) := \{\rho; k \rightarrow V | \rho(1) = 0, \rho(gh) = \rho(g) + g\rho(h) \text{ for all } g, h \in K\}. \quad (69)$$

The one-coboundary is defined as

$$B^1(K, V) := \{\rho \in Z^1(K, V) | \rho(g) = gv - v \text{ for some } v \in V\}. \quad (70)$$

The one-cohomology is defined as their quotient:

$$H^1(K, V) := Z^1(K, V) / B^1(K, V) \quad (71)$$

We can see the vector system in the space group, which satisfies the condition

$$\tau(gh) \equiv \tau(g) + g \cdot \tau(h) \pmod{\mathbb{Z}^n \pmod{\text{lattice translations}}} \quad (72)$$

is a kind of cocycle. Furthermore, the one-coboundary is interpreted as the shift of origin; we can observe this from the conjugation operation:

$$\{1|s\}^{-1}\{g|t\}\{1|s\} = \{g|(gs - s) + t\} \quad (73)$$

Thus, the vector system could be understood in the context of one-cohomology.

The above definition of the one-cohomology is derived from the general theory of group cohomology. Let G be a finite group and M be a module. Let $C^n(G, M)$ be the set functions from $G^n = (g_1, g_2, \dots, g_n)$ to M . The differential ($d^n : C^n(G, M) \rightarrow C^{n+1}(G, M)$) is defined as

$$\begin{aligned} d^n(f)(g_0, g_1, \dots, g_n) &= g_0 \cdot f(g_1, \dots, g_n) \\ &+ \sum_j^n (-1)^j f(g_0, \dots, g_{j-2}, g_{j-1}g_j, g_{j+1}, \dots, g_n) \\ &+ (-1)^{n+1} f(g_0, g_1, \dots, g_{n-1}). \end{aligned} \quad (74)$$

It satisfies

$$d^n \circ d^{n-1} = 0. \quad (75)$$

The n-cocycle $Z^i(G, M)$ is defined as $\text{Ker}(d^n)$, and the n-coboundary is as $\text{Im}(d^{n-1})$. The n-th cohomology group is defined as $H^i(G, M) := Z^i(G, M)/B^i(G, M)$.

2. The possible fractional translations with one point group

We make use of following matrices (as explained elsewhere in this article) in order to define the crystallographic group in the diamond crystal lattice:

```
gap>M1:=[[0,0,1,1/4],[1,0,0,1/4],[0,-1,0,1/4],[0,0,0,1]];
gap>M2:[[0,0,-1,0],[0,-1,0,0],[1,0,0,0],[0,0,0,1]];
gap>S:=AffineCrystGroupOnLeft([M1,M2]);
gap>P:=PointGroup(S);
```

In this definition, the fractional translation is given a priori. With regard to this, there is a question: what is the possible fractional translation compatible to the point group of the diamond crystal? Is it uniquely determined? Let us inspect this problem. For example, take the face-centered lattice. For simplicity in the

following computation, the symmetry operations are represented by the “lattice axes coordinate”, by means of the vector system of the primitive lattice vectors. For this new coordinate, the new point group Q is made from the group P by the conjugation of the generators. (The symbol $\wedge$ is used for the conjugation in GAP.)

```
gap> A:=[[0,1/2,1/2],[1/2,0,1/2],[1/2,1/2,0]];
gap> Q:=P^A;
gap> Q.1;Q.2;
[ [-1, 0, 0 ], [ 0, 0, -1 ], [ 1, 1, 1 ] ]
[ [ 0, 1, 0 ], [ 0, 0, 1 ], [ -1, -1, -1 ] ]
```

The generators of the space groups are defined now by means of unknown variables. (For the heuristic purpose, we venture to employ generators different to the first definition.)

```
a:=Indeterminate(Rationals,1);
b:=Indeterminate(Rationals,2);
c:=Indeterminate(Rationals,3);
N1:= [[-1,0,0,0],[0,0,-1,0],[1,1,1,0],[0,0,0,1]];
N2:= [[0,1,0,a],[0,0,1,b],[-1,-1,-1,c],[0,0,0,1]];
```

Let us consider multiplications of two elements g_i and g_j in the point group, which yields the identity. If g_i and g_j are represented by the products of the generators, the multiplication gives a relation of the generators both in the point group and in the space group. For example, take $(Q.2*Q.1)^4=I$. This relation is lifted up to the space group as $(N2*N1)^4 \equiv \{I|T\}$, where T is a translation. The linear part of $(N2*N1)^4$ is the identity matrix; and the translation part $[2*a+2*b, 2*a+2*b, -2*a-2*b]$ must be one of translation vectors. In general, the translation part in the relation of the generators in the space group gives three linear equations with respect to unknown

variables “a”, “b”, and “c”. These equation should be equivalent to zero, modulo translation vectors; viz. they should be integer-valued.

The relations in generators in Q shall be set up now. For this purpose, each elements in the group and its inverse are represented by generators respectively, so that the product of them gives the relation in generators which yields the unity. In the following, the symbols x_1 and x_2 indicate the two generators of the group Q . For simplicity, the trivial relation only representing the unity (returned as `<identity ...>` in the GAP result) is eliminated in the list.

```
gap> MQ:=Elements(Q);;
gap> rel:=List(MQ,i->Factorization(Q,i)*Factorization(Q,i^-1));;
gap> IDENTITY:=Factorization(Q,One(Q));;
gap> rel:=Filtered(rel,i->i<>IDENTITY);
[ (x2^-1*x1*x2*x1)^2, x1*(x2*x1^-1)^2*x1^-1, (x2*x1^2)^2,
  (x2^-1*x1)^2, x1*x2^2*x1*x2^-1*x1*x2*x1^-1, x1^6,
  (x2*x1*x2^2)^2, (x2^2*x1*x2)^2, (x2*x1*x2^2*x1^2)^2,
  (x2^-1*x1)^2, (x1*x2^2*x1^2)^2, x2^4, x2*x1^3*x2^-1*x1^3,
  x1*x2^4*x1^-1, x1^-1*(x2^-1*x1)^2*x1, x2^-1*x1*x2^3*x1,
  (x2^2*x1^3)^2, (x2*x1^-1)^2, x2^4,
  x2^-1*x1^-1*(x2^-1*x1)^2*x1*x2, (x1*x2*x1)^2, (x2^-1*x1)^2,
  x1^-1*x2^-1*x1*x2^3*x1^2, x2^-1*x1*x2^3*x1,
  x1^-1*(x2^-1*x1)^2*x1, x2^2*x1*x2^-1*x1*x2, (x2*x1)^4,
  (x1^2*x2)^2, (x2*(x2*x1)^2)^2, (x2*x1*x2^2*x1)^2,
  (x1*x2^2*x1*x2)^2, x2^-1*x1^3*x2*x1^3, x2^2*x1*x2^-1*x1*x2,
  (x2*x1^-1)^2, (x2^-1*x1^-1*x2^-1*x1^2)^2 ]
```

The relations of the point group generators are lift to the space group. The matrix relations are stored in the list “relMat”; and the fractional translations are

taken out in the list “relv”. Now, if the fractional translation $[a,b,c]$ is admissible, the list “relv” must be integer-valued by the substitutions to the indeterminates. (Apropos of this, we can use symbols of unknowns as “a”, “b”, “c” for the input, whereas the GAP results are represented by “x_1”, “x_2”, “x_3”. Be careful not to confuse indeterminates and generators of the group.) The GAP program cannot invert the symbolically represented matrices N1 and N2, so we must prepare the inverses for them (N1I and N2I) by the power products.

```

N1I:=N1^5;
N2I:=N2^3;
relMat:=[ (N2I^1*N1*N2*N1)^2, N1*(N2*N1I^1)^2*N1I^1, (N2*N1^2)^2,
(N2I^1*N1)^2, N1*N2^2*N1*N2I^1*N1*N2*N1I^1, N1^6,
(N2*N1*N2^2)^2, (N2^2*N1*N2)^2, (N2*N1*N2^2*N1^2)^2, (N2I^1*N1)^2,
(N1*N2^2*N1^2)^2, N2^4, N2*N1^3*N2I^1*N1^3,
N1*N2^4*N1I^1, N1I^1*(N2I^1*N1)^2*N1, N2I^1*N1*N2^3*N1,
(N2^2*N1^3)^2, (N2*N1I^1)^2, N2^4,
N2I^1*N1I^1*(N2I^1*N1)^2*N1*N2, (N1*N2*N1)^2, (N2I^1*N1)^2,
N1I^1*N2I^1*N1*N2^3*N1^2, N2I^1*N1*N2^3*N1,
N1I^1*(N2I^1*N1)^2*N1, N2^2*N1*N2I^1*N1*N2, (N2*N1)^4,
(N1^2*N2)^2, (N2*(N2*N1)^2)^2, (N2*N1*N2^2*N1)^2,
(N1*N2^2*N1*N2)^2, N2I^1*N1^3*N2*N1^3, N2^2*N1*N2I^1*N1*N2,
(N2*N1I^1)^2, (N2I^1*N1I^1*N2I^1*N1^2)^2 ];
relv:=List(relMat,i->[i[1][4],i[2][4],i[3][4]]);
[ [ 2*x_1+x_2+x_3, -2*x_1-x_2-x_3, -2*x_1-x_2-x_3 ],
[ -2*x_1-x_2-x_3, 0, 2*x_1+x_2+x_3 ], [ -x_2-x_3, 2*x_2, 2*x_3 ],
[ 2*x_1+x_2+x_3, -2*x_1-x_2-x_3, 0 ], [ 0, 2*x_1+x_2+x_3, 0 ],
[ 0, 0, 0 ], [ 0, 0, 2*x_1+x_2+x_3 ],

```

```

[ 0, 2*x_1+x_2+x_3, -2*x_1-x_2-x_3 ], [ 0, 2*x_1+4*x_2+2*x_3, 0 ],
[ 2*x_1+x_2+x_3, -2*x_1-x_2-x_3, 0 ],
[ -2*x_1-2*x_2, 2*x_1+2*x_2, 2*x_2+2*x_3 ], [ 0, 0, 0 ],
[ 2*x_1, 2*x_2, 2*x_3 ], [ 0, 0, 0 ],
[ -2*x_1-x_2-x_3, 0, 2*x_1+x_2+x_3 ],
[ 2*x_1+x_2+x_3, -2*x_1-x_2-x_3, 0 ],
[ 2*x_1+2*x_2, 2*x_2+2*x_3, -2*x_1-2*x_2 ],
[ 2*x_1+x_2+x_3, 0, 0 ], [ 0, 0, 0 ], [ 0, -2*x_1-x_2-x_3, 0 ],
[ x_2+x_3, -2*x_3, x_2+x_3 ], [ 2*x_1+x_2+x_3, -2*x_1-x_2-x_3, 0 ]
, [ -2*x_1-x_2-x_3, 0, 2*x_1+x_2+x_3 ],
[ 2*x_1+x_2+x_3, -2*x_1-x_2-x_3, 0 ],
[ -2*x_1-x_2-x_3, 0, 2*x_1+x_2+x_3 ],
[ 0, 2*x_1+x_2+x_3, -2*x_1-x_2-x_3 ],
[ 2*x_1+2*x_2, 2*x_1+2*x_2, -2*x_1-2*x_2 ],
[ -x_2-x_3, -x_2-x_3, 2*x_2 ],
[ 4*x_1+4*x_2+2*x_3, -x_2-x_3, -4*x_1-2*x_2 ],
[ 4*x_1+2*x_2, x_2+x_3, x_2+x_3 ],
[ -4*x_1-4*x_2-2*x_3, 4*x_1+2*x_2, x_2+x_3 ],
[ 2*x_1+2*x_2+2*x_3, -2*x_1, -2*x_2 ],
[ 0, 2*x_1+x_2+x_3, -2*x_1-x_2-x_3 ], [ 2*x_1+x_2+x_3, 0, 0 ],
[ 2*x_2+2*x_3, -2*x_1-2*x_3, 2*x_1+2*x_3 ] ]

```

Since there are duplicates in the linear equations of the fractional translation, the unique ones should be extracted by

```

gap> Unique(Flat(relv*a^0));
[ 2*x_1+x_2+x_3, -2*x_1-x_2-x_3, 0, -x_2-x_3, 2*x_2, 2*x_3,
  2*x_1+4*x_2+2*x_3, -2*x_1-2*x_2, 2*x_1+2*x_2, 2*x_2+2*x_3, 2*x_1,

```

$x_2+x_3, -2*x_3, 4*x_1+4*x_2+2*x_3, -4*x_1-2*x_2, 4*x_1+2*x_2,$
 $-4*x_1-4*x_2-2*x_3, 2*x_1+2*x_2+2*x_3, -2*x_1, -2*x_2,$
 $-2*x_1-2*x_3, 2*x_1+2*x_3]$

It is necessary to use an input such as “relv*a^0”, so that all entries in the list should be polynomials, for the convenience of sorting, by dint of the fact a^0 is the unity as a polynomial. Now we have following four equations to be integer-valued:

x_2+x_3
 $2*x_1$
 $2*x_2$
 $2*x_3$

In $\mathbb{Q}/\mathbb{Z}$, there are four representatives of the fractional translations, as are given below, with the primitive lattice vectors accompanied to them. (The translation vectors are computed by the substitution in the list “relv”, from which the basis vectors are extracted by the GAP built-in command “BaseIntMat(mat)”.)

Fractional translation	Translation vectors
$[0, 1/2, 1/2]$	$[[1, 0, 0], [0, 1, 0], [0, 0, 1]]$
$[1/2, 0, 0]$	$[[1, 0, 0], [0, 1, 0], [0, 0, 1]]$
$[1/2, 1/2, 1/2]$	$[[1, 1, 1], [0, 2, 0], [0, 0, 2]]$

TABLE XXII. The fractional translations and the translation vectors.

To inspect the validity, by means of GAP built-in command, the possible space groups with a given point group can be computed. In order to check the computed fractional translations, it is enough to see the generators of the space group and the primitive translation vectors.

```

gap> SS:=SpaceGroupsByPointGroupOnLeft(Q);;
gap> Display(List(SS,GeneratorsOfGroup));

```

```

[ [ [ [ -1, 0, 0, 0 ], [ 0, 0, -1, 0 ], [ 1, 1, 1, 0 ], [ 0, 0, 0, 1 ] ],
    [ [ 0, 1, 0, 0 ], [ 0, 0, 1, 0 ], [ -1, -1, -1, 0 ], [ 0, 0, 0, 1 ] ],
    [ [ 1, 0, 0, 1 ], [ 0, 1, 0, 0 ], [ 0, 0, 1, 0 ], [ 0, 0, 0, 1 ] ],
    [ [ 1, 0, 0, 0 ], [ 0, 1, 0, 1 ], [ 0, 0, 1, 0 ], [ 0, 0, 0, 1 ] ],
    [ [ 1, 0, 0, 0 ], [ 0, 1, 0, 0 ], [ 0, 0, 1, 1 ], [ 0, 0, 0, 1 ] ] ],
[ [ [ -1, 0, 0, 0 ], [ 0, 0, -1, 0 ], [ 1, 1, 1, 0 ], [ 0, 0, 0, 1 ] ],
    [ [ 0, 1, 0, 0 ], [ 0, 0, 1, 1/2 ], [ -1, -1, -1, 1/2 ], [ 0, 0, 0, 1 ] ],
    [ [ 1, 0, 0, 1 ], [ 0, 1, 0, 0 ], [ 0, 0, 1, 0 ], [ 0, 0, 0, 1 ] ],
    [ [ 1, 0, 0, 0 ], [ 0, 1, 0, 1 ], [ 0, 0, 1, 0 ], [ 0, 0, 0, 1 ] ],
    [ [ 1, 0, 0, 0 ], [ 0, 1, 0, 0 ], [ 0, 0, 1, 1 ], [ 0, 0, 0, 1 ] ] ],
[ [ [ -1, 0, 0, 0 ], [ 0, 0, -1, 0 ], [ 1, 1, 1, 0 ], [ 0, 0, 0, 1 ] ],
    [ [ 0, 1, 0, 1/2 ], [ 0, 0, 1, 0 ], [ -1, -1, -1, 0 ], [ 0, 0, 0, 1 ] ],
    [ [ 1, 0, 0, 1 ], [ 0, 1, 0, 0 ], [ 0, 0, 1, 0 ], [ 0, 0, 0, 1 ] ],
    [ [ 1, 0, 0, 0 ], [ 0, 1, 0, 1 ], [ 0, 0, 1, 0 ], [ 0, 0, 0, 1 ] ],
    [ [ 1, 0, 0, 0 ], [ 0, 1, 0, 0 ], [ 0, 0, 1, 1 ], [ 0, 0, 0, 1 ] ] ],
[ [ [ -1, 0, 0, 0 ], [ 0, 0, -1, 0 ], [ 1, 1, 1, 0 ], [ 0, 0, 0, 1 ] ],
    [ [ 0, 1, 0, 1/2 ], [ 0, 0, 1, 1/2 ], [ -1, -1, -1, 1/2 ], [ 0, 0, 0, 1 ] ],
    [ [ 1, 0, 0, 1 ], [ 0, 1, 0, 0 ], [ 0, 0, 1, 0 ], [ 0, 0, 0, 1 ] ],
    [ [ 1, 0, 0, 0 ], [ 0, 1, 0, 1 ], [ 0, 0, 1, 0 ], [ 0, 0, 0, 1 ] ],
    [ [ 1, 0, 0, 0 ], [ 0, 1, 0, 0 ], [ 0, 0, 1, 1 ], [ 0, 0, 0, 1 ] ] ] ]

```

```
gap> Display(List(SS,TranslationBasis));
```

```

[ [ [ 1, 0, 0 ], [ 0, 1, 0 ], [ 0, 0, 1 ] ],
  [ [ 1, 0, 0 ], [ 0, 1, 0 ], [ 0, 0, 1 ] ],
  [ [ 1, 0, 0 ], [ 0, 1, 0 ], [ 0, 0, 1 ] ],
  [ [ 1, 0, 0 ], [ 0, 1, 0 ], [ 0, 0, 1 ] ] ]

```

There are four space groups with the point group Q . The last three of the GAP result is the same fractional translation in Table XXII. However, their translational vectors are different: the latter has larger translational vectors. This is because the GAP computation implicitly includes the primitive translations of the unit cube in generators of the space groups.

Readers may question about the relationship between the fractional translation computed now and those of the definition of the space group given in the first part of this section. The generators defined earlier are rewritten in the lattice axes coordinate as:

```
gap> MM1:=[[-1,0,0,1/4],[0,0,-1,1/4],[1,1,1,1/4],[0,0,0,1]];
gap> MM2:=[[0,1,0,0],[0,0,1,0],[-1,-1,-1,0],[0,0,0,1]];
gap> S2:=AffineCrystGroupOnLeft([MM1,MM2]);
```

We can apply the shift of the origin to this space group by means of the conjugation $\{E| -s\}\{R|t\}\{E|s\} = \{R|t + (R - I) \cdot s\}$. If the matrix $R - I$ is normal, we can annihilate the fractional translation. Let us apply such a conjugation to the generators. (The command M^T is the abbreviation of the conjugation $T^{-1} \cdot M \cdot T$.)

```
gap> T:=[[1,0,0,1/8],[0,1,0,-3/8],[0,0,1,5/8],[0,0,0,1]];
gap> MM1^T;
[ [-1, 0, 0, 0 ], [ 0, 0, -1, 0 ], [ 1, 1, 1, 0 ], [ 0, 0, 0, 1 ] ]
gap> MM2^T;
[ [ 0, 1, 0, -1/2 ], [ 0, 0, 1, 1 ], [ -1, -1, -1, -1 ], [ 0, 0, 0, 1 ] ]
```

Thus we can see that the shift of the origin generates the space group, which is equivalent to that composed by matrices $N1$ and $N2$ with $[a,b,c]=[-1/2, 1, -1] \cong [1/2, 0, 0]$. Incidentally, let us generate other representation of generators:

```
N1:=[[-1,0,0,a],[0,0,-1,b],[1,1,1,c],[0,0,0,1]];
```

```
N2:=[[0,1,0,0],[0,0,1,0],[-1,-1,-1,0],[0,0,0,1]];
```

The linear equations for the fractional translation are given as

```
[ 0, 4*x_3, -2*x_2-2*x_3, -2*x_2+2*x_3, -x_2+x_3, x_2-x_3,
2*x_2+2*x_3, -4*x_1-4*x_2-4*x_3, -2*x_1-2*x_3, -2*x_1+2*x_3,
-2*x_1-4*x_2-2*x_3, -2*x_1-2*x_2, -2*x_1-2*x_2-4*x_3,
-2*x_1-x_2-x_3, -2*x_1+2*x_2, 2*x_1-2*x_3, 2*x_1+2*x_3,
2*x_1-2*x_2, 2*x_1+x_2+x_3, 2*x_1+2*x_2+4*x_3,
2*x_1+4*x_2+2*x_3, 4*x_1+4*x_2+4*x_3 ]
```

From them, seven possible vectors of $[a,b,c]$ ($=[x_1,x_2,x_3]$) are obtained as

```
[ 0, 1/2, 1/2 ], [ 1/4, 1/4, 1/4 ], [ 1/4, 3/4, 3/4 ],
[ 1/2, 0, 0 ], [ 1/2, 1/2, 1/2 ], [ 3/4, 1/4, 1/4 ],
[ 3/4, 3/4, 3/4 ] ]
```

We can see one of the fractional translations is $[1/4,1/4,1/4]$.

Whereas the GAP computation goes as

```
gap> Q2:=Group(Q.1,Q.2);
Group([ [ [ -1, 0, 0 ], [ 0, 0, -1 ], [ 1, 1, 1 ] ],
[ [ 0, 1, 0 ], [ 0, 0, 1 ], [ -1, -1, -1 ] ] ])
gap> Q2=Q;
true
gap> SS2:=SpaceGroupsByPointGroupOnLeft(Q2);
[ <matrix group with 5 generators>, <matrix group with 5 generators>
, <matrix group with 5 generators>,
<matrix group with 5 generators> ]
gap> List(SS2,GeneratorsOfGroup);
```

```

[ [ [ 0, 1, 0, 0 ], [ 0, 0, 1, 0 ], [ -1, -1, -1, 0 ], [ 0, 0, 0, 1 ] ],
  [ [ -1, 0, 0, 0 ], [ 0, 0, -1, 0 ], [ 1, 1, 1, 0 ], [ 0, 0, 0, 1 ] ],
  [ [ 1, 0, 0, 1 ], [ 0, 1, 0, 0 ], [ 0, 0, 1, 0 ], [ 0, 0, 0, 1 ] ],
  [ [ 1, 0, 0, 0 ], [ 0, 1, 0, 1 ], [ 0, 0, 1, 0 ], [ 0, 0, 0, 1 ] ],
  [ [ 1, 0, 0, 0 ], [ 0, 1, 0, 0 ], [ 0, 0, 1, 1 ], [ 0, 0, 0, 1 ] ] ],
[ [ [ 0, 1, 0, 0 ], [ 0, 0, 1, 0 ], [ -1, -1, -1, 0 ], [ 0, 0, 0, 1 ] ],
  [ [ -1, 0, 0, 0 ], [ 0, 0, -1, 1/2 ], [ 1, 1, 1, 1/2 ], [ 0, 0, 0, 1 ] ],
  [ [ 1, 0, 0, 1 ], [ 0, 1, 0, 0 ], [ 0, 0, 1, 0 ], [ 0, 0, 0, 1 ] ],
  [ [ 1, 0, 0, 0 ], [ 0, 1, 0, 1 ], [ 0, 0, 1, 0 ], [ 0, 0, 0, 1 ] ],
  [ [ 1, 0, 0, 0 ], [ 0, 1, 0, 0 ], [ 0, 0, 1, 1 ], [ 0, 0, 0, 1 ] ] ],
[ [ [ 0, 1, 0, 0 ], [ 0, 0, 1, 0 ], [ -1, -1, -1, 0 ], [ 0, 0, 0, 1 ] ],
  [ [ -1, 0, 0, 1/4 ], [ 0, 0, -1, 1/4 ], [ 1, 1, 1, 1/4 ], [ 0, 0, 0, 1 ] ],
  [ [ 1, 0, 0, 1 ], [ 0, 1, 0, 0 ], [ 0, 0, 1, 0 ], [ 0, 0, 0, 1 ] ],
  [ [ 1, 0, 0, 0 ], [ 0, 1, 0, 1 ], [ 0, 0, 1, 0 ], [ 0, 0, 0, 1 ] ],
  [ [ 1, 0, 0, 0 ], [ 0, 1, 0, 0 ], [ 0, 0, 1, 1 ], [ 0, 0, 0, 1 ] ] ],
[ [ [ 0, 1, 0, 0 ], [ 0, 0, 1, 0 ], [ -1, -1, -1, 0 ], [ 0, 0, 0, 1 ] ],
  [ [ -1, 0, 0, 1/4 ], [ 0, 0, -1, 3/4 ], [ 1, 1, 1, 3/4 ], [ 0, 0, 0, 1 ] ],
  [ [ 1, 0, 0, 1 ], [ 0, 1, 0, 0 ], [ 0, 0, 1, 0 ], [ 0, 0, 0, 1 ] ],
  [ [ 1, 0, 0, 0 ], [ 0, 1, 0, 1 ], [ 0, 0, 1, 0 ], [ 0, 0, 0, 1 ] ],
  [ [ 1, 0, 0, 0 ], [ 0, 1, 0, 0 ], [ 0, 0, 1, 1 ], [ 0, 0, 0, 1 ] ] ] ]

```

Four space groups are generated by GAP: non-zero fractional translations are three in number:

```

[ 0, 1/2, 1/2 ], [ 1/4, 1/4, 1/4 ], [ 1/4, 3/4, 3/4 ]

```

Apparently the GAP result is lacking in some of fractional translations computed just before by means of linear equations. The GAP result should rather be interpreted as

the basis vectors for the possible fractional translations. The other possible fractional translations can be generated from this basis set.

It is well to remind readers of the point that the setting up of the admissible fractional translations (which is called “vector system” in the mathematical context) is nothing other than the computation of the one-cohomology. In the above example, the fractional translation in the generator N1 is chosen to be zero from the outset. It is possible to assume the non-zero translation in N1. However, a shift of the origin can cancel a non-zero fractional translation as we have seen. The shift of the origin could be caused by the conjugation, which corresponds to the choice of the representative of the elements in the map of the one-cohomology.

3. *Group extension*

The space group of the crystal, is determined by the following short exact sequence, or the group extension:

$$1 \rightarrow K \rightarrow E \xrightarrow{\pi} G \rightarrow 1 \quad (76)$$

with the condition that there exists a normal subgroup of N in E which is isomorphic to K and that E/K is isomorphic to G . The group E is called an extension of G by K . The equivalence classes of extension of E are computed by a concept of the cohomological algebra, i.e. two-cohomology (denoted as $H^2(G, K) = Z^2(G, K)/B^2(G, K)$). In order to understand this concept, however, one should get acquainted of the language of commutative algebra, especially concerning with homological algebra, which would necessitate long explanation.¹⁹ Thus if the reader would get interested with these topics, he should try advanced mathematical textbooks. However, the viewpoint of cohomological algebra might be useful in material designing, especially in

studying the algebraic aspects of crystallography. For example, the Bravais lattice in two- or three- dimensional crystals can be classified by two-cohomology.

For simplicity, consider the two-dimensional case. Let $P = \langle x, y | x^2 = y^2 = (xy)^2 = 1 \rangle$, which acts on $T = \mathbb{Z}^2$ through $M_x = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$ and $M_y = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. The action on T is written as $\{ {}^x e_1 = e_1^{-1}, {}^x e_2 = e_2, {}^y e_1 = e_1, {}^y e_2 = e_2^{-1} \}$. ($e_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $e_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$).

Let us extend this group, and, if possible, let us construct space groups which have this group as their point groups. (This example is taken from the lecture note of Webb.²⁰ For theoretical details, consult with that article and references therein.)

There is a general procedure (Zassenhauss algorithm) to compute two-cohomology, which is based on the following theorem.

Theorem 1. *Let P be a finite group given by the representation*

$$P = \langle x_1, x_2, \dots, x_d | r_1, r_2, \dots, r_t \rangle.$$

Let n be the dimension of the space, and T be a module. From the relators r_i , a matrix $\Lambda \in M_{nt,nd}(\mathbb{Z})$ is computed, and the elements Λ_{ij} are defined as

$$r_i - 1 = \sum_{j=1}^d \Lambda_{ij} (x_j - 1) \quad (i = 1, \dots, t).$$

Then the two-cohomology is given by

$$H^2(P, T) \cong \{x \in (\mathbb{R}T)^d | \Lambda \cdot x \in T^t\} / (\text{Ker } \Lambda + T^d). \quad (77)$$

This definition says that the representative elements in two-cohomology are given as $(v_1, \dots, v_d)$, the concatenation of the vectors in $\mathbb{R}T^n$, (from which the component in $\text{Ker } \Lambda + T^d$ should be factored out), so as to be

$$\Lambda \begin{pmatrix} v_1 \\ \vdots \\ v_d \end{pmatrix} \in T^t. \quad (78)$$

The integer matrix Λ can be converted into its Smith normal form

$$\begin{pmatrix} b_1 & & & & & \\ & b_2 & & & & \\ & & \ddots & & & \\ & & & b_l & & \\ & & & & 0 & \\ & & & & & \ddots \\ & & & & & & 0 \end{pmatrix} \quad (79)$$

with $b_i \neq 0$, dividing b_j for $i < j$. (A matrix $A \in M_{m,n}(\mathbb{Z})$ can be converted into the diagonal form as this, by means matrix operation $P \cdot A \cdot Q$ with $P \in GL(m, \mathbb{Z})$ and $Q \in GL(n, \mathbb{Z})$.)

Then $H^2(P, T) \cong \mathbb{Z}/b_1\mathbb{Z} \oplus \dots \oplus \mathbb{Z}/b_l\mathbb{Z}$. Now the relators in P are lifted in the extension of P by T as

$$\begin{pmatrix} r_1 \\ r_2 \\ \vdots \\ r_t \end{pmatrix} = \Lambda \cdot v \quad (\forall v \in H^2(P, T)). \quad (80)$$

The vector systems are given as $\{x_i|v_i\}$ ($i = 1, \dots, d$) in the crystallography.²¹

In the aforesaid question, the matrix Λ is computed as

$$\Lambda = \begin{pmatrix} \Lambda_{x^2,x} & \Lambda_{x^2,y} \\ \Lambda_{y^2,x} & \Lambda_{y^2,y} \\ \Lambda_{(xy)^2,x} & \Lambda_{(xy)^2,y} \end{pmatrix} = \begin{pmatrix} x+1 & 0 \\ 0 & y+1 \\ xy+1 & xyx+x \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (81)$$

From this, it can be concluded that $H^2(P, T) = \mathbb{Z}/2\mathbb{Z} \oplus \mathbb{Z}/2\mathbb{Z}$. The homomorphism representing the two-cohomology, which determines the extension of the group, is generated from these vectors:

$$\left\{ \begin{pmatrix} \frac{1}{2}e_2 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \frac{1}{2}e_1 \end{pmatrix} \right\} = \left\{ \begin{pmatrix} 0 \\ 1/2 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1/2 \\ 0 \end{pmatrix} \right\} \quad (82)$$

The linear combination of them (with integer coefficients, of 0 or 1) admits four possible mappings. The relators in the extension E are obtained from the entries in

$$\Lambda(c_1 \cdot e_1 + c_2 \cdot e_2) = \begin{pmatrix} \hat{\Lambda}_{x^2} \\ \hat{\Lambda}_{y^2} \\ \hat{\Lambda}_{(xy)^2} \end{pmatrix}. \text{ They are listed as: They generate four different}$$

extensions in table XXIV. The extensions of type 2 and type 3 are isomorphic, since they are converted with each other by interchanging x and y , and e_1 and e_2 .

We can see the relators of the extensions provide the relations which determine the vector system in the non-symmorphic crystal, with the point group P . (To obtain

	type 1	type 2	type 3	type 4
$\hat{\Lambda}_{x^2}$	$0 \cdot e_1 + 0 \cdot e_2$	$0 \cdot e_1 + 1 \cdot e_2$	$0 \cdot e_1 + 0 \cdot e_2$	$0 \cdot e_1 + 1 \cdot e_2$
$\hat{\Lambda}_{y^2}$	$0 \cdot e_1 + 0 \cdot e_2$	$0 \cdot e_1 + 0 \cdot e_2$	$1 \cdot e_1 + 0 \cdot e_2$	$1 \cdot e_1 + 1 \cdot e_2$
$\hat{\Lambda}_{(xy)^2}$	$0 \cdot e_1 + 0 \cdot e_2$	$0 \cdot e_1 + 0 \cdot e_2$	$0 \cdot e_1 + 0 \cdot e_2$	$0 \cdot e_1 + 0 \cdot e_2$

TABLE XXIII. Four possible types of relators in the extensions.

type 1	$\langle x, y, e_1, e_2 x^2 = y^2 = (xy)^2 = [e_1, e_2] = 1, {}^x e_1 = e_1^{-1}, {}^x e_2 = e_2, {}^y e_1 = e_1, {}^y e_2 = e_2^{-1} \rangle$
type 2	$\langle x, y, e_1, e_2 x^2 = e_2, y^2 = (xy)^2 = [e_1, e_2] = 1, {}^x e_1 = e_1^{-1}, {}^x e_2 = e_2, {}^y e_1 = e_1, {}^y e_2 = e_2^{-1} \rangle$
type 3	$\langle x, y, e_1, e_2 y^2 = e_1, x^2 = (xy)^2 = [e_1, e_2] = 1, {}^x e_1 = e_1^{-1}, {}^x e_2 = e_2, {}^y e_1 = e_1, {}^y e_2 = e_2^{-1} \rangle$
type 4	$\langle x, y, e_1, e_2 x^2 = e_2, y^2 = e_1, (xy)^2 = [e_1, e_2] = 1, {}^x e_1 = e_1^{-1}, {}^x e_2 = e_2, {}^y e_1 = e_1, {}^y e_2 = e_2^{-1} \rangle$

TABLE XXIV. Four types of the extension. e_1 and e_2 should be assumed to be translations $\{E|e_1\}$ and $\{E|e_2\}$, rather than vectors.

the vector system, it is enough to re-express x, y as the augmented matrix forms of the space groups, with indeterminate fractional translations. The e_1 and e_2 are also represented by matrices as translations. The equivalence relations in the entries of the matrix products in the group multiplications will give the vector systems, as was demonstrated elsewhere in this article. In that demonstration, the vector system was also derived from cohomological algebra, not from two-cohomology, but from one-cohomology.) From this simple example, we can observe some importance of homological algebra, which provides us the criterion of the existence of the non-symmorphic crystal, in accordance with the non-triviality of two-cohomology. On the other hand, if the two-cohomology is trivial, or of zero-mapping, the extension of the group simply becomes a semidirect product, which is always a symmorphic crystal. In this case of zero two-cohomology, the exact sequence splits, in the sense that there is a homomorphism $s : G \rightarrow H$ such as $\pi \circ s = \text{id}_G$. It can be proved that an extension (or, the short exact sequence as above) is split if and only if the group H is the semidirect product of N and G . (We should remember this: elsewhere in this article, the point group of non-symmorphic crystal is constructed by means

of semidirect product. In that computation, the point group of non-symmorphic crystal is not directly obtained as a semidirect product, but extracted as one of its subgroups. So there is no contradiction against the above statement.)

Now the relationship is established among the symmorphic properties of crystals, the splitting extension of group, and the two-cohomology, as is shown in the table below.

type 1	$\{M_x 0\}, \{M_y 0\}, \{E e_1\}, \{E e_2\}$
type 2	$\{M_x \frac{1}{2}e_2\}, \{M_y 0\}, \{E e_1\}, \{E e_2\}$
type 3	$\{M_x 0\}, \{M_y \frac{1}{2}e_1\}, \{E e_1\}, \{E e_2\}$
type 4	$\{M_x \frac{1}{2}e_2\}, \{M_y \frac{1}{2}e_1\}, \{E e_1\}, \{E e_2\}$

TABLE XXV. The generators of the four types of the space groups classified by the two-cohomology.

In getting through this section, two necessary points for the computations in GAP are given. The first is how to derive the relators, or the finite representation: the second is the computation of the Smith Normal form. (The two-cohomology can be computed by GAP built-in command, for the case of finite group G and a module M , over a *finite field*. Because of this assumption, the GAP built-in command is not applicable to the above example, in which the module M is $\mathbb{Z}^n$.)

A definition is now needed: a group G is polycyclic if there is a series of subgroups

$$G = C_1 > C_2 > \cdots > C_n > C_{n+1} = 1,$$

where C_{i+1} is normal in C_i and C_i/C_{i+1} is a cyclic group. The generators of G is given by a sequence $G := (g_1, \dots, g_n)$ such that $C_i = \langle C_{i+1}, g_i \rangle$. As a finite solvable group, the point group of the crystal is polycyclic, which is composed from the polycyclic generating system.²² We have defined the point groups by means of matrix generators, or the multiplication table. These groups can be converted into

isomorphic polycyclic groups, and then, polycyclic groups are converted into finitely presented groups with relators. The conversion goes as follows:

```
gap> A:=[ [ 0, 0, 1 ], [ 1, 0, 0 ], [ 0, -1, 0 ] ];
gap> B:=[ [ 0, 0, -1 ], [ 0, -1, 0 ], [ 1, 0, 0 ] ];
gap> G:=Group(A,B);
Group([ [ [ 0, 0, 1 ], [ 1, 0, 0 ], [ 0, -1, 0 ] ],
        [ [ 0, 0, -1 ], [ 0, -1, 0 ], [ 1, 0, 0 ] ] ])
gap> p:=Pcgs(G);
Pcgs([ [ [ 0, 0, 1 ], [ 0, 1, 0 ], [ -1, 0, 0 ] ],
        [ [ 1, 0, 0 ], [ 0, 1, 0 ], [ 0, 0, -1 ] ],
        [ [ 0, 0, -1 ], [ -1, 0, 0 ], [ 0, 1, 0 ] ],
        [ [ 1, 0, 0 ], [ 0, -1, 0 ], [ 0, 0, -1 ] ],
        [ [ -1, 0, 0 ], [ 0, -1, 0 ], [ 0, 0, 1 ] ] ])
gap> iso:=IsomorphismFpGroupByPcgs(p,"g");
CompositionMapping( [ (1,4,6,8)(2,3,5,7), (1,4)(2,3)(5,7)(6,8),
        (3,6,7)(4,5,8), (1,7)(2,8)(3,6)(4,5), (1,3)(2,4)(5,8)(6,7) ] ->
[ g1, g2, g3, g4, g5 ], <action isomorphism> )
gap> fp:=Image(iso);
<fp group of size 48 on the generators [ g1, g2, g3, g4, g5 ]>
gap> RelatorsOfFpGroup(fp);
[ g1^2*g5^-1*g4^-1, g2^-1*g1^-1*g2*g1*g5^-1*g4^-1,
  g3^-1*g1^-1*g3*g1*g5^-1*g4^-1*g3^-1, g4^-1*g1^-1*g4*g1*g5^-1*g4^-1,
  g5^-1*g1^-1*g5*g1*g5^-1*g4^-1, g2^2, g3^-1*g2^-1*g3*g2*g4^-1,
  g4^-1*g2^-1*g4*g2, g5^-1*g2^-1*g5*g2, g3^3, g4^-1*g3^-1*g4*g3*g5^-1*g4^-1,
  g5^-1*g3^-1*g5*g3*g4^-1, g4^2, g5^-1*g4^-1*g5*g4, g5^2 ]
```

The command “Pcgs(G)” returns the polycyclic generating system of G . (In

this example, the generators are accessible through the list `p[1],...p[5].`) The command “`IsomorphismOfFpGroupByPcgs(p,”g”)`” gives the map which converts the polycyclic generating system into a finitely represented group. As the image of this isomorphism, the polycyclic group is given. However, the polycyclic generating system is not minimal. To generate the minimal one, we should do as this:

```
gap> iso:=IsomorphismFpGroupByGenerators(G,GeneratorsOfGroup(G));
<composed isomorphism:[ [ [ 0, 0, 1 ], [ 1, 0, 0 ], [ 0, -1, 0 ] ],
[ [ 0, 0, -1 ], [ 0, -1, 0 ], [ 1, 0, 0 ] ] ]->[ F1, F2 ]>
gap> fp:=Image(iso);
<fp group of size 48 on the generators [ F1, F2 ]>
gap> RelatorsOfFpGroup(fp);
[ F2^4, (F1*F2^-1)^2, F1^6, (F1*F2*F1)^2 ]
gap> [G.2^4,(G.1*G.2^-1)^2,G.1^6,(G.1*G.2*G.1)^2];
[ [ [ 1, 0, 0 ], [ 0, 1, 0 ], [ 0, 0, 1 ] ],
[ [ 1, 0, 0 ], [ 0, 1, 0 ], [ 0, 0, 1 ] ],
[ [ 1, 0, 0 ], [ 0, 1, 0 ], [ 0, 0, 1 ] ],
[ [ 1, 0, 0 ], [ 0, 1, 0 ], [ 0, 0, 1 ] ] ]
```

The smith normal form is also computed by GAP:

```
gap> M:=[[0,0,0,0],[0,2,0,0],[0,0,0,0],[0,0,2,0],[0,0,0,0],[0,0,0,0]];
gap> SmithNormalFormIntegerMat(M);
[ [ 2, 0, 0, 0 ], [ 0, 2, 0, 0 ], [ 0, 0, 0, 0 ], [ 0, 0, 0, 0 ],
[ 0, 0, 0, 0 ], [ 0, 0, 0, 0 ] ]
```

H. Remarks to this section

In this section, the technical details which would be important in the actual application in the computational group theory in the field of solid state physics are explained. The chosen topics are as follows: the algorithm to determine the symmetry of the crystal; the computation of the compatibility relation, which is useful in the discussion of the splitting of the energy spectra with the reduction of the structural symmetry; the concept of the semi-direct product, which is applicable to the preparation of the character table of the super-cell structure; the concept of the group extension, by means of cohomology, which can be utilized to design the crystal lattice. The author hopes that the readers of this article would get familiar with these technical or advanced topics in order to deepen the knowledge of the group theory, applicable to concrete problems in material science. The small programs presented in this article can be executed in a desk-top PC. They are composed in accordance with the elementary formulas and definitions in the references and textbooks, so that they should be as readable as possible, thus they are not always effective in speed, and some part of them could be replaced by built-in functions in GAP. In the preceding sections of this article, the topics are taken from the solid state physics. In the forthcoming sections, however, the application to the quantum chemistry (applicable to the isolated system, equipped with a certain symmetry, without periodicity) shall be discussed in a parallel way as the solid state physics, where the importance of the symmetry in the quantum dynamics in the molecule shall be illustrated in the different light.

VII. SYMMETRY IN C_{60}

The C_{60} molecule is characterized by the peculiar structure, that of soccer-ball, composed of 60 atoms, 90 bonds, and 12 pentagons, and 60 hexagons. The group theoretical symmetry is of the icosahedral type, which contains 120 symmetric operations and 10 irreducible representations, according to which, the eigenstates are classified and the origins of degeneracies in energy spectrum are explained. We begin from the construction of the symmetric operations by means of permutations of atoms, generate the icosahedral group by GAP, compute the irreducible representations, and compose the projection operators. We execute the electronic structure calculations of the molecule, and analyze the wave-functions from the viewpoint of their irreducible representation. Furthermore, some concepts of symmetries (to which physicists pays little notice) are presented also by the analysis of the computer algebra. Throughout the study, it is necessary that whole subgroups of icosahedral symmetry should be extracted and classified by equivalence, and we will see that the utilization of the computer algebra is effective for this purpose.

A. The initial set-up

The C_{60} molecule (in Fig. 6) is projected on a plane as in the Fig. 7. The vertexes are numbered from 1 to 60, where we follow the following rule: the two atoms numbered as I and $I+30$ are located in the opposite poles in the molecular sphere. The pentagons are also numbered from 1 to 12 (with under-bars), and two pentagons numbered as I and $I+6$ are opposed with each other. There are two types of bonds, single and double, having slightly different lengths, distinguished by broad and broken segments in the figure. The icosahedral group are generated by three basic operations and represented by the permutations of atoms as follows. The group

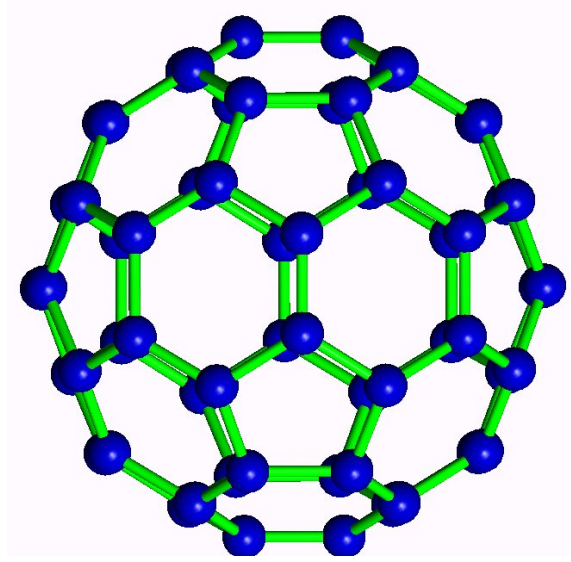


FIG. 6. A C_{60} molecule.

is the direct product of the fifth alternating group “A5” (the 5-th alternating group) and the group of the inversion “I”. The generators are represented by permutations:

```
gap> g1:=(1, 14, 20)(2, 15, 16)(3, 11, 17)(4, 12, 18)(5, 13, 19)
(6, 58, 22)(7, 57, 23)( 8, 56, 24)( 9, 60, 25)( 10, 59, 21)
( 31, 44, 50)( 32, 45, 46)( 33, 41, 47)( 34, 42, 48)( 35, 43, 49)
( 36, 28, 52)( 37, 27, 53)( 38, 26, 54)( 39, 30, 55)( 40, 29, 51);
gap> g2:=( 1, 5, 4, 3, 2)( 6,26,21,16,11)( 7,27,22,17,12)( 8,28,23,18,13)
( 9,29,24,19,14)(10,30,25,20,15)(31,35,34,33,32)(36,56,51,46,41)
(37,57,52,47,42)(38,58,53,48,43)(39,59,54,49,44)(40,60,55,50,45);
gap> g3:=( 1, 31)( 2, 32)( 3, 33)( 4, 34)( 5, 35)( 6, 36)( 7, 37)( 8, 38)
( 9, 39)( 10, 40)( 11, 41)( 12, 42)( 13, 43)( 14, 44)( 15, 45)( 16, 46)
( 17, 47)( 18, 48)( 19, 49)( 20, 50)( 21, 51)( 22, 52)( 23, 53)( 24, 54)
( 25, 55)( 26, 56)( 27, 57)( 28, 58)( 29, 59)( 30, 60);
```

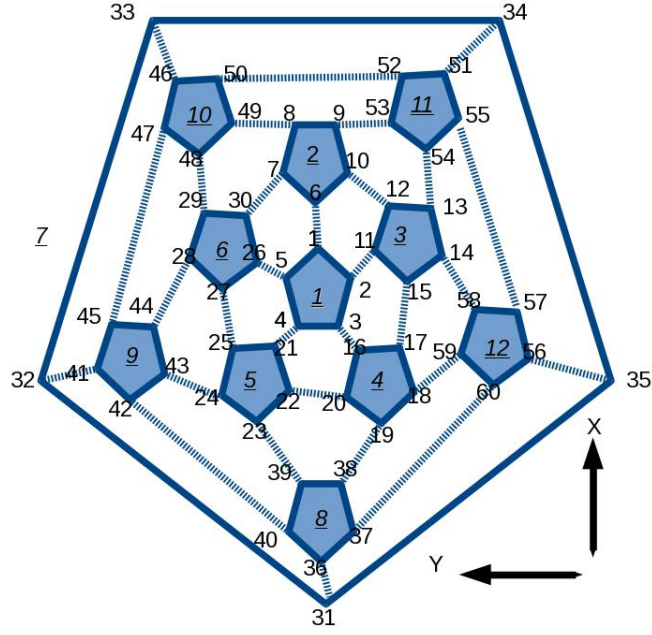


FIG. 7. The projected image of C_{60} on a plane.

The elements g_1 (the rotation by 120 degrees) and g_2 (that by 72 degrees) generate “A5” and g_3 generates “I”. The permutation, denoted by $(a, b, c, d, \dots, x)$, should be interpreted as the replacement of atoms in the following way: the atom located at the site “a” is replaced by that at the site “b”, that at “b” by that at “c”, then in turn and finally, the last entry “x” by the first “a”.²³ The usage of sixty

symbols for the definition of the group is superfluous, and in fact, twelve symbols (representing the 12 vertexes of the icosahedron, or the 12 pentagons in the molecule) will do. If it is unnecessary to use the geometrical image, one can use 7 symbols, since, the icosahedral group is the direct product of the 5-th alternating group A_5 and the inversion I , as the former requires five symbols “1,2,3,4,5” and the latter two symbols “6,7”. The equivalence of these different definition is assured by constructing isomorphisms among them, which is an easy task for the computer algebra.

The group is constructed as

```
gap> gp:=Group(g1,g2,g3);
```

For the later utilization, it is more convenient to generate the group by means of matrices (which represents the permutations on sixty vertexes). We use the built-in function “ListPerm()” which computes the action on the permutation on the list [1,2,...,60].

```
gap> p11:=ListPerm(g1);
[ 14, 15, 11, 12, 13, 58, 57, 56, 60, 59, 17, 18, 19, 20, 16, 2, 3, 4, 5, 1,
  10, 6, 7, 8, 9, 54, 53, 52, 51, 55, 44, 45, 41, 42, 43, 28, 27, 26, 30, 29,
  47, 48, 49, 50, 46, 32, 33, 34, 35, 31, 40, 36, 37, 38, 39, 24, 23, 22, 21,
  25 ]
gap> p12:=ListPerm(g2);;
gap> p13:=ListPerm(g3);;
```

These three lists are converted into three matrices by means of this user-defined function.

```
ListToMat:=function(l)
  local size,h,i,j;
```

```

size:=Size(l);
h:=List([1..size],i->List([1..size],j->0));
for i in [1..size] do
  h[i][l[i]]:=1;
od;
return h;
end;

```

```

gap> m1:=ListToMat(pl1);;
gap> m2:=ListToMat(pl2);;
gap> m3:=ListToMat(pl3);;

```

The irreducible representations are computed now.²⁴

```

gap> g:=Group(m1,m2,m3);
gap> irr:=Irr(g);
gap> Size(irr);
10

```

The characters for each element can be listed as numeral tables.

```

gap> elm:=Elements(g);
gap> A1:=List(elm,g->g^irr[1]);;
gap> A2:=List(elm,g->g^irr[2]);;
.....
gap> A10:=List(elm,g->g^irr[10]);;

```

The notation $g^{\text{irr}[X]}$ means the computation of the character value of the element “g” by the X-th representation in this context.

The characters of the irreducible representations are orthogonal and normalized.

```

gap> A1*A1;
120
gap> A2*A2;
120
gap> A1*A2;
0

```

The virtual character is decomposed into the direct sum.

```

gap> (4*A1+2*A2)*TransposedMat([A1,A2,A3,A4,A5,A6,A7,A8,A9,A10])/Size(elm);
[4, 2, 0, 0, 0, 0, 0, 0, 0, 0]

```

There are 10 conjugacy classes and 10 irreducible representations. They are shown in the tables XXVI and XXVII. In table XXVI, the second row shows the number of elements in each conjugacy classes (CL1,...,CL10), and the ten rows bellow are characters for each of the ten irreducible representations (I.1,...,I.10). The last row (I.Tr) shows the trace of the group elements as matrices, which is a virtual character (not irreducible). The notation $E(5)$ means a complex number, the fifth root of the unity $\exp(2\sqrt{-1}\pi/5)$, thus the characters are real-valued. Simply the computed result by GAP is tabulated here, as it is. The projector on the p -th irreducible representation is computed by the formula

$$P^{(p)} = \frac{l(p)}{|G|} \sum_{T \in G} \chi^{(p)*}(T) \cdot O(T)$$

by summing up the elements T of the group G , where $l(p)$ is the dimension of the p -th irreducible representation, g the order of the group, $\chi(p)$ the character, $O(T)$ the operation of the group (which would be represented as matrices and applied to the vector representation of the wave function. The irreducible representation of the

	CL1	CL2	CL3	CL4	CL5	CL6	CL7	CL8	CL9	CL10
	1	12	12	20	20	15	12	1	12	15
I.1	1	1	1	1	1	1	1	1	1	1
I.2	1	-1	1	-1	1	-1	-1	-1	1	1
I.3	3	$-E(5)-E(5)^4$	$-E(5)^2-E(5)^3$	0	0	-1	$-E(5)^2-E(5)^3$	3	$-E(5)-E(5)^4$	-1
I.4	3	$-E(5)^2-E(5)^3$	$-E(5)-E(5)^4$	0	0	-1	$-E(5)-E(5)^4$	3	$-E(5)^2-E(5)^3$	-1
I.5	3	$E(5)^2+E(5)^3$	$-E(5)-E(5)^4$	0	0	1	$E(5)+E(5)^4$	-3	$-E(5)^2-E(5)^3$	-1
I.6	3	$E(5)+E(5)^4$	$-E(5)^2-E(5)^3$	0	0	1	$E(5)^2+E(5)^3$	-3	$-E(5)-E(5)^4$	-1
I.7	4	-1	-1	1	1	0	-1	4	-1	0
I.8	4	1	-1	-1	1	0	1	-4	-1	0
I.9	5	0	0	-1	-1	1	0	5	0	1
I.10	5	0	0	1	-1	-1	0	-5	0	1
I.Tr	60	0	0	0	0	4	0	0	0	0

TABLE XXVI. The table of characters of the irreducible representation of the icosahedral group.

	The representatives
CL1	<identity ...>
CL2	$x1^{-1}x2^{-2}x3$
CL3	$x2^{-1}x1x2x1$
CL4	$x3x2x1x2^2$
CL5	$x2^{-2}x1x2x1$ (also including $x1$)
CL6	$x3x2^2x1x2^2$
CL7	$x3x2^2$
CL8	$x3$
CL9	$x1^{-1}x2^{-2}$ (also including $x2$)
CL10	$x1x2x1$

TABLE XXVII. The representatives in the conjugacy classes of the irreducible representations of the icosahedral group. The generators of the groups are represented by symbols $x1...xN$, as are numbered by GAP. In this case $x1=m1, x2=m2, x3=m3$.

wave function is determined numerically, by the condition that the application of the projector should keep the wave function as it is, or delete it.)

B. The analysis of the eigenstates

Now that we have the irreducible representations and the symmetry operations, we can construct the projection operators.

At first, we assume a model of C_{60} , where, in each vertex, one s or π orbital is located. The inter-atomic interactions are limited to those among three different neighboring sites, as are signified by single and double bonds. We permit two different strengths of interactions in the Fock matrix H , according to two types of the bonding. We neglect the overlap matrix elements between different sites, the overlapping matrix S being the unity. A computation is executed by the above assumption, with the values of $H_{\text{single}}=-2$ (on the single bonds in the pentagons), $H_{\text{double}}=-1$ (on the double bonds in the hexagons).

Before the electronic structure computation, we can deduce a prediction from the group theory. The group elements given by the matrices which represent the replacements of the 60 vertexes provide us the trace representation $I.\text{Tr}$. The virtual representation is decomposed by the irreducible representations (as the sum of row vectors in the table):

$$I.\text{Tr} = 1 \times I.1 + 0 \times I.2 + 1 \times I.3 + 1 \times I.4 + 2 \times I.5 + 2 \times I.6 + 2 \times I.7 + 2 \times I.8 + 3 \times I.9 + 2 \times I.10.$$

This relation tells us that the 60 dimensional vector space (on which the matrix group acts) is divided into the ten irreducible components, given as the ten irreducible representations of the group. The multiplicity of X-th component is equal to the coefficient to “I.X”. One of these components, belonging to “I.2”, is a null space in this case. The wave functions, computed as the eigenvectors of the Fock matrix, are also subject to this division of the vector space.

Let us verify this. The eigenstates and the corresponding irreducible represen-

tations are shown in the following list. The abbreviations as “I.”, “D.”, “E” denote the index of the irreducible representation, the degeneracy of the energy, and the energies. The values of the energies are listed in the bracket. If the bracket is blank, the eigenstates in correspondence with the irreducible representations do not exist. The number of different eigenvalues in each irreducible representation is equal to the multiplicity in the above relation between I.Tr and I.1,...,I.10.

```

I.1  D.1 E. [ -5.0000 ]
I.2  D.1 E. [ None ]
I.3  D.3 E. [ 4.2361 ]
I.4  D.3 E. [ -0.2361 ]
I.5  D.3 E. [ -4.6542, -0.5819 ]
I.6  D.3 E. [ -3.6765, 2.9126 ]
I.7  D.4 E. [ -1.4495, 3.4495 ]
I.8  D.4 E. [ -2.1623, 4.1623 ]
I.9  D.5 E. [ -4.0642, -1.6946, 2.7588 ]
I.10 D.5 E. [ -1.0000, 3.0000 ]

```

For a realistic quantum chemistry computation of C_{60} , the similar analysis is possible. For simplicity, one can make use of the amplitudes of 1s orbitals, because those orbitals are transformed among themselves, without mixing with other types, 2s, 2p, 3s, 3p. Except for one special case where the amplitudes of 1s orbital are null, the correspondence between the eigenstates and the irreducible representations can be well established. The result is listed in the following list. (The last entry of the list I.0 is for the case of the failures in the identification.) Even in the case of the failure of the analysis, the degeneracy is single, and one can conclude the corresponding irreducible representation is I.1 or I.2, that of 1-dimension. The numbers of the different eigenvalues in the each irreducible representations are predicable by means of

the decomposition of the trace representation of the character of the transformation matrices of the 1s,2s,2px,2py,2pz,3s,3px,3py,3pz orbitals. (The p orbitals are transformed by the same matrices prepared for the vibrational mode of the molecule, as will be discussed later.)

I.1	D.1	E. [7 different eigenvalues]
I.2	D.1	E. [?]
I.3	D.3	E. [11 different eigenvalues]
I.4	D.3	E. [11 different eigenvalues]
I.5	D.3	E. [16 different eigenvalues]
I.6	D.3	E. [16 different eigenvalues]
I.7	D.4	E. [24 different eigenvalues]
I.8	D.4	E. [24 different eigenvalues]
I.9	D.5	E. [25 different eigenvalues]
I.10	D.5	E. [20 different eigenvalues]
I.0	D.1	E. [2 different eigenvalues]

C. The analysis again, against the failure in the identification

As the degeneracy of the energy is one, one can see the levels denoted as I.0 in the previous section belong to the representation I.1 or I.2. The characters of the one-dimensional representation in table XXVI are shown here again (in table XXVIII).

	CL1	CL2	CL3	CL4	CL5	CL6	CL7	CL8	CL9	CL10
I.1	1	1	1	1	1	1	1	1	1	1
I.2	1	-1	1	-1	1	-1	-1	-1	1	1

TABLE XXVIII. The one-dimensional irreducible representations.

To distinguish the representation I.1 and I.2 with ease, one may apply the element in the conjugacy class 8 (the inversion). By the inversion, one vertex moves to the opposite site with respect to the center of the geometry, and the coefficients of p-orbitals change signs. The amplitudes of the wave-functions (in the two atoms located in the antipodes positions) in I.0 are typically obtained as in table XXIX.

CA	1S	0
	2S	0
	2PX	X
	2PY	Y
	2PZ	Z
CB	1S	0
	2S	0
	2PX	X
	2PY	Y
	2PZ	Z

TABLE XXIX. The amplitudes of the wave-function (coefficients for each orbital) in two opposing atoms.

The inversion changes the sign of non-zero coefficients. We must recall that the wave-functions are basis functions of some irreducible representations, and the traces of their transformation matrices are the characters. Since the traces are -1 in the above cases, the wave-functions belong to the representation I.2. The reason of the failure in the analysis by the projection operators applied on s orbitals are fundamental one: the projection operator of I.2 over s orbitals is exactly the zero-matrix, which gives rise to exact zero amplitudes in s orbitals (i.e. the null space.) The reason of the existence of the orbitals of the I.2 is that the actual C_{60} molecule has the symmetry of the inversion and the carbon atom has p-orbitals.

D. The perturbation and the symmetry

We often have to compute matrix elements in the perturbation theory such as

$$\langle \psi_i | V_p | \psi_j \rangle = [I_i | I_p | I_j] = [I_i | I_p * I_j]. \quad (83)$$

The product of the perturbation potential and the wave function belongs to the direct product of the representation, which is decomposed into the direct sum

$$I_p * I_j = \sum_k A_k^{p,j} I_k. \quad (84)$$

We can determine beforehand whether this matrix element would be zero or not, only from the group theoretical consideration: if the two irreducible representations in the inner product are the same, the matrix element will be non-zero. In the system with the high symmetry, the group theoretical constraint is so strong that it annihilates many matrix elements. However, the symmetry is reduced, there is a possibility where the matrix element will become non-zero. Indeed there is no symmetry, there is no group theoretical constraint which annihilates the matrix elements. And if one uses the group theory, he can see the least reduction of the symmetry where the matrix element will become non-zero. For the irreducible representation of group g ramifies in the subgroup s as follows.

$$I_p^g = C_{i,1}^{(g,s)} I_1^s + C_{i,2}^{(g,s)} I_2^s + \cdots + C_{i,M}^{(g,s)} I_M^s. \quad (85)$$

One can find the subgroup where the non-zero matrix element will exist, by tracing the sequence of subgroups (in the subgroup lattice) and checking the possible combinations of the ramified irreducible representations. In this stage, the concrete style of the structural deformation is not discussed yet.

One of the important perturbation potential is that of optical transition, such as $E \cdot r$. Now we determine the irreducible representation to which the perturbation $E \cdot r$ (or the spatial vector r) belongs. We now construct icosahedral group from the rotation matrices in three-dimensional Euclidean space, acting on the twelve vertexes of one icosahedron.

The twelve vertexes in one icosahedron are given by

- 1 [0, 0, 1]
- 2 [$\frac{2}{5}E(5) - \frac{2}{5}E(5)^2 - \frac{2}{5}E(5)^3 + \frac{2}{5}E(5)^4$, 0,
 $\frac{1}{5}E(5) - \frac{1}{5}E(5)^2 - \frac{1}{5}E(5)^3 + \frac{1}{5}E(5)^4$]
- 3 [$-\frac{3}{5}E(5) - \frac{2}{5}E(5)^2 - \frac{2}{5}E(5)^3 - \frac{3}{5}E(5)^4$,
 $-\frac{1}{5}E(20) + \frac{1}{5}E(20)^9 + \frac{2}{5}E(20)^{13} - \frac{2}{5}E(20)^{17}$,
 $\frac{1}{5}E(5) - \frac{1}{5}E(5)^2 - \frac{1}{5}E(5)^3 + \frac{1}{5}E(5)^4$]
- 4 [$\frac{2}{5}E(5) + \frac{3}{5}E(5)^2 + \frac{3}{5}E(5)^3 + \frac{2}{5}E(5)^4$,
 $-\frac{2}{5}E(20) + \frac{2}{5}E(20)^9 - \frac{1}{5}E(20)^{13} + \frac{1}{5}E(20)^{17}$,
 $\frac{1}{5}E(5) - \frac{1}{5}E(5)^2 - \frac{1}{5}E(5)^3 + \frac{1}{5}E(5)^4$]
- 5 [$\frac{2}{5}E(5) + \frac{3}{5}E(5)^2 + \frac{3}{5}E(5)^3 + \frac{2}{5}E(5)^4$,
 $\frac{2}{5}E(20) - \frac{2}{5}E(20)^9 + \frac{1}{5}E(20)^{13} - \frac{1}{5}E(20)^{17}$,
 $\frac{1}{5}E(5) - \frac{1}{5}E(5)^2 - \frac{1}{5}E(5)^3 + \frac{1}{5}E(5)^4$],
- 6 [$-\frac{3}{5}E(5) - \frac{2}{5}E(5)^2 - \frac{2}{5}E(5)^3 - \frac{3}{5}E(5)^4$,
 $\frac{1}{5}E(20) - \frac{1}{5}E(20)^9 - \frac{2}{5}E(20)^{13} + \frac{2}{5}E(20)^{17}$,
 $\frac{1}{5}E(5) - \frac{1}{5}E(5)^2 - \frac{1}{5}E(5)^3 + \frac{1}{5}E(5)^4$]
- 7 [0, 0, -1]
- 8 [$-\frac{2}{5}E(5) + \frac{2}{5}E(5)^2 + \frac{2}{5}E(5)^3 - \frac{2}{5}E(5)^4$, 0,
 $-\frac{1}{5}E(5) + \frac{1}{5}E(5)^2 + \frac{1}{5}E(5)^3 - \frac{1}{5}E(5)^4$]
- 9 [$\frac{3}{5}E(5) + \frac{2}{5}E(5)^2 + \frac{2}{5}E(5)^3 + \frac{3}{5}E(5)^4$,
 $\frac{1}{5}E(20) - \frac{1}{5}E(20)^9 - \frac{2}{5}E(20)^{13} + \frac{2}{5}E(20)^{17}$,

```

-1/5*E(5)+1/5*E(5)^2+1/5*E(5)^3-1/5*E(5)^4 ]
10 [ -2/5*E(5)-3/5*E(5)^2-3/5*E(5)^3-2/5*E(5)^4,
      2/5*E(20)-2/5*E(20)^9+1/5*E(20)^13-1/5*E(20)^17,
      -1/5*E(5)+1/5*E(5)^2+1/5*E(5)^3-1/5*E(5)^4 ]
11 [ -2/5*E(5)-3/5*E(5)^2-3/5*E(5)^3-2/5*E(5)^4,
      -2/5*E(20)+2/5*E(20)^9-1/5*E(20)^13+1/5*E(20)^17,
      -1/5*E(5)+1/5*E(5)^2+1/5*E(5)^3-1/5*E(5)^4 ]
12 [ 3/5*E(5)+2/5*E(5)^2+2/5*E(5)^3+3/5*E(5)^4,
      -1/5*E(20)+1/5*E(20)^9+2/5*E(20)^13-2/5*E(20)^17,
      -1/5*E(5)+1/5*E(5)^2+1/5*E(5)^3-1/5*E(5)^4 ]

```

The three generators of the group are as follows:

```

gap> f1:=(1,2,3)(4,6,11)(5,10,12)(7,8,9);;
gap> f2:=(2,6,5,4,3)(8,12,11,10,9);;
gap> f3:=(1,7)(2,8)(3,9)(4,10)(5,11)(6,12);;

```

These permutations are represented by the rotation matrices as

```

gap> f1:=[ [ 3/10*E(5)+1/5*E(5)^2+1/5*E(5)^3+3/10*E(5)^4,
             -1/10*E(20)+1/10*E(20)^9+1/5*E(20)^13-1/5*E(20)^17,
             2/5*E(5)-2/5*E(5)^2-2/5*E(5)^3+2/5*E(5)^4 ],
            [ 1/2*E(20)-1/2*E(20)^9, -1/2*E(5)-1/2*E(5)^4, 0 ],
            [ -3/5*E(5)-2/5*E(5)^2-2/5*E(5)^3-3/5*E(5)^4,
              1/5*E(20)-1/5*E(20)^9-2/5*E(20)^13+2/5*E(20)^17,
              1/5*E(5)-1/5*E(5)^2-1/5*E(5)^3+1/5*E(5)^4 ] ];;
gap> f2:=[ [ 1/2*E(5)+1/2*E(5)^4, -1/2*E(20)+1/2*E(20)^9, 0 ],
            [ 1/2*E(20)-1/2*E(20)^9, 1/2*E(5)+1/2*E(5)^4, 0 ], [ 0, 0, 1 ] ];;
gap> f3:=[ [ -1, 0, 0 ], [ 0, -1, 0 ], [ 0, 0, -1 ] ];;

```

	Dimension	Operator	The characters of [f1,f2,f3]	
N.1	1	$[[0, 0, 0], [0, 0, 0], [0, 0, 0]]$	$[1, 1, 1]$	
N.2	1	$[[0, 0, 0], [0, 0, 0], [0, 0, 0]]$	$[1, 1, -1]$	
N.3	3	$[[0, 0, 0], [0, 0, 0], [0, 0, 0]]$	$[0, -E(5)^2 - E(5)^3, 3]$	(I.4 in table XXVI)
N.4	3	$[[0, 0, 0], [0, 0, 0], [0, 0, 0]]$	$[0, -E(5) - E(5)^4, 3]$	(I.3 in XXVI)
N.5	3	$[[1, 0, 0], [0, 1, 0], [0, 0, 1]]$	$[0, -E(5)^2 - E(5)^3, -3]$	
N.6	3	$[[0, 0, 0], [0, 0, 0], [0, 0, 0]]$	$[0, -E(5) - E(5)^4, -3]$	
N.7	4	$[[0, 0, 0], [0, 0, 0], [0, 0, 0]]$	$[1, -1, 4]$	
N.8	4	$[[0, 0, 0], [0, 0, 0], [0, 0, 0]]$	$[1, -1, -4]$	
N.9	5	$[[0, 0, 0], [0, 0, 0], [0, 0, 0]]$	$[-1, 0, 5]$	
N.10	5	$[[0, 0, 0], [0, 0, 0], [0, 0, 0]]$	$[-1, 0, -5]$	

TABLE XXX. The projection operators. Be careful that the computation by GAP returns the representations (N.1,...,N.10) in the slightly different order from those in table XXVI(I.1,...,I.10).

The ten projection operators are computed as in table XXX. The operators, except that of the fifth representation, are exactly zeros. The symmetry operations on one vector, which is subject to the icosahedral symmetry, are only representable in the fifth irreducible representation, and the perturbation term $E \cdot r$ is represented by the fifth representation. (The fifth representation can be distinguished from others, as such having characters $[0, -E(5)^2 - E(5)^3, -3]$ for three generators. Especially, the rotation of 72 degrees should have the character value $-E(5)^2 - E(5)^3$. The rotation by 72 degrees and its inverse (f2 and f2⁻¹) have the same character value, because they are conjugate.²⁵)

E. The possible deformation in the reduced symmetry

We can construct molecular geometry which is admissible in each subgroup. If the vertexes are dislocated as $V(i) \rightarrow V(i) + d(i)$, the set of $d(i)$ should satisfy a certain geometrical constraint in the symmetry operation in the subgroup. We should take note of this : since the icosahedral group which includes 120 operations and acts on

60 vertexes in one C_{60} , there are two operations, both of which equally transfers one atomic site into same, but another site. If the dislocations of atoms are still subject to the icosahedral symmetry, there is a constraint. When the atom at the site $V[i]$ moves to $V[j]$ by the operation R , it must be

$$R \cdot V[i] = V[j], \quad \text{and} \quad R \cdot (V[i] + d[i]) = V[j] + d[j],$$

i.e.

$$R \cdot d[i] = d[j].$$

If there are two possible transformations R and Q , it must be

$$R \cdot d[i] = Q \cdot d[i].$$

If we chose $T=R^{-1}Q$, then $T \cdot d[i]=d[i]$, and the possible dislocation is the solution of the equation $(T - E) \cdot d[i] = 0$ (E : the unit matrix). In the case of the icosahedral symmetry in C_{60} , such a T is the reflection at the plain in which one double bond and its antipodes are located.

In general, the dislocations $d[i]$ on all of the vertex are generated as follows. For example, take $V[1]$, and find the operation R , Q , T as above, and then find a possible solution d of $(T - E) \cdot d = 0$ as the generator. The application of the 120 operations on $V[1]+d$ shall generate 60 sites, which are represented by $V[i]+d[i]$, and the set of $d[i]$ is obtained. (This is equivalent to the projection on the trivial irreducible representation, in which the basis set is invariant under the group action.) In a subgroup, the symmetric operations does not act transitively, and the “orbit” of one vertex by the symmetry operations (which covers all of the vertex in C_{60} by the icosahedral symmetry) splits into several subsets, as we will see later. For each subsets, we construct independent d , the generator of the dislocation in each

subset. If the subgroups contains the reflection, the dislocations on the atoms has similar constraints to d (being fixed on one of the reflectional plane) as in the case of the icosahedral symmetry. On the contrary, when the reflection is missing in the subgroup, we can chose arbitrary generator of dislocations in each sub-orbits. One should note that the center of mass will not be kept, since $d[1]+d[2]+\dots+d[60]$ is not equal to 0 in general.

Concerning with this topic, we can classify the vibrational mode of C_{60} according to the group theory. The procedure is to form the direct product of the virtual representation with respect to the replacement of atoms and the irreducible representation of the symmetry operations on the space vector, and then to decompose it into the direct sum. One will find that the vibrational mode in the icosahedral symmetry includes the duplicated trivial irreducible representation, to which the degrees of the freedom is two. The geometrical interpretation of this is that the possible distortion which keeps the icosahedral symmetry is confined in one plane as discussed above.

F. The reduction of the symmetry, from the view point of the orbit in the permutation

The full symmetry of C_{60} is the icosahedral group are generated by “g1”, “g2”, “g3” in the previous section, and it has 164 subgroups. All of the subgroups are computed as

```
gap> gr:=Group(g1,g2,g3);
gap> AS:=AllSubgroups(gr);;
```

The list of the subgroups is given in the descending order of the sizes of the subgroups, and the largest of them (No.164) is the icosahedral.

```
gap> irrA:=Irr(AS[164]);
```

Take a subgroup No.162. This group is of the order 24, and the irreducible representation is also computed.

```
gap> irrB:=Irr(AS[162]);;
```

The irreducible representations of these groups are given in tables XXXI,XXXII,XXXIII, and XXXIV.

	CL1	CL2	CL3	CL4	CL5	CL6	CL7	CL8	CL9	CL10
No.1	1	1	1	1	1	1	1	1	1	1
No.2	1	-1	1	1	1	-1	1	-1	-1	-1
No.3	3	-1	$-E(5)-E(5)^4$	$-E(5)^2-E(5)^3$	-1	$-E(5)^2-E(5)^3$	0	0	3	$-E(5)-E(5)^4$
No.4	3	-1	$-E(5)^2-E(5)^3$	$-E(5)-E(5)^4$	-1	$-E(5)-E(5)^4$	0	0	3	$-E(5)^2-E(5)^3$
No.5	3	1	$-E(5)-E(5)^4$	$-E(5)^2-E(5)^3$	-1	$E(5)^2+E(5)^3$	0	0	-3	$E(5)+E(5)^4$
No.6	3	1	$-E(5)^2-E(5)^3$	$-E(5)-E(5)^4$	-1	$E(5)+E(5)^4$	0	0	-3	$E(5)^2+E(5)^3$
No.7	4	0	-1	-1	0	-1	1	1	4	-1
No.8	4	0	-1	-1	0	1	1	-1	-4	1
No.9	5	1	0	0	1	0	-1	-1	5	0
No.10	5	-1	0	0	1	0	-1	1	-5	0

TABLE XXXI. The character table of the group AS[164].

	Representative	Size
CL1	<identity ...>	1
CL2	$x1^{-1}x2^{-2}x3x1x2x1$	15
CL3	$x2^{-1}$	12
CL4	$x2^{-2}$	12
CL5	$x2^{-2}x1x2$	15
CL6	$x2^2x1x2^2x1^{-1}x3$	12
CL7	$x2^2x1x2$	20 (including g1)
CL8	$x2^{-1}x1^{-1}x2^{-2}x1^{-1}x3$	20
CL9	$x3$	1
CL10	$x2^{-1}x3$	12

TABLE XXXII. The conjugacy classes of the group AS[164].

The branching relation from the group of No.164 to that of No.162 is computed now. The characters of the elements of the group of No.162 are computed and listed

	CL1	CL2	CL3	CL4	CL5	CL6	CL7	CL8
No.1	1	1	1	1	1	1	1	1
No.2	1	-1	-1	1	1	-1	1	-1
No.3	1	-1	$-E(3)$	$E(3)$	$E(3)^2$	$-E(3)^2$	1	-1
No.4	1	-1	$-E(3)^2$	$E(3)^2$	$E(3)$	$-E(3)$	1	-1
No.5	1	1	$E(3)^2$	$E(3)^2$	$E(3)$	$E(3)$	1	1
No.6	1	1	$E(3)$	$E(3)$	$E(3)^2$	$E(3)^2$	1	1
No.7	3	1	0	0	0	0	-1	-3
No.8	3	-1	0	0	0	0	-1	3

TABLE XXXIII. The character table of the group AS[162].

Representative	Size
CL1 <identity ...>	1
CL2 $x2^{-1}x1^{-1}x2^{-2}x3x1x2x1$	3
CL3 $x1^{-1}x2^{-2}x1^{-1}x3$	4
CL4 $x2^{-1}x1x2$	4
CL5 $x2^{-2}x1$	4
CL6 $x1x2^2x1^{-1}x2^{-1}x3$	3
CL7 $x2x1^{-1}$	3
CL8 $x3$	1

TABLE XXXIV. The conjugacy classes of the group AS[162].

in two ways: the one is by the irreducible representations of the group of No.164, and the another by those of the group of No.162. The representations in first list are decomposed as the summations of the entries in the second list, and the result is the branching relation.

```
gap> LA:=List(irrA,a->List(Elements(AS[162]),g->g^a));
[ [ 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1 ],
.....
.....
[ 5, -1, 1, -1, -1, 1, -1, 1, 1, -1, 1, -1, -5, 1, -1, 1, 1, -1, 1, -1, -1,
1, -1, 1 ] ]
```

```

gap> LB:=List(irrB,a->List(Elements(AS[162]),g->g^a));
[ [ 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1 ],
.....
.....
0 ], [ 3, -1, 0, 0, 0, 0, -1, -1, 0, 0, 0, 0, 3, -1, 0, 0, 0, 0, -1,
-1, 0, 0, 0, 0 ] ]
gap> LA*TransposedMat(LB)/Size(AS[162]);

```

The result returns as the matrix in the bellow: the irreducible representations are ramified as

	No.164	->	No.162
[[1, 0, 0, 0, 0, 0, 0, 0],	1	->	1
[0, 1, 0, 0, 0, 0, 0, 0],	2	->	2
[0, 0, 0, 0, 0, 0, 0, 1],	3	->	8
[0, 0, 0, 0, 0, 0, 0, 1],	4	->	8
[0, 0, 0, 0, 0, 0, 1, 0],	5	->	7
[0, 0, 0, 0, 0, 0, 1, 0],	6	->	7
[1, 0, 0, 0, 0, 0, 0, 1],	7	->	1 + 8
[0, 1, 0, 0, 0, 0, 1, 0],	8	->	2 + 7
[0, 0, 0, 0, 1, 1, 0, 1],	9	->	5 + 6 + 8
[0, 0, 1, 1, 0, 0, 1, 0]]	10	->	3 + 4 + 7

One can see the change in the geometry by checking the “orbit” of the vertex “1” and the bond “[1,6]”. In the icosahedral symmetry, the vertex is transferred to other sixty vertexes transitively, and this double bond is transferred to all other thirty double bonds.

```

gap> List(Elements(AS[164]),g->OnPoints(1,g));

```

```
[ 1, 1, 2, 2, 3, 3, 4, 4, 5, 5, 6, 6, 7, 7, 8, 8, 9, 9, 10, 10, 11, 11, 12,
 12, 13, 13, 14, 14, 15, 15, 16, 16, 17, 17, 18, 18, 19, 19, 20, 20, 21, 21,
 22, 22, 23, 23, 24, 24, 25, 25, 26, 26, 27, 27, 28, 28, 29, 29, 30, 30, 31,
 31, 32, 32, 33, 33, 34, 34, 35, 35, 36, 36, 37, 37, 38, 38, 39, 39, 40, 40,
 41, 41, 42, 42, 43, 43, 44, 44, 45, 45, 46, 46, 47, 47, 48, 48, 49, 49, 50,
 50, 51, 51, 52, 52, 53, 53, 54, 54, 55, 55, 56, 56, 57, 57, 58, 58, 59, 59,
 60, 60 ]
```

```
gap> BONDA:=Unique(List(Elements(AS[164]),g->OnSets([1,6],g)));
[ [ 1, 6 ], [ 2, 11 ], [ 3, 16 ], [ 4, 21 ], [ 5, 26 ], [ 7, 30 ], [ 8, 49 ],
[ 9, 53 ], [ 10, 12 ], [ 13, 54 ], [ 14, 58 ], [ 15, 17 ], [ 18, 59 ],
[ 19, 38 ], [ 20, 22 ], [ 23, 39 ], [ 24, 43 ], [ 25, 27 ], [ 28, 44 ],
[ 29, 48 ], [ 31, 36 ], [ 32, 41 ], [ 33, 46 ], [ 34, 51 ], [ 35, 56 ],
[ 37, 60 ], [ 40, 42 ], [ 45, 47 ], [ 50, 52 ], [ 55, 57 ] ]
```

In the symmetry of the subgroup No.162, in contrast, the vertex “1” is transferred only to 24 other vertexes. The orbit of single vertexes (which covers the whole system in the case of the subgroup 164) splits into three subsets. Similarly the bond “[1,6]” is not transferred transitively, only to 24 of double bonds. The remaining six double bounds are transferred among themselves. This situation can be interpreted that one of the double bonds (one of these connecting one pentagon with five neighbors) slightly changes the length, while those of remaining four bonds are unchanged.

```
gap> List(Elements(AS[162]),g->OnPoints(1,g));
[ 1, 5, 9, 10, 11, 15, 18, 19, 21, 22, 27, 28, 31, 35, 39, 40, 41, 45, 48,
 49, 51, 52, 57, 58 ]
gap> List(Elements(AS[162]),g->OnPoints(2,g));
[ 2, 4, 8, 6, 12, 14, 17, 20, 25, 23, 26, 29, 32, 34, 38, 36, 42, 44, 47, 50,
 55, 53, 56, 59 ]
```

```

gap> List(Elements(AS[162]),g->OnPoints(3,g));
[ 3, 3, 7, 7, 13, 13, 16, 16, 24, 24, 30, 30, 33, 33, 37, 37, 43, 43, 46, 46,
  54, 54, 60, 60 ]
gap> BONDB:=Unique(List(Elements(AS[162]),g->OnSets([1,6],g)));
gap> Sort(BONDB);
gap> BONDB;
[ [ 1, 6 ], [ 2, 11 ], [ 4, 21 ], [ 5, 26 ], [ 8, 49 ], [ 9, 53 ],
  [ 10, 12 ], [ 14, 58 ], [ 15, 17 ], [ 18, 59 ], [ 19, 38 ], [ 20, 22 ],
  [ 23, 39 ], [ 25, 27 ], [ 28, 44 ], [ 29, 48 ], [ 31, 36 ], [ 32, 41 ],
  [ 34, 51 ], [ 35, 56 ], [ 40, 42 ], [ 45, 47 ], [ 50, 52 ], [ 55, 57 ] ]

```

The splitting of the energy degeneracy with the symmetry reduction is verified numerically, for example, by a model computation, in which the matrix elements of these two split orbits of double bonds take slightly different values, in correspondence with the change in the symmetry. In this computation, the elements of the Fock matrix which belong to the one of the split orbit (including six bonds, the complementary part of BONDB in BONDA) are enhanced slightly, multiplied by 1.005. The energy spectra at HOMO and LUMO are computed as follows. (The positions of HOMO and LUMO are ambiguous in this case. We presently assume that the half of the 60 eigenstates are occupied by 60 electrons. The left and right columns shows the spectra of the full and the reduced symmetries. The HOMO and LUMO belong to the irreducible representations of No.10 and No.5 of the character table of the group AS[164], and the splitting of the spectra is deduced from the above relation.)

HOMO : Split from one fivefold degeneracy

to one threefold degeneracy and two single degeneracies.

```

26  -1.00000000  ->  -1.00000021
27  -1.00000000  ->  -1.00000021

```

```

28 -1.0000000 -> -1.0000021
29 -1.0000000 -> -1.0000000
30 -1.0000000 -> -1.0000000

```

In this case, two single states still have the same energy levels. This is due to the fact that the two single states belong to two of the one-dimensional irreducible representation which are complex-conjugates with each other. As the eigenvalue problem is the real-valued one, these two eigenvalues should be equal owing to the invariance by the complex conjugation acting on it. It could also be interpreted as of the time-reversal symmetry in the context of the quantum-physics.

LUMO: Without splitting.

```

31 -0.5818861 -> -0.5810887
32 -0.5818861 -> -0.5810887
33 -0.5818861 -> -0.5810887

```

The symmetry reduction from the icosahedral group to one of the subgroup of order 24 can be realized clearly, as supposed in this computation. On the other hand, the difference between the icosahedral group and the maximal subgroup AS[163] (the 5-th alternating group: A5) is more subtle. The splitting of the “orbits” by the group action does not occur in the transposition of the bonds between nearest or second-nearest neighbors. The length of the single or double bonds is also unique in A5 symmetry, and the change in the symmetry could be seen in the “orbit” of the bonds among more distant neighbors. Take the bond of [1,11].

```

gap> lg:=List(Elements(AS[164]),i->OnSets([1,11],i));
[ [ 1, 11 ], [ 1, 26 ], [ 2, 6 ], [ 2, 16 ], [ 3, 11 ], [ 3, 21 ], [ 4, 16 ],
  [ 4, 26 ], [ 5, 6 ], [ 5, 21 ], [ 6, 30 ], [ 6, 12 ], [ 1, 7 ], [ 7, 49 ],
  [ 8, 30 ], [ 8, 53 ], [ 9, 49 ], [ 9, 12 ], [ 1, 10 ], [ 10, 53 ],

```

```

[ 10, 11 ], [ 11, 17 ], [ 2, 12 ], [ 12, 54 ], [ 10, 13 ], [ 13, 58 ],
[ 14, 54 ], [ 14, 17 ], [ 2, 15 ], [ 15, 58 ], [ 15, 16 ], [ 16, 22 ],
[ 3, 17 ], [ 17, 59 ], [ 15, 18 ], [ 18, 38 ], [ 19, 59 ], [ 19, 22 ],
[ 3, 20 ], [ 20, 38 ], [ 20, 21 ], [ 21, 27 ], [ 4, 22 ], [ 22, 39 ],
[ 20, 23 ], [ 23, 43 ], [ 24, 39 ], [ 24, 27 ], [ 4, 25 ], [ 25, 43 ],
[ 25, 26 ], [ 7, 26 ], [ 5, 27 ], [ 27, 44 ], [ 25, 28 ], [ 28, 48 ],
[ 29, 44 ], [ 7, 29 ], [ 5, 30 ], [ 30, 48 ], [ 31, 41 ], [ 31, 56 ],
[ 32, 36 ], [ 32, 46 ], [ 33, 41 ], [ 33, 51 ], [ 34, 46 ], [ 34, 56 ],
[ 35, 36 ], [ 35, 51 ], [ 36, 60 ], [ 36, 42 ], [ 31, 37 ], [ 19, 37 ],
[ 38, 60 ], [ 23, 38 ], [ 19, 39 ], [ 39, 42 ], [ 31, 40 ], [ 23, 40 ],
[ 40, 41 ], [ 41, 47 ], [ 32, 42 ], [ 24, 42 ], [ 40, 43 ], [ 28, 43 ],
[ 24, 44 ], [ 44, 47 ], [ 32, 45 ], [ 28, 45 ], [ 45, 46 ], [ 46, 52 ],
[ 33, 47 ], [ 29, 47 ], [ 45, 48 ], [ 8, 48 ], [ 29, 49 ], [ 49, 52 ],
[ 33, 50 ], [ 8, 50 ], [ 50, 51 ], [ 51, 57 ], [ 34, 52 ], [ 9, 52 ],
[ 50, 53 ], [ 13, 53 ], [ 9, 54 ], [ 54, 57 ], [ 34, 55 ], [ 13, 55 ],
[ 55, 56 ], [ 37, 56 ], [ 35, 57 ], [ 14, 57 ], [ 55, 58 ], [ 18, 58 ],
[ 14, 59 ], [ 37, 59 ], [ 35, 60 ], [ 18, 60 ] ]

```

On the other hand, the “orbit” by A5 includes only 60 bonds.

```

gap> la5:=List(Elements(AS[163]),i->OnSets([1,11],i));
[ [ 1, 11 ], [ 2, 16 ], [ 3, 21 ], [ 4, 26 ], [ 5, 6 ], [ 6, 30 ], [ 7, 49 ],
[ 8, 53 ], [ 9, 12 ], [ 1, 10 ], [ 10, 11 ], [ 12, 54 ], [ 13, 58 ],
[ 14, 17 ], [ 2, 15 ], [ 15, 16 ], [ 17, 59 ], [ 18, 38 ], [ 19, 22 ],
[ 3, 20 ], [ 20, 21 ], [ 22, 39 ], [ 23, 43 ], [ 24, 27 ], [ 4, 25 ],
[ 25, 26 ], [ 27, 44 ], [ 28, 48 ], [ 7, 29 ], [ 5, 30 ], [ 31, 56 ],
[ 32, 36 ], [ 33, 41 ], [ 34, 46 ], [ 35, 51 ], [ 36, 42 ], [ 31, 37 ],
[ 38, 60 ], [ 19, 39 ], [ 23, 40 ], [ 41, 47 ], [ 32, 42 ], [ 40, 43 ],

```

```
[ 24, 44 ], [ 28, 45 ], [ 46, 52 ], [ 33, 47 ], [ 45, 48 ], [ 29, 49 ],
[ 8, 50 ], [ 51, 57 ], [ 34, 52 ], [ 50, 53 ], [ 9, 54 ], [ 13, 55 ],
[ 37, 56 ], [ 35, 57 ], [ 55, 58 ], [ 14, 59 ], [ 18, 60 ] ]
```

The remaining 60 bonds are located in the separated orbit now.

```
gap> la5_2:=List(Elements(AS[163]),i->OnSets([2,6],i));
[ [ 2, 6 ], [ 3, 11 ], [ 4, 16 ], [ 5, 21 ], [ 1, 26 ], [ 1, 7 ], [ 8, 30 ],
[ 9, 49 ], [ 10, 53 ], [ 6, 12 ], [ 2, 12 ], [ 10, 13 ], [ 14, 54 ],
[ 15, 58 ], [ 11, 17 ], [ 3, 17 ], [ 15, 18 ], [ 19, 59 ], [ 20, 38 ],
[ 16, 22 ], [ 4, 22 ], [ 20, 23 ], [ 24, 39 ], [ 25, 43 ], [ 21, 27 ],
[ 5, 27 ], [ 25, 28 ], [ 29, 44 ], [ 30, 48 ], [ 7, 26 ], [ 35, 36 ],
[ 31, 41 ], [ 32, 46 ], [ 33, 51 ], [ 34, 56 ], [ 31, 40 ], [ 36, 60 ],
[ 19, 37 ], [ 23, 38 ], [ 39, 42 ], [ 32, 45 ], [ 40, 41 ], [ 24, 42 ],
[ 28, 43 ], [ 44, 47 ], [ 33, 50 ], [ 45, 46 ], [ 29, 47 ], [ 8, 48 ],
[ 49, 52 ], [ 34, 55 ], [ 50, 51 ], [ 9, 52 ], [ 13, 53 ], [ 54, 57 ],
[ 35, 60 ], [ 55, 56 ], [ 14, 57 ], [ 18, 58 ], [ 37, 59 ] ]
```

The bonds, equivalent to “[1,11]”, with the unique length in the icosahedral symmetry, are permitted to have two different lengths in the A5 symmetry. The deformation from the icosahedral symmetry to that of A5 is realized not in the bond structures between the nearest or the second-nearest neighbors, but those between remoter atomic sites. By such deformation into A5 symmetry, the two pentagons, located in the antipodes positions, can rotate themselves in the opposite directions with each other.

G. The symmetry in the eigenstates (hidden one)

The irreducible representations of the same dimension show a certain similarity in the icosahedral group. For example, in table XXVI, the representations of I.3 and I.4 or I.5 and I.6 seem to be interchangeable, if we replace $E(5), E(5)^2, E(5)^3, E(5)^4$ among themselves. This suggests a certain kind of affinity of the basis functions of the wave functions. This is a symmetry in the context of the Galois theory, especially of the cyclotomic field, and manifest itself in the secular equation of the energy spectrum.

	CL1	CL2	CL3	CL4	CL5	CL6	CL7	CL8	CL9	CL10
I.3	3	$-E(5)-E(5)^4$	$-E(5)^2-E(5)^3$	0	0	-1	$-E(5)^2-E(5)^3$	3	$-E(5)-E(5)^4$	-1
I.4	3	$-E(5)^2-E(5)^3$	$-E(5)-E(5)^4$	0	0	-1	$-E(5)-E(5)^4$	3	$-E(5)^2-E(5)^3$	-1
I.5	3	$E(5)^2+E(5)^3$	$-E(5)-E(5)^4$	0	0	1	$E(5)+E(5)^4$	-3	$-E(5)^2-E(5)^3$	-1
I.6	3	$E(5)+E(5)^4$	$-E(5)^2-E(5)^3$	0	0	1	$E(5)^2+E(5)^3$	-3	$-E(5)-E(5)^4$	-1

TABLE XXXV. The three dimensional irreducible representations in the icosahedral group.

Let us start again at the model computation of the electronic structure of C_{60} . The eigenvalue problem is solved by one of the functions in the GAP package. By this, the secular equation is decomposed into polynomials with coefficients over the specified field, and the “generalized” eigenstates for these polynomials are obtained. (The eigenvalues are computed as the set of polynomials, each of which has a part of eigenvalues as the roots. The eigenstates of the matrix H are the solutions of the matrix equation $p(H) \cdot x = 0$, where $p(t)$ is one of these polynomials.)

Let “hh” be the Fock matrix, used in the model computation of the electronic structure of C_{60} , with the same parameter as in the previous section. The generators of the group $g1, g2, g3$ are the same as defined previously. The eigenvalue problem is solved now. The last part of the following computation is to extract the basis set of the eigenspaces. (The secular equation is representable as the product of polynomials

equipped the parameter for the transfer integrals. See the appendix G.)

```

Hgen:=function(GP,a)
  local i,h,tuples;
  h:=List([1..60],i->List([1..60],j->0));
  tuples:=Orbit(GP,a,OnTuples);
  for i in tuples
  do
    h[i[1]][i[2]]:=1;
  od;
  return h;
end;

gap> G:=Group(g1,g2,g3);
gap> h1:=Hgen(G,[1,2]);
gap> h2:=Hgen(G,[1,6]);
gap> hh:=-2*h1-h2;
gap> ge:=GeneralizedEigenvalues(Rationals,hh);
[ x_1-3,  x_1+1,  x_1+5,  x_1^2-4*x_1-1,  x_1^2-2*x_1-9,
  x_1^2-2*x_1-5,  x_1^3+3*x_1^2-9*x_1-19,
  x_1^4+6*x_1^3-4*x_1^2-54*x_1-29 ]
gap> gs:=GeneralizedEigenspaces(Rationals,hh);;
gap> gsbas:=List(gs,i->Basis(i));;

```

The eight polynomials of the eigenvalues, decomposed up to the field of rational number are given as the table XXXVI, and The basis vectors in the eigenspace are allotted into the irreducible representations.

No.	Polynomial	Eigenspace dimension	Degeneracy of one eigenvalue	Irreducible representation
1	x_1-3	5	5	I.10
2	x_1+1	5	5	I.10
3	x_1+5	1	1	I.1
4	$x_1^2-4*x_1-1$	6	3	I.3,I.4
5	$x_1^2-2*x_1-9$	8	4	I.8
6	$x_1^2-2*x_1-5$	8	4	I.7
7	$x_1^3+3*x_1^2-9*x_1-19$	15	3	I.9
8	$x_1^4+6*x_1^3-4*x_1^2-54*x_1-29$	12	3	I.5,I.6

TABLE XXXVI. The classification of the solutions of the generalized eigenvalue problem. The irreducible representations are those presented in table XXVI.

The representations of I.3 and I.4 or I.5 and I.6 belong to the same eigenspace, specified by the same polynomial. The automorphism of the cyclotomic field $(E(5)+E(5)^4 \rightarrow E(5)^2 + E(5)^3)$, which forms a group, interchanges these pairs of the irreducible representation, and consequently, also interchanges the vector solutions x of the equation $p(H) \cdot x = 0$. From the viewpoint of the Galois theory, Let us review the situation. Take the last polynomial of the four degrees. The 8-th polynomial in the above table has C_4 as the Galois group,²⁷ and the four roots are transported with each other by the operation of this group(as $1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 1$, by a certain sequential order of the roots.)

Let us represent this Galois group concretely as the operation of the eigenvectors. The polynomial splits in four polynomials of one degree in the 15-th cyclotomic field $\mathbb{Q}_{15}$ (see the remark.²⁶) The generalized eigenvalue problem is solved again in this field, for which $CF(15)$ is the notation in GAP.)

```
gap> ge2:=GeneralizedEigenvalues(CF(15),hh);
[ x_1-3, x_1+1, x_1+5, x_1+(E(5)+3*E(5)^2+3*E(5)^3+E(5)^4),
  x_1+(3*E(5)+E(5)^2+E(5)^3+3*E(5)^4),
  x_1+(E(15)+E(15)^2+E(15)^4+3*E(15)^7+3*E(15)^8+E(15)^11+E(15)^13+E(15)^14),
```

No.	Polynomial	Eigenspace dimension	Irreducible representation
1	x_1-3	5	10
2	x_1+1	5	10
3	x_1+5	1	1
4	$x_1+(E(5)+3E(5)^2+3E(5)^3+E(5)^4)$	3	3
5	$x_1+(3E(5)+E(5)^2+E(5)^3+3E(5)^4)$	3	4
6	$x_1+(E(15)+E(15)^2+E(15)^4+3E(15)^7+3E(15)^8+E(15)^{11}+E(15)^{13}+E(15)^{14})$	3	6
7	$x_1+(E(15)+E(15)^2+3E(15)^4+E(15)^7+E(15)^8+3E(15)^{11}+E(15)^{13}+E(15)^{14})$	3	5
8	$x_1+(E(15)+3E(15)^2+E(15)^4+E(15)^7+E(15)^8+E(15)^{11}+3E(15)^{13}+E(15)^{14})$	3	6
9	$x_1+(3E(15)+E(15)^2+E(15)^4+E(15)^7+E(15)^8+E(15)^{11}+E(15)^{13}+3E(15)^{14})$	3	5
10	$x_1^2-2x_1-9$	8	8
11	$x_1^2-2x_1-5$	8	7
12	$x_1^3+3x_1^2-9x_1-19$	15	9

TABLE XXXVII. The classification of the solutions of the generalized eigenvalue problem in $\mathbb{Q}_{15}$.

$x_1+(E(15)+E(15)^2+3E(15)^4+E(15)^7+E(15)^8+3E(15)^{11}+E(15)^{13}+E(15)^{14})$,
 $x_1+(E(15)+3E(15)^2+E(15)^4+E(15)^7+E(15)^8+E(15)^{11}+3E(15)^{13}+E(15)^{14})$,
 $x_1+(3E(15)+E(15)^2+E(15)^4+E(15)^7+E(15)^8+E(15)^{11}+E(15)^{13}+3E(15)^{14})$,
 $x_1^2-2x_1-9, x_1^2-2x_1-5, x_1^3+3x_1^2-9x_1-19$]

```
gap> gs2:=GeneralizedEigenspaces(CF(15),hh);;
gap> gsbas2:=List(gs2,i->Basis(i));;
```

The Galois group of $\mathbb{Q}_{15}$ is computed as.

```
gap> GaloisGroup(CF(15));
<group with 2 generators>
gap> g:=GaloisGroup(CF(15));
<group with 2 generators>
```

```
gap> g.1;
ANFAutomorphism( CF(15), 11 )
gap> g.2;
ANFAutomorphism( CF(15), 7 )
```

The generator $g.1$ is the map, replacing $E(15) \rightarrow E(15)^{11}$, of order 2, and $g.2$, $E(15) \rightarrow E(15)^7$, of order 4. The latter generator, in table XXXVII, transports the 6-th eigenspace to the 7-th, the 7-th to the 8-th, in turn, and the 10-th to the 6-th, generating the group C_4 (the forth cyclic group.), realizing the Galois group of the polynomial $x_1^4 + 6x_1^3 - 4x_1^2 - 54x_1 - 29$ as the following computation verifies.

```
gap> ge2[6]*ge2[7]*ge2[8]*ge2[9]=ge[8];
true

gap> for j in [1..3] do;
> Print(RootsOfPolynomial(ge2[6])[1]^g.2=RootsOfPolynomial(ge2[7])[1]);
> Print(RootsOfPolynomial(ge2[7])[1]^g.2=RootsOfPolynomial(ge2[8])[1]);
> Print(RootsOfPolynomial(ge2[8])[1]^g.2=RootsOfPolynomial(ge2[9])[1]);
> Print(RootsOfPolynomial(ge2[9])[1]^g.2=RootsOfPolynomial(ge2[6])[1]);
>od;
truetruetruetruetruetruetruetruetruetrue

gap> for j in [1..3] do;
> Print(List(gsbas2[6][j],x->x^g.2)=gsbas2[7][j]);
> Print(List(gsbas2[7][j],x->x^g.2)=gsbas2[8][j]);
> Print(List(gsbas2[8][j],x->x^g.2)=gsbas2[9][j]);
> Print(List(gsbas2[9][j],x->x^g.2)=gsbas2[6][j]);
```


functions are transformed with each other by operations of a group, which is different from that of the structural symmetry of the molecule.

We can approach the hidden symmetry in another direction: there is an automorphism on the icosahedral group which interchanges these two irreducible representations. For simplicity, we reduce the problem in A5. (The icosahedral group is constructed from this by the direct product with the inversion.) The generators of A5 are g1 and g2, (given as the permutations in the previous section.)

```
gap> G:=Group(g1,g2);;
gap> Irr(G);;
```

The character table is as follows (written briefly by a list in GAP).

```
[[ 1, 1, 1, 1, 1 ],
 [ 3, -E(5)-E(5)^4, -E(5)^2-E(5)^3, -1, 0 ],
 [ 3, -E(5)^2-E(5)^3, -E(5)-E(5)^4, -1, 0 ],
 [ 4, -1, -1, 0, 1 ],
 [ 5, 0, 0, 1, -1 ] ]
```

The conjugacy classes are computed now. (As the list of the classes is given as the permutations, it is transformed to the representations by generators, to make the list as brief as possible. The symbols x1 and x2 represent g1 and g2 respectively.)

```
gap> A:=List(ConjugacyClasses(G),Elements);;
gap> B:=List(A,i->List(i,j->Factorization(G,j)));
[ [ <identity ...> ],
  [ x2^-1, x2, x2*x1*x2, x1*x2, x2^2*x1, x2*x1, x2^-1*x1^-1, x2^-2*x1^-1,
    x2^-1*x1^-1*x2^-1, x1^-1*x2^-1, x1*x2^2, x1^-1*x2^-2 ],
  [ x2^-2, x2^2, x2^2*x1*x2^2*x1^-1, x1*x2^2*x1^-1, (x1*x2^2)^2,
```

```

(x2^-1*x1^-1*x2^-1)^2, (x2*x1*x2)^2, x2^-1*x1^-1*x2^-2*x1*x2,
(x2^2*x1)^2, x1^-1*x2^-2*x1, (x2*x1)^2, x2^-1*x1*x2*x1 ],
[ x2^-2*x1*x2, x2^-1*x1, x2*x1^-1, x2^2*x1^-1*x2^-1, x2^2*x1*x2^2,
x1^-1*x2^-2*x1*x2*x1, x1*x2*(x2*x1)^2, (x2*x1*x2)^2*x1,
(x2^2*x1)^2*x2*x1, x2^-1*x1^-1*x2^-2*x1*x2*x1, x2*x1*x2^2*x1^-1,
(x2*x1*x2)^2*x2, (x2^2*x1)^2*x2, x2^-1*x1^-1*x2^-2*x1, x1*x2*x1 ],
[ x2^2*x1*x2, x2^-1*x1*x2, x2^-2*x1, x1, x2^2*x1^-1, x1^-1,
x2^-2*x1^-1*x2^-1, x2*x1^-1*x2^-1, x2^-1*x1^-1*x2^-2, x2*x1*x2^2,
x2^-1*x1^-1*x2^-2*x1^-1, x1^-1*x2^-2*x1^-1, x1^-1*x2^-2*x1^-1*x2^-1,
x1*x2^2*x1^-1*x2^-1, x1*x2^2*x1*x2, x1^-1*x2^-2*x1*x2, x1*x2^2*x1,
x2*x1*x2^2*x1, x2*(x2*x1)^2, x2^-2*x1*x2*x1 ] ]

```

The group of all automorphism is computed as

```
gap> AUALL:=AutomorphismGroup(G);
```

Take first of the generator, AUALL.1.

```

gap> AUALL.1;
[ (1,14,20)(2,15,16)(3,11,17)(4,12,18)(5,13,19)(6,58,22)(7,57,23)
(8,56,24)(9,60,25)(10,59,21)(26,54,38)(27,53,37)(28,52,36)(29,51,40)
(30,55,39)(31,44,50)(32,45,46)(33,41,47)(34,42,48)(35,43,49),
(1,2,3,4,5)(6,11,16,21,26)(7,12,17,22,27)(8,13,18,23,28)(9,14,19,24,29)
(10,15,20,25,30)(31,32,33,34,35)(36,41,46,51,56)(37,42,47,52,57)
(38,43,48,53,58)(39,44,49,54,59)(40,45,50,55,60) ] ->
[ (1,57,45)(2,56,44)(3,60,43)(4,59,42)(5,58,41)(6,55,47)(7,54,46)(8,53,50)
(9,52,49)(10,51,48)(11,35,28)(12,34,29)(13,33,30)(14,32,26)
(15,31,27)(16,37,24)(17,36,25)(18,40,21)(19,39,22)(20,38,23),
(1,59,9,16,55)(2,58,10,17,54)(3,57,6,18,53)(4,56,7,19,52)

```

(5,60,8,20,51)(11,14,12,15,13)(21,35,30,38,50)(22,34,26,37,49)
 (23,33,27,36,48)(24,32,28,40,47)(25,31,29,39,46)(41,44,42,45,43)]

This automorphism maps g1 and g2 in the following way.

```
gap> Factorization(G,Image(AUALL.1,g1));
x2*(x2*x1)^2
gap> Factorization(G,Image(AUALL.1,g2));
x1^-1*x2^-2*x1
```

The two conjugacy classes (of the second and of the third) are interchanged with each other, while the other classes are unchanged. This causes the exchange of the character values and that of the two irreducible representation (of No.2 and No.3). Let us verify this. The image of the automorphism on the elements of the conjugacy class 2 is computed and sorted as

```
gap> imgCl2:=List(A[2], a ->Image(AUALL.1,a));;
gap> SortedList(List(imgCl2,i->Factorization(G,i)));
[ x2^-2, x2^2, x1^-1*x2^-2*x1, x1*x2^2*x1^-1, x2^-1*x1*x2*x1, (x2*x1)^2,
  (x1*x2^2)^2, (x2^-1*x1^-1*x2^-1)^2, x2^-1*x1^-1*x2^-2*x1*x2, (x2*x1*x2)^2,
  x2^2*x1*x2^2*x1^-1, (x2^2*x1)^2 ]
```

The sorted list of the conjugacy class 3 is:

```
gap> SortedList(B[3]);
[ x2^-2, x2^2, x1^-1*x2^-2*x1, x1*x2^2*x1^-1, x2^-1*x1*x2*x1, (x2*x1)^2,
  (x1*x2^2)^2, (x2^-1*x1^-1*x2^-1)^2, x2^-1*x1^-1*x2^-2*x1*x2, (x2*x1*x2)^2,
  x2^2*x1*x2^2*x1^-1, (x2^2*x1)^2 ]
```

These two list are identical. As the automorphism AUALL.1 has the order 2, the conjugacy classes 2 and 3, or the irreducible representation (of No.2 and No.3), are interchanged with each other by this automorphism.

As the each element of the group A5 has a correspondence with one of vertex of the C_{60} molecule, this automorphism can be interpreted as a geometrical operation, that of the replacement of vertex. But this replacement of atoms does not conserve the bonding structure between nearest neighbors. This means that this replacement of atoms is not the symmetry operation on the C_{60} .

H. The super-symmetries

In this section, we will see that we can construct a symmetry higher than the icosahedral one. The icosahedral group is the direct product of A5 and I. If the one of the components, the group A5, is extended to a larger group, the direct product is a super-group of the icosahedral one. The bonding structure of the C_{60} is representable by the pairs of the sequential numbers of the two vertex, and it can be interpreted as the “orbit” of these pairs by the action of the icosahedral group. Then the orbit of the pairs of vertex, generated by the action of this new larger group, provides us with the bonding structure in the higher symmetry. The guiding principle is based the following observation: in the previous section, we have seen the existence of a certain group automorphism which interchanges two of the irreducible representation. If a group, including A5 and this group automorphism, could be constructed, the two three-dimensional irreducible representations will be merged into one. And if a molecule obeys this higher symmetry, the electronic structure will show different features, such as sixfold degeneracies. Now, concerning with the extension of a group, the concept of the semi-direct product (with the automorphism group) is usable.²⁸ For this purpose, we should construct a group composed from

all of the automorphisms on the group A5. Taking this automorphism group or its subgroups, we can construct the semi-direct product with the group A5. The necessary computation is executed in the following way. As the full automorphism group of A5 is too large, we take a small subgroup of this (a subgroup generated by one of the generators of this group).

```
gap> G:=Group(g1,g2);
gap> AUALL:=AutomorphismGroup(G);
gap> p:=SemidirectProduct(Group(AUALL.1),G);
```

The newly created group “p” is larger than A5 (the group “G”), and contains A5 as a subgroup. The three generators are given as

```
gap> p.1;
(3,16,22)(4,17,18)(5,13,19)(6,14,20)(7,15,21)(8,60,24)(9,59,25)(10,58,26)
(11,62,27)(12,61,23)(28,56,40)(29,55,39)(30,54,38)(31,53,42)(32,57,41)
(33,46,52)(34,47,48)(35,43,49)(36,44,50)(37,45,51)
gap> p.2;
(3,7,6,5,4)(8,28,23,18,13)(9,29,24,19,14)(10,30,25,20,15)(11,31,26,21,16)(12,
32,27,22,17)(33,37,36,35,34)(38,58,53,48,43)(39,59,54,49,44)(40,60,55,50,
45)(41,61,56,51,46)(42,62,57,52,47)
gap> p.3;
(1,2)(4,61)(5,11)(6,18)(7,57)(8,21)(9,28)(10,42)(12,46)(13,54)(14,39)
(15,49)(16,59)(17,44)(19,51)(20,26)(22,47)(23,58)(25,34)(27,45)(29,36)
(31,55)(32,43)(33,50)(37,38)(40,48)(41,60)(52,53)
```

The first and the second generators are inherited from A5, and the third is the new one. They are represented by 62 symbols. The symbols from 3 to 62 correspond to the 60 vertexes in one C_{60} . The extension of the group introduces extra symbols “1”

and “2”. We can give a geometrical interpretation to this group in the following way. From the 62 symbols, we can construct a bonding system which contains 120 atoms, located in the double C_{60} molecules. The atoms will be indexed as $[i,j]$ ($i=3,\dots,62$, and $j=1,2$) by the duplication of single C_{60} . This structure (C_{120}) is regulated by the symmetry of the new extended group. The operation p.1 and p.2 are the rotations by 120 and 72 degrees. The operation p.3 interchanges 60 vertexes between two C_{60} shells. To see this, we have only to compute the orbit of the vertex at $[I,J]$ by these operations. The permutation (1,2), applied to the latter element of the pairs, represents the exchange of vertexes between the two C_{60} .

By means of a function defined below, the bonding structure in the this new symmetry can be set up in matrices (of 120×120 dimension). If one bond is bridged between the vertex $[i[1],i[2]]$ and $[i[3],i[4]]$, the corresponding element in the networking matrix is set to be the unity.

```
listforh:=function(A)
  local h,i1,i2,i3,i4,k,l,i;
  h:=List([1..120],i->List([1..120],j->0));
  for i in A do
    i1:=i[1];
    i2:=i[2];
    i3:=i[3];
    i4:=i[4];
    k:=(i1-2)+60*(i2-1);
    l:=(i3-2)+60*(i4-1);
    h[k][l]:=1;
    h[l][k]:=1;
  od;
```

```

return h;
end;

```

The orbits of the double bond [3,1,4,1] (read as from [3,1] to [4,1]), the single bond [3,1,8,1], and the bond between the first and the second C_{60} (such as [3,1,4,2], a possible example, taken par hazard) are computed into the lists “A1”, “B1”, “C1” as bellow. The bonding structures generated from them are represented by three matrices “a1”, “b1”, “c1”.

```

gap> A1:=Orbit(p,[3,1,4,1],OnTuples);
[ [ 3, 1, 4, 1 ], [ 16, 1, 17, 1 ], [ 4, 1, 5, 1 ], [ 3, 2, 61, 2 ],
  [ 22, 1, 18, 1 ], [ 21, 1, 22, 1 ], [ 59, 2, 44, 2 ], [ 17, 1, 13, 1 ],
  [ 5, 1, 6, 1 ], [ 61, 2, 11, 2 ], [ 16, 2, 23, 2 ], [ 4, 2, 41, 2 ],
  ...(omitted hereafter)...
gap> B1:=Orbit(p,[3,1,8,1],OnTuples);
gap> C1:=Orbit(p,[3,1,4,2],OnTuples);
gap> a1:=listforh(A1);
gap> b1:=listforh(B1);
gap> c1:=listforh(C1);

```

In the C_{60} , the symmetry operation of the icosahedral symmetry includes the inversion. The inversion itself is not included in the new group, but we can furnish this operation with first sixty vertex (from the third to the sixty-second) in the same manner as the icosahedral case. And the inversion in the second 60 vertexes can be written in the following way. The second sixty vertex are transported from the first sixty, by the operation $p.3$. If the inversions on the first and second 60 vertexes are denoted as $I1, I2$, they are related by the conjugation $I2 := (p.3) \cdot I1 \cdot (p.3)^{-1}$ (symbolically written here). The inversion on the total system is written by their

union as

$$\begin{pmatrix} I1 & 0 \\ 0 & I2 \end{pmatrix}$$

where the each entry is assumed to be 60×60 dimensional matrix.

The destinations of the vertexes by the inversion “g3” in one C_{60} shell are stored in the list bellow.

```
gap> ListInv:=List([1..60],i->OnPoints(i,g3));
```

The destinations of the vertexes in the first C_{60} shell to the second one, by the operation “p.3”, is stored in the list bellow.

```
gap> mconjg:=List([3..62],i->OnPoints(i,p.3))-2;
```

The inversions in the first and the second C_{60} shell are composed now (as matrices “invrs”, “invrs2”, and by uniting them, the inversion in the full system is computed, as in the matrix “ivfull”).

```
gap> invrs:=List([1..60],i->List([1..60],j->0));
gap> mc:=List([1..60],i->List([1..60],j->0));
gap> for i in [1..60] do
    invrs[i][ListInv[i]]:=1;
    mc[i][mconjg[i]]:=1;
od;
gap> invrs2:=mc*invrs*mc^-1;
gap> ivfull:=List([1..120],i->List([1..120],j->0));
gap> for i in [1..60] do
    for j in [1..60] do
        ivfull[i][j]:=invrs[i][j];
```

```

    ivfull[i+60][j+60]:=invrs2[i][j];
  od;
od;

```

The generators of the group “p”, as the symmetry operations of the 120 atoms, are also represented by matrices. At first we prepare the lists to represent the permutation.

```

gap> l1:=List([1..2],j->List([3..62],i->(OnPoints(i,p.1)+60*(j-1))));
gap> l1:=Flat(l1);
gap> l2:=List([1..2],j->List([3..62],i->(OnPoints(i,p.2)+60*(j-1))));
gap> l2:=Flat(l2);
gap> l3:=List([1..2],j->List([3..62],i->(OnPoints(i,p.3)+60*(OnPoints(j,p.3)-1))));
gap> l3:=Flat(l3);

```

The permutations are transformed to the matrix forms by this function.

```

ListToMat:=function(l)
  local size,h,i,j;
  size:=Size(l);
  h:=List([1..size],i->List([1..size],j->0));
  for i in [1..size] do
    h[i][l[i]]:=1;
  od;
  return h;
end;

```

```

gap> P1:=ListToMat(l1-2);
gap> P2:=ListToMat(l2-2);

```

```
gap> P3:=ListToMat(13-2);
```

We must examine the congruence of the computed data, by checking whether the matrices representing the bonding structure are subject to the symmetry of the extended group. For this purpose, we can compute the commutators between these matrices (“a1”, “b1”, “c1”) and the generators of this group (P1,P2,P3 and ivfull): the results should be zero. The matrices “a1” and “b1” pass the test, but “c1” not. As the matrix “c1” is not conserved by the matrix of the inversion “ivfull” (or not commutable), the symmetrization is necessary for the construction of the Fock matrix. One of the Fock matrix is given as, fixing the values of the transfer integrals,

```
gap> hh:=-2*a1-b1-1/2*(c1+ivfull*c1*ivfull);
```

The generalized eigenvalue problems is solved up to in the field of rational numbers.

```
gap> gev:=GeneralisedEigenvalues(Rationals,hh);
[ x_1-3, x_1+1, x_1+3, x_1+7, x_1^2-4*x_1-13/4, x_1^2-4*x_1-2,
x_1^2-2*x_1-81/4, x_1^2-2*x_1-9/4, x_1^2-12, x_1^2-21/4,
x_1^3+5*x_1^2-4*x_1-24, x_1^4+6*x_1^3-6*x_1^2-60*x_1-36 ]
gap> ges:=GeneralisedEigenspaces(Rationals,hh);
[ <vector space over Rationals, with 10 generators>,
<vector space over Rationals, with 15 generators>,
<vector space over Rationals, with 1 generators>,
<vector space over Rationals, with 1 generators>,
<vector space over Rationals, with 8 generators>,
<vector space over Rationals, with 12 generators>,
<vector space over Rationals, with 8 generators>,
<vector space over Rationals, with 8 generators>,
```

```

<vector space over Rationals, with 10 generators>,
<vector space over Rationals, with 8 generators>,
<vector space over Rationals, with 15 generators>,
<vector space over Rationals, with 24 generators> ]

```

The group is composed and the irreducible representation is computed now.

```

gap> irr:=Irr(Group(P1,P2,P3,ivfull));
[ Character( CharacterTable( <matrix group of size 240 with 4 generators> ),
[ 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1 ] ),
Character( CharacterTable( <matrix group of size 240 with 4 generators> ),
[ 1, -1, -1, -1, -1, -1, 1, 1, 1, 1, 1, 1, 1, -1 ] ),
Character( CharacterTable( <matrix group of size 240 with 4 generators> ),
[ 1, -1, -1, -1, 1, 1, 1, -1, 1, -1, 1, -1, -1, 1 ] ),
Character( CharacterTable( <matrix group of size 240 with 4 generators> ),
[ 1, 1, 1, 1, -1, -1, 1, -1, 1, -1, 1, -1, -1, -1 ] ),
Character( CharacterTable( <matrix group of size 240 with 4 generators> ),
[ 4, -2, 1, 0, 1, -2, 0, -1, -1, 1, 1, 0, 4, 0 ] ),
Character( CharacterTable( <matrix group of size 240 with 4 generators> ),
[ 4, 2, -1, 0, -1, 2, 0, -1, -1, 1, 1, 0, 4, 0 ] ),
Character( CharacterTable( <matrix group of size 240 with 4 generators> ),
[ 4, -2, 1, 0, -1, 2, 0, 1, -1, -1, 1, 0, -4, 0 ] ),
Character( CharacterTable( <matrix group of size 240 with 4 generators> ),
[ 4, 2, -1, 0, 1, -2, 0, 1, -1, -1, 1, 0, -4, 0 ] ),
Character( CharacterTable( <matrix group of size 240 with 4 generators> ),
[ 5, 1, 1, -1, 1, 1, 1, 0, 0, -1, -1, 1, 5, -1 ] ),
Character( CharacterTable( <matrix group of size 240 with 4 generators> ),
[ 5, -1, -1, 1, -1, -1, 1, 0, 0, -1, -1, 1, 5, 1 ] ),

```

```

Character( CharacterTable( <matrix group of size 240 with 4 generators> ),
[ 5, 1, 1, -1, -1, -1, 1, 0, 0, 1, -1, -1, -5, 1 ] ),
Character( CharacterTable( <matrix group of size 240 with 4 generators> ),
[ 5, -1, -1, 1, 1, 1, 1, 0, 0, 1, -1, -1, -5, -1 ] ),
Character( CharacterTable( <matrix group of size 240 with 4 generators> ),
[ 6, 0, 0, 0, 0, 0, 0, -2, 1, 1, 0, 0, -2, 6, 0 ] ),
Character( CharacterTable( <matrix group of size 240 with 4 generators> ),
[ 6, 0, 0, 0, 0, 0, 0, -2, -1, 1, 0, 0, 2, -6, 0 ] ) ]

```

Solution	Representation	Dimension
x_1-3	[11, 12]	5
x_1+1	[10, 11, 12]	5
x_1+3	[2]	1
x_1+7	[1]	1
$x_1^2-4x_1-13/4$	[6]	4
$x_1^2-4x_1-2$	[13]	6
$x_1^2-2x_1-81/4$	[8]	4
$x_1^2-2x_1-9/4$	[7]	4
x_1^2-12	[10]	5
$x_1^2-21/4$	[5]	4
$x_1^3+5x_1^2-4x_1-24$	[9]	5
$x_1^4+6x_1^3-6x_1^2-60x_1-36$	[14]	6

TABLE XXXIX. The correspondence between the solutions of the generalized eigenvalue problem and the irreducible representations. The left column shows the polynomial, the center the corresponding irreducible representation by sequential numbers, and the right the dimension of the irreducible representation.

The four eigenvalues, as the solutions of “ $x_1^4+6x_1^3-6x_1^2-60x_1-36$ ”, composed by the <vector space over Rationals, with 24 generators>, are of the sixfold degeneracies, allotted to the 14th irreducible representation, which we have expected to see in this structure. Although this example is rather an imaginary one, it suggests us the importance of the concept of “group extension” in the

artificial design of the electronic structure in molecular systems of high symmetries. Usually we argue the electronic structure from the viewpoint of the splitting of the degeneracies in accordance with the reduction of the symmetry, but we will be able to proceed in the inverse direction by actually composing the “super-group”.

I. Remarks to this section

In this section, with the viewpoint of the group theory, we analyze the electronic properties of C_{60} . The group theoretical properties of the icosahedral symmetry of C_{60} are computed by a computer algebra program package GAP, and the obtained results are utilized to the analysis. We started at a traditional way in order to classify the eigenstates into irreducible representations. However, the possible applications of the computer algebra are not limited to this sort of the rather classical analysis, since we can construct the group and extract the group theoretical properties more freely and adroitly by the computer algebra than by the utilization of the group theoretical data given in some references. We can construct the all of the subgroups of the icosahedral symmetry. By means of the “orbitals” of the movement of the vertex by the symmetry operations, the correspondence between the subgroup and the possible deformation of the molecule can be established. The change in the energy spectra and the existence of the zero or nonzero transition moments could be discussed qualitatively, without massive computation. Furthermore, through the construction of the semi-direct group of the icosahedral group, the structure equipped with a symmetry higher than that of the icosahedral symmetry, can be generated. The interest with relation to the “molecular design” is as follows: the higher symmetry in the semi-direct product merges some of the irreducible representations into one, and gives rise to a higher degeneracy of the energy spectra. These examples suggest the importance of the group theoretical viewpoint in the material design, re-armored

(or revived) by the modern computational tools, developed as “computer algebra” among mathematicians.

VIII. ANALYSIS OF VIBRATIONAL MODE IN C_{60}

In this section, the computation of the vibrational modes of the C_{60} by means of the computer algebra is demonstrated. The C_{60} molecule has the unique symmetry, comparable to one soccer-ball (see Fig. 6). The symmetry of the molecule is described by the icosahedral group, and this group is represented by the permutation of 60 vertexes or the group of rotation matrices operating on them. Owing to this high symmetry, the molecule shows peculiar electronic and dynamic properties, both of scientific and industrial interest, and the vibrational mode might be one of the principal phenomena in governing the quantum dynamics in it. As a tool of the computation, we utilize the software GAP, developed in the field of the pure mathematics¹². This software can construct the symmetry group and compute the irreducible representations and other group-theoretical properties and enable us to put into practice the application in the material science, possibly in a modernized way. The computation presented hereafter will be useful to the working physicists and the students, who want to deepen the understanding of the group theory that are given in the textbooks^{2,4,5,8,9}.

A. The vibrational modes of C_{60}

The atoms and the pentagons in the molecule are provided with sequential numbers as in Fig. 7 in the preceding section. The symmetry operations on the spatial vectors on the vertexes of C_{60} are made by the direct products of the two types of matrices. The first type R_i represents the replacement of 60 vertexes and the

second type G_i the rotation and the reflection of the spatial vectors. The symmetry operations on the spatial vectors placed into 60 vertexes are represented as this:

$$O_i = R_i^f \otimes G_i, \quad (86)$$

where R_i and G_i should represent the equivalent operation, and the superscript f is the group automorphism in the group R . The matrices generates the icosahedral group, and the trace of O_i provides us with the trace representation $\chi^{tr}(O_i)$ (not irreducible). The decomposition of the trace representation by means of the irreducible representations indicates the distinct modes of the vibration, and the projection operators composed by O_i can generate the basis vectors for them. And to obtain the vibrational mode, the degrees of the freedoms of the translation and the rotation of the molecule should be removed:

$$\chi^{tr} - \chi^{Trans} - \chi^{Rot}. \quad (87)$$

The presence of the automorphism f is inevitable. Consider the operation $r = (1, 2, 3, 4, 5) \cdots (\cdots)$. This operation, as the rotation G , acts on the dislocated vertexes ($V([j] \rightarrow V[j] + d[j])$):

$$\begin{aligned} G(V[1] + d[1]) &= V[2] + G \cdot d[1] \\ G(V[2] + d[2]) &= V[3] + G \cdot d[2] \\ G(V[3] + d[3]) &= V[4] + G \cdot d[3] \\ G(V[4] + d[4]) &= V[5] + G \cdot d[4] \\ G(V[5] + d[5]) &= V[1] + G \cdot d[5] \\ &\dots\dots\dots \end{aligned}$$

The operation on $d[i]$ should be represented as

$$\begin{pmatrix} 0 & 0 & 0 & 0 & G & \cdots \\ G & 0 & 0 & 0 & 0 & \cdots \\ 0 & G & 0 & 0 & 0 & \cdots \\ 0 & 0 & G & 0 & 0 & \cdots \\ 0 & 0 & 0 & G & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} d[1] \\ d[2] \\ d[3] \\ d[4] \\ d[5] \\ \vdots \end{pmatrix}$$

so that the rotation to $d[j]$ should be located at the correct position, while the permutation r is represented in the form which is the transposition of that operation:

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 1 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 1 & \cdots \\ 1 & 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

It happens that the permutation r should act on $d[j]$ as its transposition, or its inverse. And the product of the operations is given by $(R_1, G_1) \circ (R_2, G_2) = (R_2 \cdot R_1, G_1 \cdot G_2)$, with inverse directions for R_i and G_i . This observation shows the inadequacy of the simple definition of the direct product $R_i \otimes G_i$ as the symmetry operation. However, the naive redefinition, such as $R_i^{-1} \otimes G_i$ for all i , does not work well. Now we can make use the fact the conjugation ($A \rightarrow M \cdot A \cdot M^{-1}$) is an automorphism which preserves the sequential order of the group multiplication; we should find the elements which inverts the generators of the group by the conjugation in order to define the exact symmetry operations, the products of which go from

right to left both for R_i^f and G_i . Indeed this can be done in the final stage of the computation. So, before stepping into it, let us execute the naive computation (with the direct product $R_i \otimes G_j$). Concerning with the dimension counting of the basis set, such a computation does not fail.

The icosahedral group is defined in several ways. We prepare the twelve points, located at the centers of the pentagons in the molecule (or the vertexes in the icosahedron) as follows. $E(5)$ is the fifth root of the unity, $\exp(2\pi i/5)$, and the symbolically presented data are all real. (The data and results are given by the expressions in GAP.)

- 1 $[0, 0, 1],$
- 2 $[2/5 * E(5) - 2/5 * E(5)^2 - 2/5 * E(5)^3 + 2/5 * E(5)^4,$
 $0,$
 $1/5 * E(5) - 1/5 * E(5)^2 - 1/5 * E(5)^3 + 1/5 * E(5)^4],$
- 3 $[-3/5 * E(5) - 2/5 * E(5)^2 - 2/5 * E(5)^3 - 3/5 * E(5)^4,$
 $1/5 * E(20) - 1/5 * E(20)^9 - 2/5 * E(20)^{13} + 2/5 * E(20)^{17},$
 $1/5 * E(5) - 1/5 * E(5)^2 - 1/5 * E(5)^3 + 1/5 * E(5)^4],$
- 4 $[2/5 * E(5) + 3/5 * E(5)^2 + 3/5 * E(5)^3 + 2/5 * E(5)^4,$
 $2/5 * E(20) - 2/5 * E(20)^9 + 1/5 * E(20)^{13} - 1/5 * E(20)^{17},$
 $1/5 * E(5) - 1/5 * E(5)^2 - 1/5 * E(5)^3 + 1/5 * E(5)^4],$
- 5 $[2/5 * E(5) + 3/5 * E(5)^2 + 3/5 * E(5)^3 + 2/5 * E(5)^4,$
 $-2/5 * E(20) + 2/5 * E(20)^9 - 1/5 * E(20)^{13} + 1/5 * E(20)^{17},$
 $1/5 * E(5) - 1/5 * E(5)^2 - 1/5 * E(5)^3 + 1/5 * E(5)^4],$
- 6 $[-3/5 * E(5) - 2/5 * E(5)^2 - 2/5 * E(5)^3 - 3/5 * E(5)^4,$
 $-1/5 * E(20) + 1/5 * E(20)^9 + 2/5 * E(20)^{13} - 2/5 * E(20)^{17},$
 $1/5 * E(5) - 1/5 * E(5)^2 - 1/5 * E(5)^3 + 1/5 * E(5)^4],$
- 7 $[0, 0, -1],$

- 8 $[-2/5 * E(5) + 2/5 * E(5)^2 + 2/5 * E(5)^3 - 2/5 * E(5)^4,$
 $0,$
 $-1/5 * E(5) + 1/5 * E(5)^2 + 1/5 * E(5)^3 - 1/5 * E(5)^4],$
- 9 $[3/5 * E(5) + 2/5 * E(5)^2 + 2/5 * E(5)^3 + 3/5 * E(5)^4,$
 $-1/5 * E(20) + 1/5 * E(20)^9 + 2/5 * E(20)^{13} - 2/5 * E(20)^{17},$
 $-1/5 * E(5) + 1/5 * E(5)^2 + 1/5 * E(5)^3 - 1/5 * E(5)^4],$
- 10 $[-2/5 * E(5) - 3/5 * E(5)^2 - 3/5 * E(5)^3 - 2/5 * E(5)^4,$
 $-2/5 * E(20) + 2/5 * E(20)^9 - 1/5 * E(20)^{13} + 1/5 * E(20)^{17},$
 $-1/5 * E(5) + 1/5 * E(5)^2 + 1/5 * E(5)^3 - 1/5 * E(5)^4],$
- 11 $[-2/5 * E(5) - 3/5 * E(5)^2 - 3/5 * E(5)^3 - 2/5 * E(5)^4,$
 $2/5 * E(20) - 2/5 * E(20)^9 + 1/5 * E(20)^{13} - 1/5 * E(20)^{17},$
 $-1/5 * E(5) + 1/5 * E(5)^2 + 1/5 * E(5)^3 - 1/5 * E(5)^4],$
- 12 $[3/5 * E(5) + 2/5 * E(5)^2 + 2/5 * E(5)^3 + 3/5 * E(5)^4,$
 $1/5 * E(20) - 1/5 * E(20)^9 - 2/5 * E(20)^{13} + 2/5 * E(20)^{17},$
 $-1/5 * E(5) + 1/5 * E(5)^2 + 1/5 * E(5)^3 - 1/5 * E(5)^4]$

These twelve points are transported among themselves by these three operations $(g1, g2, g3)$. The three operations $(g1, g2, g3)$ induces the three permutations $(f1, f2, f3)$ on the 12 vertexes of the icosahedron, and $(r1, r2, r3)$ on 60 vertexes in the C_{60} .

```
gap> g1:= [ [ 3/10 * E(5) + 1/5 * E(5)^2 + 1/5 * E(5)^3 + 3/10 * E(5)^4,
-1/10 * E(20) + 1/10 * E(20)^9 + 1/5 * E(20)^{13} - 1/5 * E(20)^{17},
2/5 * E(5) - 2/5 * E(5)^2 - 2/5 * E(5)^3 + 2/5 * E(5)^4 ],
[ 1/2 * E(20) - 1/2 * E(20)^9, -1/2 * E(5) - 1/2 * E(5)^4, 0 ],
[ -3/5 * E(5) - 2/5 * E(5)^2 - 2/5 * E(5)^3 - 3/5 * E(5)^4,
1/5 * E(20) - 1/5 * E(20)^9 - 2/5 * E(20)^{13} + 2/5 * E(20)^{17},
1/5 * E(5) - 1/5 * E(5)^2 - 1/5 * E(5)^3 + 1/5 * E(5)^4 ] ];
```

```
gap> g2:=[ [ 1/2*E(5)+1/2*E(5)^4, 1/2*E(20)-1/2*E(20)^9, 0 ],
[ -1/2*E(20)+1/2*E(20)^9, 1/2*E(5)+1/2*E(5)^4, 0 ], [ 0, 0, 1 ] ];
```

```
gap> g3:=[ [ -1, 0, 0 ], [ 0, -1, 0 ], [ 0, 0, -1 ] ];
```

```
gap> G:=Group(g1,g2,g3);
```

```
gap> f1:=(1,2,3)(4,6,11)(5,10,12)(7,8,9);
```

```
gap> f2:=(2,3,4,5,6)(8,9,10,11,12);
```

```
gap> f3:=(1,7)(2,8)(3,9)(4,10)(5,11)(6,12);
```

```
gap> F:=Group(f1,f2,f3);
```

```
gap> r1:=( 1, 14, 20)( 2, 15, 16)( 3, 11, 17)( 4, 12, 18)( 5, 13, 19)
( 6, 58, 22)( 7, 57, 23)( 8, 56, 24)( 9, 60, 25)( 10, 59, 21)
( 31, 44, 50)( 32, 45, 46)( 33, 41, 47)( 34, 42, 48)( 35, 43, 49)
( 36, 28, 52)( 37, 27, 53)( 38, 26, 54)( 39, 30, 55)( 40, 29, 51);
```

```
gap> r2:=( 1, 2, 3, 4, 5)( 6, 11, 16, 21, 26)( 7, 12, 17, 22, 27)
( 8, 13, 18, 23, 28)( 9, 14, 19, 24, 29)( 10, 15, 20, 25, 30)( 31, 32, 33, 34, 35)
( 36, 41, 46, 51, 56)( 37, 42, 47, 52, 57)( 38, 43, 48, 53, 58)( 39, 44, 49, 54, 59)
( 40, 45, 50, 55, 60);
```

```
gap> r3:=( 1, 31)( 2, 32)( 3, 33)( 4, 34)( 5, 35)( 6, 36)( 7, 37)( 8, 38)
( 9, 39)( 10, 40)( 11, 41)( 12, 42)( 13, 43)( 14, 44)( 15, 45)( 16, 46)( 17, 47)
( 18, 48)( 19, 49)( 20, 50)( 21, 51)( 22, 52)( 23, 53)( 24, 54)( 25, 55)( 26, 56)
( 27, 57)( 28, 58)( 29, 59)( 30, 60);
```

```
gap> R:=Group(r1,r2,r3);
```

```
gap> Irr(R);
```

The command “Irr(R)” returns the character table of R, a part of which is listed in table XL:

Rep	Dim	[f1,f2,f3]	
N.1	1	[1, 1, 1]	A_g
N.2	1	[1, 1, -1]	A_u
N.3	3	[0, -E(5)-E(5)^4, 3]	F_{2g}
N.4	3	[0, -E(5)^2-E(5)^3, 3]	F_{1g}
N.5	3	[0, -E(5)-E(5)^4, -3]	F_{2u}
N.6	3	[0, -E(5)^2-E(5)^3, -3]	F_{1u}
N.7	4	[1, -1, 4]	H_g
N.8	4	[1, -1, -4]	H_u
N.9	5	[-1, 0, 5]	G_g
N.10	5	[-1, 0, -5]	G_u

TABLE XL. The characters of the generators in ten irreducible representations of the icosahedral group.

We use the group R as the standard. The isomorphism from R to G is set up at the three generators (from [R.1,R.2,R.3] to [G.1,G.2,G.3].)

```
gap> hom:=GroupHomomorphismByImages(R,G,[R.1,R.2,R.3],[G.1,G.2,G.3]);
```

It is necessary to judge the irreducible representations to which the translation belongs. The projectors (applicable to three-dimensional spatial vectors) are computed now for this purpose. They are defined as

$$P^{(p)} = \frac{l(p)}{|G|} \sum_{T \in G} \chi^{(p)*}(T) \cdot O(T)$$

by summing up the elements T of the group G , where $l(p)$ is the dimension of the p -th irreducible representation, $|G|$ the order of the group, $\chi(p)$ the character, $O(T)$ the operation of the group. The gap script is given as³⁰:

```

Projopr:=function(irr,Em,hom)
#
# irr:Irreducible representation of the group.
# Em :Elements in the group.
# hom:Homomorphism of the permutation group to the matrix group
#
return List(irr,i->Sum(List(Em,j->j^i*Image(hom,j)))/Size(Em)*i[1]);
end;

```

The result is given in table XLI. The non-zero one exists only in the representation N.6, so we conclude the spatial translation belongs to this representation.

	Operator
N.1	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
N.2	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
N.3	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
N.4	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
N.5	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
N.6	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
N.7	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
N.8	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
N.9	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
N.10	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$

TABLE XLI. The projection operators for the spatial vectors.

There is another necessity to judge the representation of the spatial rotations. The group operation T on the rotation matrix M is defined as the product from both sides, $T \cdot M \cdot T^t$. This operation should be treated with care. This product is also a rotation matrix, but the summation of such products not. Thus the projection operator defined as above will not generate the proper rotation matrix, if it is naively applied to the rotation matrices. Concerning this, the exponential map is useful,

which is defined as

$$M = \exp(A),$$

$$T \cdot M \cdot T^t = \exp(T \cdot A \cdot T^t).$$

The pre-image A of the rotation M is the skew-symmetric matrix. The projection operator should be applied to the linear space of these pre-images. The gap computation for the determination of the irreducible representation is now presented. The projectors are computed by the formula

$$P^{(p)}(A) = \frac{l(p)}{|G|} \sum_{T \in G} \chi^{(p)*}(T) T \cdot A \cdot T^t$$

by means of the function

```
ProjoprR:=function(irr,Em,MM,hom)
  return List(irr,i->Sum(List(Em,j->j^i*Image(hom,j)
    *MM*TransposedMat(Image(hom,j))))/Size(Em)*i[1]);
end;
```

The computation is done now.

```
gap> x:=Indeterminate(Rationals,"x");
gap> y:=Indeterminate(Rationals,"y");
gap> z:=Indeterminate(Rationals,"z");
gap> MM:=[[0*x,x,y],[-x,0*x,z],[-y,-z,0*x]];
gap> ProjoprR(Irr(R),Elements(R),MM,hom);
```

(See the remark²⁹.)

The non-zero projector is the forth one. The spatial rotations belongs to the fourth representation (N.4)³¹.

	Operator
N.1	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
N.2	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
N.3	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
N.4	$\begin{bmatrix} 0 & x & y \\ -x & 0 & z \\ -y & -z & 0 \end{bmatrix}$
N.5	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
N.6	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
N.7	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
N.8	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
N.9	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
N.10	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$

TABLE XLII. The projection operators for the rotations.

Now we construct the symmetry operation ($O_i = R_i \otimes G_i$) on the spatial vectors on the 60 vertexes. The following function converts a permutation R_i to an integer matrix which represents the replacement of vertexes.

```
ListToMat:=function(l)
  local size,h,i,j;
  size:=Size(l);
  h:=List([1..size],i->List([1..size],j->0));
  for i in [1..size] do
    h[i][l[i]]:=1;
  od;
  return h;
end;
```

The following function constructs the direct product of R_i and G_i . The isomorphism “iso” from the group R to G convert an element “rr” (in R) to the equivalence in G exactly. In the generated matrix, the non-zero entries in R_i are replaced by G_i

(the rotation), as this.

$$R_i = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 1 & 0 & 0 & \cdots & 0 \\ \vdots & & & & \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix} \rightarrow R_i \otimes G_i = \begin{pmatrix} 0 & G_i & 0 & \cdots & 0 \\ G_i & 0 & 0 & \cdots & 0 \\ \vdots & & & & \vdots \\ 0 & 0 & 0 & \cdots & G_i \end{pmatrix}$$

```

LargeMatrix:=function(rr,iso)
  local l,rmat,rrimg,i,i1,i2,n,m;
  l:=ListPerm(rr,60);
  rmat:=List([1..Size(l)*3],i->List([1..Size(l)*3],j->0));
  rrimg:=Image(iso,rr);
  for i in [1..Size(l)]
  do
    i1:=i-1;i2:=l[i]-1;
    for n in [1..3]
    do
      for m in [1..3]
      do
        rmat[3*i1+n][3*i2+m]:=rrimg[n][m];
      od;
    od;
  od;
  return rmat;
end;

```

The projector function, composed from the direct product, is defined as:

```

ProjoprE:=function(irr,Em,hom2)

```

```

#
# irr:Irreducible representation.
# Em :Elements of the group R.
# hom:Isomorphism from the group R to the group G.
#
return List(irr,i->Sum(List(Em,j->j^i*LargeMatrix(j,hom2)))/Size(Em)*i[1]);
end;

```

We can compute now the basis set of the mode of deformation³². The projectors are placed in the list of ten matrices (of dimension 180) (PRJE[1]...PRJE[10]), and each of them does the projection on each irreducible representations (N.1...N.10). The basis vectors for the each vibrational mode are generated from the column vectors of the corresponding projector. In the computation the list “BASSIZE” gives us the dimensions of each modes.

```

gap> PRJE:=ProjoprE(Irr(R),Elements(R),hom2);;
gap> BAS:=List(PRJE,i->BaseMat(TransposedMat(i))));;
gap> BASSIZE:=List(BAS,Size);
[ 2, 1, 12, 12, 15, 15, 24, 24, 40, 35 ]
gap> BAS;
[ [ [ 1, E(20)-E(20)^9+E(20)^13-E(20)^17, 0, 2*E(5)+E(5)^2+E(5)^3+2*E(5)^4,
      -E(20)^13+E(20)^17, 0, -2*E(5)-2*E(5)^4, 0, 0,
      2*E(5)+E(5)^2+E(5)^3+2*E(5)^4, E(20)^13-E(20)^17, 0, 1,
      -E(20)+E(20)^9-E(20)^13+E(20)^17, 0,
      -1/5*E(5)+1/5*E(5)^2+1/5*E(5)^3-1/5*E(5)^4,
      1/5*E(20)-1/5*E(20)^9+3/5*E(20)^13-3/5*E(20)^17,
      12/5*E(5)+8/5*E(5)^2+8/5*E(5)^3+12/5*E(5)^4,
      -6/5*E(5)-4/5*E(5)^2-4/5*E(5)^3-6/5*E(5)^4,

```

.....
.....

At present projectors “PRJE[i]” are defined by the “bare” forms, using the direct product $R_i \otimes G_i$. and they should be modified to the correct ones, such as $M_f \cdot \text{PRJE}[i] \cdot M_f^{-1}$, composed by the direct product $R_i^f \otimes G_i$, where f is a conjugation which inverts the generators of the permutation group R . There are two candidates for such automorphisms.

```
gap> RPC:=Filtered(Elements(R),x->List([R.1,R.2,R.3],i->i^x)=[R.1^-1,R.2^-1,R.3^-1])
[ (1,4)(2,3)(6,21)(7,25)(8,24)(9,23)(10,22)(11,16)(12,20)(13,19)(14,18)(15,
  17)(27,30)(28,29)(31,34)(32,33)(36,51)(37,55)(38,54)(39,53)(40,52)(41,
  46)(42,50)(43,49)(44,48)(45,47)(57,60)(58,59),
  (1,34)(2,33)(3,32)(4,31)(5,35)(6,51)(7,55)(8,54)(9,53)(10,52)(11,46)(12,
  50)(13,49)(14,48)(15,47)(16,41)(17,45)(18,44)(19,43)(20,42)(21,36)(22,
  40)(23,39)(24,38)(25,37)(26,56)(27,60)(28,59)(29,58)(30,57) ]
gap> RPC[1]*r3=RPC[2];
true
```

The conjugation is computed as a matrix through this function.

```
ConjugMatrix:=function(rr)
  local l,rmat,vmat,i,i1,i2,n,m;
  l:=ListPerm(rr,60);
  vmat:=List([1..Size(l)*3],i->List([1..Size(l)*3],j->0));
  for i in [1..Size(l)]
  do
    i1:=i-1;i2:=l[i]-1;
    for n in [1..3]
```

```

do
  vmat[3*i1+n][3*i2+n]:=1;
od;
od;
return vmat;
end;

gap> PCM:=ConjugMatrix(RPC[1]);
gap> PRJEC:=List(PRJE,i->i^PCM);;
gap> BASC:=List(PRJEC,i->BaseMat(TransposedMat(i)));;
gap> BASCSIZE:=List(BASC,Size);
[ 2, 1, 12, 12, 15, 15, 24, 24, 40, 35 ]

```

In fact, in order to obtain the correct vibrational modes, it is enough to multiply the matrix “PCM” for the conjugation to the basis vectors “BAS” computed by the bare projectors. If we neglect such corrections, it happens that the “breathing mode” would not belong to the trivial representation.

To check the validity, the characters of χ^{Tr} and those by the irreducible representations are computed in the two lists “CTRC” and “CIRR”. The irreducible representation of χ^{Vec} is located at the sixth component of CIRR, and that of χ^{Rot} is at the fourth.

```

CTRC:=List(Elements(R),i->Trace(ListToMat(ListPerm(i,60))));
CIRR:=List(Irr(R),r->List(Elements(R),i->i^r));

```

The $\chi^{Tr} \times \chi^{Vec}$ is computed and decomposed.

```

gap> List([1..Size(R)],i->CTRC[i]*CIRR[6][i])*TransposedMat(CIRR)/Size(R);
[ 2, 1, 4, 4, 5, 5, 6, 6, 8, 7 ]

```

```
gap> List([1..10], i->BASSIZE[i]/Irr(R)[i][1]);
[ 2, 1, 4, 4, 5, 5, 6, 6, 8, 7 ]
```

These results are the multiplicities to each irreducible representation (in theory and in computation) and shows the validity of the computation. The direct product of the characters (i.e. the vibrational mode plus extra terms) is decomposed as

$$\chi^{tr} \times \chi^{Vec} = 2 \cdot N.1 + 1 \cdot N.2 + 4 \cdot N.3 + 4 \cdot N.4 + 5 \cdot N.5 + 5 \cdot N.6 + 6 \cdot N.7 + 6 \cdot N.8 + 8 \cdot N.9 + 7 \cdot N.10.$$

B. One technical problem

The modes of vibrations are decomposed into irreducible representations, some of which appear with multiplicities. Take one of the basis vectors, computed in the previous section, and apply the symmetry operations on it: for example, one of those which belong to the tenth irreducible representation. In the following computation the two lists “EMR” and “AR” contains the group elements in R and the whole of the symmetry operation, “vs” is the set of the generated vectors, “vsb”, the basis set to it, and the command RankMat(...) computes the dimension of the vector space.

```
gap> EMR:=Elements(R) ;;
gap> AR:=List(Elements(R), j->LargeMatrix(j, hom2));;
gap> vs:=List(AR, x->x*BAS[10][1]);
gab> vsb:=Basemat(vs);
gap> RankMat(vsb);
25
```

The chosen vector generates the vector space of dimension 25 by the symmetry operation³³. But the tenth irreducible representation is of dimension 5. The generated vectors span the copies of this irreducible space, not confined to one of them.

For the practical purpose, we should remove the degrees of freedoms which correspond to those of the translation and the rotation. And it is enough to the reset the dislocated origin or the disorientated axes at the proper positions when we make the structures altered by vibrations. Thus the technical problem of this kind might not be of importance. However, we can divide the multiplied irreducible spaces, so that the each component is proper minimal one, separated with each other, kept invariant under the symmetry operation. In this section two kinds of such constructions are demonstrated.

The first is to use the projectors composed from matrix representations $D_{kl}^{(p)}(O_T)$, not from characters, as was explained in the previous section. The formula is given again:

$$P_{kl}^{(p)} = \frac{l_p}{|G|} \sum_{T \in G} D_{kl}^{(p)*}(O_T) \cdot O_T.$$

The basis vectors are transformed by the matrix representation, forming the subspace which has the proper dimension of the irreducible representation. We can make the plural irreducible spaces from the column vectors of the projector one of the $P_{kk}^{(p)}$, the diagonal part of the projectors. Unfortunately, even in this construction, the generated irreducible spaces overlap with each other, not being separated. Thus we should make the separation, projecting out overlapping subspaces. At first the matrix representation is computed in the following way. (The GAP, in each run, returns the different results concerning with the matrix representation, since we can determine them up to the isomorphism, but not furthermore; there are plural possibilities.)

```
gap> irrR:=Irr(R);;
gap> irrRM:=IrreducibleRepresentations(R);;
gap> EMR:=Elements(R);;
gap> AM:=List(EMR,j->LargeMatrix(j,hom2));;
```

The projector $P_{ij}^{(p)}$ is defined as a function

```
PRJR:=function(i,j,p)
  local C,REP,dim;
  REP:=irrRM[p];
  dim:=Trace(())^REP);
  C:=List([1..Size(AM)],k->AsList(EMR[k]^REP)[i][j]*AM[k]);
  return ComplexConjugate(Sum(C))/Size(AM)*dim;
end;
```

Take the $P_{1,1}^{(10)}$ component of the projector. The basis vectors are generated from column vectors of this. As the GAP software defines the vector set by row vectors, The basis sets are computed from the transposed matrix. The basis set of the vector space is listed in “vtb”. The projectors $P_{1,1}^{(10)}, \dots, P_{5,1}^{(10)}$ are stored now for the afterward usage.

```
gap> vt:=TransposedMat(PRJR(1,1,10));;
gap> vtb:=BaseMat(vt);;
gap> PRJRS:=List([1..5],i->PRJR(i,1,10));;
```

The validity of the transformation of the partner functions is checked now.

```
gap> PRJR(2,2,10)*PRJR(2,1,10)*vtb[1]=PRJR(2,1,10)*vtb[1];
true
```

Each of the basis vector x generates the five-dimensional, irreducible vector spaces under the symmetry operation, and the vector space is composed of $P_{1,1}^{(10)} \cdot x, \dots, P_{5,1}^{(10)} \cdot x$. In the following computations, the irreducible vector space for each of basis vector is stored in the list “zz” (in the seven component $zz[1], \dots, zz[7]$). However, these irreducible spaces are overlapped with each other. The computations of the inner products show this³⁴.

```

gap> zz:=List(vtb,y->List(List([1..5],i->PRJRS[i]*y))));
gap> List(zz,a->List(zz,b->RankMat(a*TransposedMat(b))));
[ [ 5, 0, 5, 0, 0, 0, 0 ], [ 0, 5, 0, 0, 0, 0, 0 ], [ 5, 0, 5, 5, 0, 0, 0 ],
  [ 0, 0, 5, 5, 0, 5, 0 ], [ 0, 0, 0, 0, 5, 0, 0 ], [ 0, 0, 0, 5, 0, 5, 5 ],
  [ 0, 0, 0, 0, 0, 5, 5 ] ]

```

We now project out the overlapping between irreducible subspaces. We start from the one of the irreducible space, say $zz[1]$, and construct the orthogonal space to it. One of the basis vector in the latter space, if the projector $P_{1,1}^{(10)}$ is applied to it, belongs to the irreducible space invariant by $P_{1,1}^{(10)}$. This vector is chosen as the generator of another irreducible space. Similarly we construct the orthogonal space to the set of the irreducible spaces obtained until now, from this we extract the generator of another irreducible space, and proceed so on.

```

gap> B:=ShallowCopy(zz[1]);
gap> D:=[ShallowCopy(zz[1])];
gap> for n in [2..Size(zz)]
do
  OV:=BaseOrthogonalSpaceMat(B);
  xx:=BaseMat(List(OV,x->PRJRS[1]*x))[1];
  vv:=List(List([1..5],i->PRJRS[i]*xx));
  Append(B,vv);
  Append(D,[vv]);
od;

```

We generated seven separated irreducible spaces; let us check this:

```

gap> List(D,a->List(D,b->RankMat(a*TransposedMat(b))));
[ [ 5, 0, 0, 0, 0, 0, 0 ], [ 0, 5, 0, 0, 0, 0, 0 ], [ 0, 0, 5, 0, 0, 0, 0 ],

```

```
[ 0, 0, 0, 5, 0, 0, 0 ], [ 0, 0, 0, 0, 5, 0, 0 ], [ 0, 0, 0, 0, 0, 5, 0 ],
[ 0, 0, 0, 0, 0, 0, 5 ] ]
```

The vector space generated by the symmetry operations from one of the separated irreducible spaces should be orthogonal to others; let us check this:

```
gap> OO:=List(AM,o->o*D[1][1]);;
gap> List(D,d->RankMat(OO*TransposedMat(d)));
[ 5, 0, 0, 0, 0, 0, 0 ]
gap> OO:=List(AM,o->o*D[2][1]);;
gap> List(D,d->RankMat(OO*TransposedMat(d)));
[ 0, 5, 0, 0, 0, 0, 0 ]
. . . etc . . .
```

We can see that all is done well.

The second method is to divide the multiplied irreducible spaces W (as computed in the previous section, by the projectors defined by the characters) into proper minimal components, invariant under the symmetry operation. This method utilizes the coset decomposition of the group G by the subgroup H , G/H . In general, one vector v_1 in W , under the operation of the elements g_i in G , generates the set of vectors, the total number of which is equal to the order of G . Now let us take another vector w_1 , also in W , generated by the operation on the elements h_i in H , such as $w_1 = \sum_i h_i \cdot v_1$. Under the symmetry operation of G , it generates the set of vectors, the total number of which is equal to the order of G/H . The number of the generated vectors decreased in the latter case. We might expect the dimension of the basis vectors of the generated vectors would also be diminished in the latter case. And if w_1 would generate the vector space of the proper dimension of the irreducible representation, we adopt it, as the generator of the separated, proper, irreducible space. (If not, with another chose of H , this step is repeated.) Then we

project out the vector space generated by w_1 from W . We take another vector v_2 from W , make a H -invariant vector w_2 with the suitable H (if necessary, H should be chosen again) to generate the another proper irreducible space. We proceed so on until W is exhausted. This method will be applicable to the present problem in order to separate each irreducible component, even if it involves the trial-and-error, in the choice of the suitable subgroup H . At the start, the vector v_1 is taken from the multiplied irreducible spaces. The candidate vector w_i is generated by the projection of v_i into the trivial irreducible representation of the subgroup H . (Indeed, it could also be prepared by the projection of v into other irreducible representations of H , for the purpose of diminishing the number of the generated vectors by the symmetry operation.)

In order to execute this computation, the following function is prepared. The function tries to find the irreducible subspace of dimension “REPSIZ” in the operation of the group “R”. The function cuts out the subspace (as minimal as possible) from the given vector space, making use of the coset decomposition of R by the subgroups H of order “NMULTI”. In projecting out the proper irreducible component from the multiplied copies, we employ slightly different step from the above description. Let W be the initial starting place, that is, the multiplied components of the irreducible representations, from which the separated proper irreducible components $W_1, \dots, W_i$ are computed. The next candidate of the generator v_{i+1} is not taken directly from the complementary space $(W \setminus (W_1 \cup W_2 \cup \dots \cup W_i))$; instead, in the whole vector space S (of 180 dimension in this case), the orthogonal space to $W_1 \cup W_2 \cup \dots \cup W_i$, biz, $S \setminus (W_1 \cup W_2 \cup \dots \cup W_i)$ is constructed. The basis set in the latter space is projected into the irreducible representation under the consideration, and the candidate v_{i+1} is taken from this projected space (the renewed W). This treatment is to quicken the symbolic computation.

```

gopr:=function(O,v,i,hom)
  local irr;
  irr:=Irr(O);
  return Sum(List(Elements(O),j->j^irr[i]*LargeMatrix(j,hom)*v));
end;

Cutout:=function(BAS,PROJ,R,hom,NMULTI,REPSIZ)
#
# BAS      : THE VECTOR SPACE INCLUDING THE COPIES OF IRREDUCIBLE SPACES
# PROJ     : THE PROJECTORS
# R        : THE GROUP IN THE PROBLEM.
# hom      : THE HOMOMORPHISM FROM <R> TO THE MATRIX GROUP.
# NMULTI   : THE SIZE OF THE SUBGROUP TO FORM THE COSET.
# REPSIZ   : THE SIZE OF THE IRREDUCIBLE REPRESENTATION.
#
  local C,D,BASN,EA,O,l,P,p,B,OV,SI,AS,OREP,ww,OT,ith,ifind;
  C:=[];
  D:=[];
  BASN:=BAS;
  EA:=List(Elements(R),j->LargeMatrix(j,hom));;
#
# The subgroups with the order of "NMULTI" are extracted.
#
  AS:=AllSubgroups(R);
  while (BASN<>[])
  do
    Print("\n",Size(BASN),"\n");

```

```

O:=Filtered(AS,g->Order(g)=NMULTI);;
Print(O);

#
# The subgroups which generate the vector space of
# the correct dimension of the irreducible representation
# are chosen.
#
if (O=[]) then
  O:=[Group(One(R))];
fi;
l:=List([1..Size(O)],i->O);
ifind:=0;
ith:=1;
while (ifind=0 and ith<=Size(O))
do
  ww:=gopr(O[ith],BASN[1],1,hom);
  l[ith]:=RankMat(List(EA,g->g*ww));
  Print(l);
  if (l[ith]=REPSIZ) then
    ifind:=1;
    OT:=O[ith];
  fi;
  ith:=ith+1;
od;
if (ifind=0) then
  Print("CHANGE THE SUPPOSITION!\n");
return 0;

```

```

    fi;
#
# By means of the chosen subgroup, the irreducible
# vector space "B" is generated.
# It is stored in the vector space "D".
#
    B:=BaseMat(List(EA,g->g*gopr(OT,BASN[1],1,hom)));;
    Append(C,[B]);
    Append(D,B);
#
# The orthogonal space "OV" to the vector space "D" is prepared.
#
    OV:=BaseOrthogonalSpaceMat(D);
#
# The vector space "BASN" to be processed is renewed now,
# by the projection "PROJ" on the vectors in "OV".
#
    BASN:=BaseMat(List(OV,o->PROJ*o));
#
# Instead, it is possible that "BASN" is renewed
# as the intersection between "BASN" and "OV".
#
    SI:=SumIntersectionMat(BASN,OV);
    BASN:=SI[2];
#
    od;
#

```

```

# Return C, the separated subspaces.
#
  return C;
end;

```

In our problem, the latter method works well, too. We can separate out seven distinct irreducible spaces. (As for the other irreducible representations, it is successful, with the suitable choice of the coset decomposition. For example, the subgroups of order 5 operate well at the first, third, fourth, fifth, sixth, ninth and tenth irreducible representations; that of order 8 does at the seventh; that of order 4 does at the eighth.)

```

gap> H1:=Cutout(BAS[10],PRJE[10],hom2,R,5,5);;
gap> List(H1,a->List(H1,b->RankMat(a*TransposedMat(b))));
[ [ 5, 0, 0, 0, 0, 0, 0, 0 ], [ 0, 5, 0, 0, 0, 0, 0, 0 ], [ 0, 0, 5, 0, 0, 0, 0, 0 ],
  [ 0, 0, 0, 5, 0, 0, 0, 0 ], [ 0, 0, 0, 0, 5, 0, 0, 0 ], [ 0, 0, 0, 0, 0, 5, 0, 0 ],
  [ 0, 0, 0, 0, 0, 0, 5, 0 ] ]
gap> 00:=List(EA,o->o*H1[1][1]);;
gap> List(H1,d->RankMat(00*TransposedMat(d)));
[ 5, 0, 0, 0, 0, 0, 0, 0 ]
gap> 00:=List(EA,o->o*H1[2][1]);;
gap> List(H1,d->RankMat(00*TransposedMat(d)));
[ 0, 5, 0, 0, 0, 0, 0, 0 ]
. . . etc . . .

```

C. Remark to this section

In this section, the computation of the vibrational mode of C_{60} by means of the computer algebra system GAP is demonstrated. The computation can be executed by a standard desktop personal computer. Though the topic in the present article is limited to the C_{60} molecule, the way of the computation shall be applicable to other systems, such as crystal. The small programs in the article are composed as brief as possible and as comprehensible as possible, but without considerations of the optimization, such as memory usages, or the avoidance of the re-computation of same objects. So there is the possibility to improve the efficiency, although they are computable even by the standard desktop personal computer. The computed basis of the vibrational modes are obtained as the symbolic formulas, and they are convertible to the numerical program functions simply by the rewriting of strings. Some of formulas might be so lengthy that the generated program functions might be beyond the capacity of the compiler. However, the computations presented in this article can be done by the floating-point computation, started from the numerical representation of the rotation matrices, with a certain toleration to the numerical error under the threshold.

IX. CONCLUSION

The theme of this article is how to simulate the property of the material by means of electronic structure calculations with the aid of computer algebra. The collaboration of the electronic structure calculation and the computer algebra is not novel one; rather being regarded as the modernization of the union of the quantum dynamics and the group theory, the success of which was brilliantly displayed in the former half of last century. In this article, the treated topics in the group theory are

rather classical ones concerning with the character theory. However, there can be various applications of the myriad topics of mathematics. As for the combinatorics, the Polya counting theory is a typical example; it is applicable to determine the number of configurations, equivalent by some symmetry operations, for example to determine the total number of possible molecular formations indicated by a single chemical formula.³⁵ This type of computations in combinatorics can also be executed by the computer algebra. As for the application of combinatorics in quantum physics, a sort of extension of Polya counting theorem can be useful in computing the spin weight in molecules.³⁶⁻³⁸ In a recent study, it is shown that the framework of the electronic structure could be reconstructed by means of a concept in the algebraic geometry, so-called Groebner bases theory, through the utilization of symbolic computation.³⁹

In the present circumstance of the material physics, indeed, there is an awkward inclination in which one solely relies on computer powers; only by trial and errors, or, only by varying the input data, one tries to execute “material design”, without any effective guiding principle. We must admit that the computational packages have developed so complex and so vast that a common researcher, if not being an expert, would be obliged to utilize them as black boxes, without knowing the detail of the programs; fortunately those packages are so powerful and effective that one can obtain reliable results with ease. The blind reliance on these packages, however, should be avoided; the mere enumeration of results of computations, with the slight modification of input data, will be waste of computational resources. Certainly, by gathering and comparing computed results we could surmise vague tendencies, but may not go furthermore, if we do not know physical or mathematical origin. Instead, it is necessary for us to have another utensil, which will compensate for such a short-coming; the group theory, or its modernization, the computer algebra, will be of great use for this purpose. With the aid of computer algebra, advanced

concepts in group theory are easily accessible and applicable, so that we can execute systematic research of material design from the mathematical first principles, since the group theoretical view illuminates for us the mathematical principles lurking behind observable phenomena. I am certain that the computer algebra will bring forth the blessed reunion of physics and mathematics in the research of materials; the available tool for us is not limited to the classics such as Courant-Hilbert,⁴⁰ although they had been powerful in the early stages of the development of quantum dynamics. The mathematics and physics have progressed greatly since then; the forefront of these developments seems to be so esoteric that non-experts feel dismayed when urged to put it into practice. Nevertheless, one should not be timid; for the sake of ardent researchers, the computer algebra will be a most suitable guide for their efforts, and there they will find a most speedily passable bridge over the ever-deepening chasm between physics and mathematics.

Appendix A: Symmetry operations in the diamond structure (real space)

The symmetry operations in the diamond structure (in Cartesian coordinates) are given in the table. The operation on the atomic coordinate is given by $x \rightarrow R \cdot x + T1 \cdot a_1 + T2 \cdot a_2 + T3 \cdot a_3$, where (a_1, a_2, a_3) are primitive translations. There are two types of fractional translations, according to the location of the origin of the unit cell. The first, denoted as (T1,T2,T3) corresponds to the case of atomic positions of $\pm(1/8 \cdot a_1 + 1/8 \cdot a_2 + 1/8 \cdot a_3)$; the second, (T1(*),T2(*),T3(*)) corresponds to positions of $(0 \cdot a_1 + 0 \cdot a_2 + 0 \cdot a_3)$ and $(1/4 \cdot a_1 + 1/4 \cdot a_2 + 1/4 \cdot a_3)$. Although the latter case is more conventional, the former has a merit such that the coefficients of the plane-wave-expression of the wavefunctions are real-valued.

R11	R12	R13	R21	R22	R23	R31	R32	R33	T1	T2	T3	T1(*)	T2(*)	T3(*)
-----	-----	-----	-----	-----	-----	-----	-----	-----	----	----	----	-------	-------	-------

1	1	0	0	0	1	0	0	0	1	0	0	0	0	0	0
2	1	0	0	0	-1	0	0	0	-1	0.5	0	0	0	0	0
3	-1	0	0	0	1	0	0	0	-1	0	0.5	0	0	0	0
4	-1	0	0	0	-1	0	0	0	1	0	0	0.5	0	0	0
5	0	1	0	0	0	1	1	0	0	0	0	0	0	0	0
6	0	1	0	0	0	-1	-1	0	0	0.5	0	0	0	0	0
7	0	-1	0	0	0	1	-1	0	0	0	0.5	0	0	0	0
8	0	-1	0	0	0	-1	1	0	0	0	0	0.5	0	0	0
9	0	0	1	1	0	0	0	1	0	0	0	0	0	0	0
10	0	0	1	-1	0	0	0	-1	0	0.5	0	0	0	0	0
11	0	0	-1	1	0	0	0	-1	0	0	0.5	0	0	0	0
12	0	0	-1	-1	0	0	0	1	0	0	0	0.5	0	0	0
13	0	-1	0	-1	0	0	0	0	-1	0	0	0	0.25	0.25	0.25
14	0	-1	0	1	0	0	0	0	1	-0.5	0	0	0.25	0.25	0.25
15	0	1	0	-1	0	0	0	0	1	0	-0.5	0	0.25	0.25	0.25
16	0	1	0	1	0	0	0	0	-1	0	0	-0.5	0.25	0.25	0.25
17	-1	0	0	0	0	-1	0	-1	0	0	0	0	0.25	0.25	0.25
18	-1	0	0	0	0	1	0	1	0	-0.5	0	0	0.25	0.25	0.25
19	1	0	0	0	0	-1	0	1	0	0	-0.5	0	0.25	0.25	0.25
20	1	0	0	0	0	1	0	-1	0	0	0	-0.5	0.25	0.25	0.25
21	0	0	-1	0	-1	0	-1	0	0	0	0	0	0.25	0.25	0.25
22	0	0	-1	0	1	0	1	0	0	-0.5	0	0	0.25	0.25	0.25
23	0	0	1	0	-1	0	1	0	0	0	-0.5	0	0.25	0.25	0.25
24	0	0	1	0	1	0	-1	0	0	0	0	-0.5	0.25	0.25	0.25
25	-1	0	0	0	-1	0	0	0	-1	0	0	0	0.25	0.25	0.25

26	-1	0	0	0	1	0	0	0	1	-0.5	0	0	0.25	0.25	0.25
27	1	0	0	0	-1	0	0	0	1	0	-0.5	0	0.25	0.25	0.25
28	1	0	0	0	1	0	0	0	-1	0	0	-0.5	0.25	0.25	0.25
29	0	-1	0	0	0	-1	-1	0	0	0	0	0	0.25	0.25	0.25
30	0	-1	0	0	0	1	1	0	0	-0.5	0	0	0.25	0.25	0.25
31	0	1	0	0	0	-1	1	0	0	0	-0.5	0	0.25	0.25	0.25
32	0	1	0	0	0	1	-1	0	0	0	0	-0.5	0.25	0.25	0.25
33	0	0	-1	-1	0	0	0	-1	0	0	0	0	0.25	0.25	0.25
34	0	0	-1	1	0	0	0	1	0	-0.5	0	0	0.25	0.25	0.25
35	0	0	1	-1	0	0	0	1	0	0	-0.5	0	0.25	0.25	0.25
36	0	0	1	1	0	0	0	-1	0	0	0	-0.5	0.25	0.25	0.25
37	0	1	0	1	0	0	0	0	1	0	0	0	0	0	0
38	0	1	0	-1	0	0	0	0	-1	0.5	0	0	0	0	0
39	0	-1	0	1	0	0	0	0	-1	0	0.5	0	0	0	0
40	0	-1	0	-1	0	0	0	0	1	0	0	0.5	0	0	0
41	1	0	0	0	0	1	0	1	0	0	0	0	0	0	0
42	1	0	0	0	0	-1	0	-1	0	0.5	0	0	0	0	0
43	-1	0	0	0	0	1	0	-1	0	0	0.5	0	0	0	0
44	-1	0	0	0	0	-1	0	1	0	0	0	0.5	0	0	0
45	0	0	1	0	1	0	1	0	0	0	0	0	0	0	0
46	0	0	1	0	-1	0	-1	0	0	0.5	0	0	0	0	0
47	0	0	-1	0	1	0	-1	0	0	0	0.5	0	0	0	0
48	0	0	-1	0	-1	0	1	0	0	0	0	0.5	0	0	0

TABLE XLIII: Symmetry operations in the point group in the diamond unit cell. If fractional translations are set to be zero, these operations are applicable to the cubic lattice.

Appendix B: Symmetry operations in the hexagonal lattice (real space)

The symmetry operations in graphite (in Cartesian coordinates) are given in the table:

	R11	R12	R13	R21	R22	R23	R31	R32	R33	T1	T2	T3
1	1	0	0	0	1	0	0	0	1	0	0	0
2	0.5	$-\sqrt{3}/2$	0	$\sqrt{3}/2$	0.5	0	0	0	1	0	0	-0.5
3	-0.5	$-\sqrt{3}/2$	0	$\sqrt{3}/2$	-0.5	0	0	0	1	0	0	0
4	-1	0	0	0	-1	0	0	0	1	0	0	-0.5
5	-0.5	$\sqrt{3}/2$	0	$-\sqrt{3}/2$	-0.5	0	0	0	1	0	0	0
6	0.5	$\sqrt{3}/2$	0	$-\sqrt{3}/2$	0.5	0	0	0	1	0	0	-0.5
7	-0.5	$-\sqrt{3}/2$	0	$-\sqrt{3}/2$	0.5	0	0	0	-1	0	0	-0.5
8	0.5	$-\sqrt{3}/2$	0	$-\sqrt{3}/2$	-0.5	0	0	0	-1	0	0	0
9	1	0	0	0	-1	0	0	0	-1	0	0	-0.5
10	0.5	$\sqrt{3}/2$	0	$\sqrt{3}/2$	-0.5	0	0	0	-1	0	0	0
11	-0.5	$\sqrt{3}/2$	0	$\sqrt{3}/2$	0.5	0	0	0	-1	0	0	-0.5
12	-1	0	0	0	1	0	0	0	-1	0	0	0
13	-1	0	0	0	-1	0	0	0	-1	0	0	-0.5
14	-0.5	$\sqrt{3}/2$	0	$-\sqrt{3}/2$	-0.5	0	0	0	-1	0	0	0
15	0.5	$\sqrt{3}/2$	0	$-\sqrt{3}/2$	0.5	0	0	0	-1	0	0	-0.5

16	1	0	0	0	1	0	0	0	-1	0	0	0
17	0.5	$-\sqrt{3}/2$	0	$\sqrt{3}/2$	0.5	0	0	0	-1	0	0	-0.5
18	-0.5	$-\sqrt{3}/2$	0	$\sqrt{3}/2$	-0.5	0	0	0	-1	0	0	0
19	0.5	$\sqrt{3}/2$	0	$\sqrt{3}/2$	-0.5	0	0	0	1	0	0	0
20	-0.5	$\sqrt{3}/2$	0	$\sqrt{3}/2$	0.5	0	0	0	1	0	0	-0.5
21	-1	0	0	0	1	0	0	0	1	0	0	0
22	-0.5	$-\sqrt{3}/2$	0	$-\sqrt{3}/2$	0.5	0	0	0	1	0	0	-0.5
23	0.5	$-\sqrt{3}/2$	0	$-\sqrt{3}/2$	-0.5	0	0	0	1	0	0	0
24	1	0	0	0	-1	0	0	0	1	0	0	-0.5

TABLE XLIV: The symmetry operations in graphite in real space.

Appendix C: Symmetry operations in the diamond structure (wave-number space)

The symmetry operations in the diamond structure, as the rotation matrices in the reciprocal spaces are given in the table:

	R'11	R'12	R'13	R'21	R'22	R'23	R'31	R'32	R'33	T1	T2	T3
1	1	0	0	0	1	0	0	0	1	0	0	0
2	-1	0	0	-1	0	1	-1	1	0	0.5	0	0
3	0	-1	1	0	-1	0	1	-1	0	0	0.5	0
4	0	1	-1	1	0	-1	0	0	-1	0	0	0.5
5	0	1	0	0	0	1	1	0	0	0	0	0
6	0	-1	0	1	-1	0	0	-1	1	0.5	0	0
7	1	0	-1	0	0	-1	0	1	-1	0	0.5	0

8	-1	0	1	-1	1	0	-1	0	0	0	0	0	0.5
9	0	0	1	1	0	0	0	1	0	0	0	0	0
10	0	0	-1	0	1	-1	1	0	-1	0.5	0	0	0
11	-1	1	0	-1	0	0	-1	0	1	0	0.5	0	0
12	1	-1	0	0	-1	1	0	-1	0	0	0	0.5	0
13	0	-1	0	-1	0	0	0	0	-1	0	0	0	0
14	0	1	0	0	1	-1	-1	1	0	-0.5	0	0	0
15	1	0	-1	1	0	0	1	-1	0	0	-0.5	0	0
16	-1	0	1	0	-1	1	0	0	1	0	0	-0.5	0
17	-1	0	0	0	0	-1	0	-1	0	0	0	0	0
18	1	0	0	1	-1	0	1	0	-1	-0.5	0	0	0
19	0	-1	1	0	0	1	-1	0	1	0	-0.5	0	0
20	0	1	-1	-1	1	0	0	1	0	0	0	-0.5	0
21	0	0	-1	0	-1	0	-1	0	0	0	0	0	0
22	0	0	1	-1	0	1	0	-1	1	-0.5	0	0	0
23	-1	1	0	0	1	0	0	1	-1	0	-0.5	0	0
24	1	-1	0	1	0	-1	1	0	0	0	0	-0.5	0
25	-1	0	0	0	-1	0	0	0	-1	0	0	0	0
26	1	0	0	1	0	-1	1	-1	0	-0.5	0	0	0
27	0	1	-1	0	1	0	-1	1	0	0	-0.5	0	0
28	0	-1	1	-1	0	1	0	0	1	0	0	-0.5	0
29	0	-1	0	0	0	-1	-1	0	0	0	0	0	0
30	0	1	0	-1	1	0	0	1	-1	-0.5	0	0	0
31	-1	0	1	0	0	1	0	-1	1	0	-0.5	0	0
32	1	0	-1	1	-1	0	1	0	0	0	0	-0.5	0

33	0	0	-1	-1	0	0	0	-1	0	0	0	0
34	0	0	1	0	-1	1	-1	0	1	-0.5	0	0
35	1	-1	0	1	0	0	1	0	-1	0	-0.5	0
36	-1	1	0	0	1	-1	0	1	0	0	0	-0.5
37	0	1	0	1	0	0	0	0	1	0	0	0
38	0	-1	0	0	-1	1	1	-1	0	0.5	0	0
39	-1	0	1	-1	0	0	-1	1	0	0	0.5	0
40	1	0	-1	0	1	-1	0	0	-1	0	0	0.5
41	1	0	0	0	0	1	0	1	0	0	0	0
42	-1	0	0	-1	1	0	-1	0	1	0.5	0	0
43	0	1	-1	0	0	-1	1	0	-1	0	0.5	0
44	0	-1	1	1	-1	0	0	-1	0	0	0	0.5
45	0	0	1	0	1	0	1	0	0	0	0	0
46	0	0	-1	1	0	-1	0	1	-1	0.5	0	0
47	1	-1	0	0	-1	0	0	-1	1	0	0.5	0
48	-1	1	0	-1	0	1	-1	0	0	0	0	0.5

TABLE XLV: Symmetry operations in the diamond crystal
in the reciprocal space.

Appendix D: Symmetry operations in the hexagonal lattice (wave-number space)

The crystal axes are chosen to be $a_1 = (1, 0, 0)$, $a_2 = (-1/2, \sqrt{3}/2, 0)$, $a_3 = (0, 0, c)$. Then The symmetry operations as the operations in the wave-number space are given as:

	R'11	R'12	R'13	R'21	R'22	R'23	R'31	R'32	R'33	T1	T2	T3
1	1	0	0	0	1	0	0	0	1	0	0	0
2	0	-1	0	1	1	0	0	0	1	0	0	-0.5
3	-1	-1	0	1	0	0	0	0	1	0	0	0
4	-1	0	0	0	-1	0	0	0	1	0	0	-0.5
5	0	1	0	-1	-1	0	0	0	1	0	0	0
6	1	1	0	-1	0	0	0	0	1	0	0	-0.5
7	-1	-1	0	0	1	0	0	0	-1	0	0	-0.5
8	0	-1	0	-1	0	0	0	0	-1	0	0	0
9	1	0	0	-1	-1	0	0	0	-1	0	0	-0.5
10	1	1	0	0	-1	0	0	0	-1	0	0	0
11	0	1	0	1	0	0	0	0	-1	0	0	-0.5
12	-1	0	0	1	1	0	0	0	-1	0	0	0
13	-1	0	0	0	-1	0	0	0	-1	0	0	-0.5
14	0	1	0	-1	-1	0	0	0	-1	0	0	0
15	1	1	0	-1	0	0	0	0	-1	0	0	-0.5
16	1	0	0	0	1	0	0	0	-1	0	0	0
17	0	-1	0	1	1	0	0	0	-1	0	0	-0.5
18	-1	-1	0	1	0	0	0	0	-1	0	0	0
19	1	1	0	0	-1	0	0	0	1	0	0	0
20	0	1	0	1	0	0	0	0	1	0	0	-0.5
21	-1	0	0	1	1	0	0	0	1	0	0	0
22	-1	-1	0	0	1	0	0	0	1	0	0	-0.5
23	0	-1	0	-1	0	0	0	0	1	0	0	0
24	1	0	0	-1	-1	0	0	0	1	0	0	-0.5

TABLE XLVI: The symmetry operations in graphite in reciprocal space.

Appendix E: The computation of Wyckoff positions by GAP

Computations for space groups can be executed by means of “Cryst” package in GAP. Though the manual of this package is provided, the description is too curt and the computed result is too unfriendly for beginners to utilize. So in this section, the usage of this package is illustrated.

The crystallographic group is defined at first (in this example, with minimal generators):

```
gap> M1:=[[0,0,1,0],[1,0,0,0],[0,-1,0,0],[1/4,1/4,1/4,1]];
gap> M2:=[[0,0,-1,0],[0,-1,0,0],[1,0,0,0],[0,0,0,1]];
gap> S:=AffineCrystGroup([M1,M2]);
```

The point group is obtained by:

```
gap> P:=PointGroup(S);
```

The Wyckoff positions are computed now:

```
gap> W:=WyckoffPositions(S);
[ < Wyckoff position, point group 4, translation := [ 1/8, 3/8, 7/8 ],
  basis := [ ] >
  , < Wyckoff position, point group 4, translation := [ 1/8, 3/8, 3/8 ],
  basis := [ ] >
```

```

, < Wyckoff position, point group 5, translation := [ 1/4, 1/4, 3/4 ],
basis := [ ] >
, < Wyckoff position, point group 5, translation := [ 1/4, 1/4, 1/4 ],
basis := [ ] >
, < Wyckoff position, point group 3, translation := [ 0, 0, 0 ],
basis := [ [ 1, -1, -1 ] ] >
, < Wyckoff position, point group 6, translation := [ 1/4, 1/4, 1/2 ],
basis := [ [ 0, 0, 1 ] ] >
, < Wyckoff position, point group 7, translation := [ 0, 1/4, 7/8 ],
basis := [ [ 1/2, 1/2, 0 ] ] >
, < Wyckoff position, point group 2, translation := [ 0, 0, 0 ],
basis := [ [ 1/2, -1/2, 0 ], [ 0, 0, 1 ] ] >
, < Wyckoff position, point group 1, translation := [ 0, 0, 0 ],
basis := [ [ 1/2, 0, 1/2 ], [ 0, 1/2, 1/2 ], [ 0, 0, 1 ] ] >
]

```

The returned result is the list of the generating set of the Wyckoff positions. The expression such as

```

, < Wyckoff position, point group 3, translation := [ 0, 0, 0 ],
basis := [ [ 1, -1, -1 ] ] >

```

indicates the information of a generator for the Wyckoff positions, which is located at the segment $[0,0,0]+t[1,-1,-1]$, where t is arbitrary real number inasmuch that the segment is confined in the unit cell. Now we get nine generators. The computed result, therefore, should be read as,

```

[ 1/8, 3/8, 7/8 ]
[ 1/8, 3/8, 3/8 ]

```

```

[ 1/4, 1/4, 3/4 ]
[ 1/4, 1/4, 1/4 ]
[ 0, 0, 0 ]+t[ 1, -1, -1 ]
[ 1/4, 1/4, 1/2 ]+t[ 0, 0, 1 ]
[ 0, 1/4, 7/8 ]+t[ 1/2, 1/2, 0 ]
[ 0, 0, 0 ]+t1[ 1/2, -1/2, 0 ]+t2[ 0, 0, 1 ]
[ 0, 0, 0 ]+t1[ 1/2, 0, 1/2 ]+t2[ 0, 1/2, 1/2 ]+t3[ 0, 0, 1 ]

```

The first four are single points, but the remaining five are one-dimensional segments, two-dimensional planes, or, a three-dimensional shape. (The last of them is the arbitrary position in the unit cell.) Let us pay attention to the fourth of them. It is the position of one carbon atom in the minimal diamond unit cell; which is moved to $[0,0,0]$ (the position of another Carbon atom) by means of symmetry operations. In order to obtain whole of the Wyckoff positions, the equivalent coordinate points (orbits by the symmetry operations) can be evaluated in the following way.

The total numbers of the equivalent coordinate points are given by

```

gap> List(WyckoffPositions(S),x->Size(WyckoffOrbit(x)));
[ 4, 4, 2, 2, 8, 12, 24, 24, 48 ]

```

For each generating points, the equivalents coordinates can be computed separately:

```

gap> WyckoffOrbit(WyckoffPositions(S)[1]);
[ < Wyckoff position, point group 4, translation := [ 1/8, 3/8, 7/8 ],
  basis := [ ] >
  , < Wyckoff position, point group 4, translation := [ 3/8, 1/8, 7/8 ],
  basis := [ ] >
  , < Wyckoff position, point group 4, translation := [ 3/8, 3/8, 5/8 ],

```

```

basis := [ ] >
, < Wyckoff position, point group 4, translation := [ 1/8, 1/8, 5/8 ],
basis := [ ] >
]
gap> WyckoffOrbit(WyckoffPositions(S)[2]);
[ < Wyckoff position, point group 4, translation := [ 1/8, 3/8, 3/8 ],
basis := [ ] >
, < Wyckoff position, point group 4, translation := [ 3/8, 1/8, 3/8 ],
basis := [ ] >
, < Wyckoff position, point group 4, translation := [ 3/8, 3/8, 1/8 ],
basis := [ ] >
, < Wyckoff position, point group 4, translation := [ 1/8, 1/8, 1/8 ],
basis := [ ] >
]
gap> .....
gap> WyckoffOrbit(WyckoffPositions(S)[8]);
[ < Wyckoff position, point group 2, translation := [ 0, 0, 0 ],
basis := [ [ 1/2, -1/2, 0 ], [ 0, 0, 1 ] ] >
, < Wyckoff position, point group 2, translation := [ 1/4, 1/4, 1/4 ],
basis := [ [ -1/2, 0, 1/2 ], [ 0, -1, 0 ] ] >
, < Wyckoff position, point group 2, translation := [ 0, 0, 0 ],
.....
.....
]

```

Appendix F: Subgroup lattice

In this article, the sequence of crystalline symmetry reduction is displayed by means of the mathematical concept of the lattice of subgroups, in which the inclusion relations among them are illustrated as a graph. The GAP computation can be done as follows:

```
gap> M1:=[[0,1,0],[0,0,1],[1,0,0]];
[ [ 0, 1, 0 ], [ 0, 0, 1 ], [ 1, 0, 0 ] ]
gap> M2:=[[0,1,0],[-1,0,0],[0,0,1]];
[ [ 0, 1, 0 ], [ -1, 0, 0 ], [ 0, 0, 1 ] ]
gap> G:=Group(M1,M2);
Group([ [ [ 0, 1, 0 ], [ 0, 0, 1 ], [ 1, 0, 0 ] ],
      [ [ 0, 1, 0 ], [ -1, 0, 0 ], [ 0, 0, 1 ] ] ])
gap> Size(G);
24
gap> l:=LatticeSubgroups(G);
<subgroup lattice of Group(
[ [ [ 0, 1, 0 ], [ 0, 0, 1 ], [ 1, 0, 0 ] ],
  [ [ 0, 1, 0 ], [ -1, 0, 0 ], [ 0, 0, 1 ] ] ]), 11 classes,
30 subgroups>
gap> ConjugacyClassesSubgroups(l);
[ Group([], [ [ 1, 0, 0 ], [ 0, 1, 0 ], [ 0, 0, 1 ] ])^G,
  Group([ [ [ 1, 0, 0 ], [ 0, -1, 0 ], [ 0, 0, -1 ] ] ])^G,
  Group([ [ [ -1, 0, 0 ], [ 0, 0, -1 ], [ 0, -1, 0 ] ] ])^G,
  Group([ [ [ 0, 1, 0 ], [ 0, 0, 1 ], [ 1, 0, 0 ] ] ])^G,
  Group([ [ [ -1, 0, 0 ], [ 0, 1, 0 ], [ 0, 0, -1 ] ],
        [ [ 1, 0, 0 ], [ 0, -1, 0 ], [ 0, 0, -1 ] ] ])^G,
```

```

Group([ [ [ -1, 0, 0 ], [ 0, 0, -1 ], [ 0, -1, 0 ] ],
        [ [ 1, 0, 0 ], [ 0, -1, 0 ], [ 0, 0, -1 ] ] ])^G,
Group([ [ [ 1, 0, 0 ], [ 0, 0, 1 ], [ 0, -1, 0 ] ],
        [ [ 1, 0, 0 ], [ 0, -1, 0 ], [ 0, 0, -1 ] ] ])^G,
Group([ [ [ -1, 0, 0 ], [ 0, 0, -1 ], [ 0, -1, 0 ] ],
        [ [ 0, 1, 0 ], [ 0, 0, 1 ], [ 1, 0, 0 ] ] ])^G,
Group([ [ [ -1, 0, 0 ], [ 0, 1, 0 ], [ 0, 0, -1 ] ],
        [ [ 1, 0, 0 ], [ 0, -1, 0 ], [ 0, 0, -1 ] ],
        [ [ -1, 0, 0 ], [ 0, 0, -1 ], [ 0, -1, 0 ] ] ])^G,
Group([ [ [ -1, 0, 0 ], [ 0, 1, 0 ], [ 0, 0, -1 ] ],
        [ [ 1, 0, 0 ], [ 0, -1, 0 ], [ 0, 0, -1 ] ],
        [ [ 0, 1, 0 ], [ 0, 0, 1 ], [ 1, 0, 0 ] ] ])^G,
Group([ [ [ -1, 0, 0 ], [ 0, 1, 0 ], [ 0, 0, -1 ] ],
        [ [ 1, 0, 0 ], [ 0, -1, 0 ], [ 0, 0, -1 ] ],
        [ [ 0, 1, 0 ], [ 0, 0, 1 ], [ 1, 0, 0 ] ],
        [ [ -1, 0, 0 ], [ 0, 0, -1 ], [ 0, -1, 0 ] ] ])^G ]
gap> DotFileLatticeSubgroups(1,"paradigm.dot");

```

The last command “DotfileLatticeSubgroups” is used to generate an output file for the visualization.

Appendix G: The analytical representation of the energy spectra of C_{60} .

In the model of C_{60} in section VII B, if we chose the transfer integral as $H_{\text{single}}=-1$ (on the single bonds in the pentagons) and $H_{\text{double}}=-y$ (on the double bonds in the hexagons), the secular equation is decomposed into the polynomial with some multiplicity in each representation, as in table XLVII. The irreducible representations I.1,...,I.10 are the same as given in the main article, at table XXVI. The energy

spectra of in the main article can be constructed from this table, setting $E = 2x$ and $y = -1/2$.

	Polynomial	multiplicity
I.1	[$x+y+2$]	1
I.2	[]	
I.3	[$x-y+(E(5)^2+E(5)^3)$]	3
I.4	[$x-y+(E(5)+E(5)^4)$]	3
I.5	[$x^2-y^2+(-E(5)-2E(5)^2-2E(5)^3-E(5)^4)*x$ + $(-E(5)-E(5)^4)*y+(2E(5)+2E(5)^4)$]	3
I.6	[$x^2-y^2+(-2E(5)-E(5)^2-E(5)^3-2E(5)^4)*x$ + $(-E(5)^2-E(5)^3)*y+(2E(5)^2+2E(5)^3)$]	3
I.7	[x^2-y^2-x-1]	4
I.8	[$x^2-y^2-x-2*y-1$]	4
I.9	[$x^3+x^2*y-x*y^2-y^3+x^2+2*x*y+y^2-3*x-y-2$]	5
I.10	[$x^2-y^2-x+y-1$]	5

TABLE XLVII. The decomposition of the secular equation.

* akihito_kikuchi@gakushikai.jp (The corresponding author)

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⁴ M. S. Dresselhaus, G. Dresselhaus, and A. Jorio, *Group Theory: Application to the Physics of Condensed Matter*, (Springer-Verlag, 2008).

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- ¹⁷ P. Etingof, O. Golberg, S. Hensel, T. Liu, A. Schwendner, D. Vaintrob, and E. Yudovina, *Introduction to representation theory*, (<http://math.mit.edu/~etingof/replect.pdf>), p76–77.
- ¹⁸ In the definition of GAP, the semidirect product of a group N with a group G (acting on N via a homomorphism α from G into the automorphism group of N) is the Cartesian product $G \times N$ with the multiplication $(g, n) \cdot (h, m) = (gh, n^{h^\alpha} m)$, since in GAP all groups act from the right. On the other hand, the familiar style for the physicists is

$\{G|n\} \cdot \{H|m\} = \{G \cdot H|n + G * m\}$, as in the crystallography; the point group acts from the left. However, these two different definitions are equivalent. This is based on this: the crystallography, the symmetry operation $\{M|t\}$ is represented by an augmented matrix, which can take two forms. The one is the matrix of the form

$$\begin{bmatrix} \mathbf{M} & \mathbf{0} \\ \mathbf{t} & \mathbf{1} \end{bmatrix}$$

acting from the right on row vectors $(x, 1)$. The another is

$$\begin{bmatrix} \mathbf{M} & \mathbf{t} \\ \mathbf{0} & \mathbf{1} \end{bmatrix}$$

acting from the left on column vectors $(x, 1)$. These two definitions are convertible by transposition and one should interpret the GAP computations by the former definition. The generators used here, (M36,M48), should be replaced with their transposed forms.

¹⁹ The construction of the two-cohomology is briefly stated here. For every $g \in G$ there are elements $e_g \in E$ with $\pi(e_g) = g$. However e_g is not unique: another element e'_g behaves similarly, if $e'_g(e_g)^{-1} \in \ker(\pi) = K$. Now we define a map $\varphi_g : k \rightarrow e_g k e_g^{-1}$, as an automorphism in K . The two-cocycle is defined by

$$f(g, h) = e_g e_h e_{gh}^{-1}.$$

For each $g \in G$, let us give an element $k_g \in K$ (by a map $k(*)$ from G to K). Then the two-coboundary is defined as

$$b(g, h) = k_g \varphi_g(k_h) k_{gh}^{-1}.$$

(It will be represented as $k(g) + g \cdot k(h) - k(gh)$ when K is a module.)

Then we have

$$f(g, h) f(gh, k) = \varphi_g(f(h, k)) f(g, hk)$$

and for another choice ($e'_g = k_g e_g$),

$$f'(g, h) = e'_g e'_h (e'_{gh})^{-1} = b(h, g) f(g, h).$$

In two-cohomology $f(*, *)$ and $f'(*, *)$ represent the same class. The elements of E is uniquely written in the form ae_g for some $a \in K$ and $g \in G$. The product is given as $(ae_g)(be_h) = a\varphi_g(b)f(g, h)e_{gh}$, which is the usual semidirect product when $f(g, h) = 1$ for all g, h .

²⁰ Peter J. Webb, “An Introduction to the Cohomology of Groups”, <http://www.math.umn.edu/~webb/oldteaching/Year2010-11/8246CohomologyNotes.pdf>.

²¹ This algorithm is a refined style of the computation of one-cohomology given in the previous section. The relation such as $xyxy = 1$ (in G) is lifted to $e_{xyxy} = 1_E$, as the relation in E . The latter is rewritten by two-cocycles

$$1_E = e_{xyxy} = f(x, yxy)^{-1} \varphi_x(f(y, xy)^{-1}) \varphi_x(\varphi_y(f(x, y)^{-1})) e_x e_y e_x e_y$$

It is furthermore rewritten as

$$e_x e_y e_x e_y = f(x, yxy) \varphi_x(f(y, xy)) \varphi_x(\varphi_y(f(x, y))).$$

The right side of this equation lies in K . The formula of $\hat{\Lambda}_{(xy)^2}$ in the algorithm represents the translational part in $e_x e_y e_x e_y$ by means of those of e_x and e_y , and it must be in $K(= T)$. To find a v such as $\Lambda \cdot v \in T$ is to fix a representative of cocycle $f(*, *)$ in two-cohomology.

²² The point group of the crystal is always solvable, by means of a famous theorem of Burnside, which relates the order of the group to the solvability.

²³ This interpretation is consistent to the operation of the permutation in GAP. For example, the permutation (3,4,5) operates on the list [1,2,3,4,5] as follows:

```
gap> ListPerm((3,4,5));
[1,2,4,5,3];
```

Here the entries 3,4,5 are replaced by 4,5,3, as our interpretation assumes.

- ²⁴ The computed irreducible representations by the group generated by the permutations and that by the matrices are listed by different orders (at least, in the result by GAP of the version 4.7.7.) This will cause some trouble in doing computations. In this article, to avoid confusion, the groups generated by different resources are given by different names even if they are isomorphic, and the generators are presented in each time of the definition.

- ²⁵ In order to see whether the elements x and y are conjugate in group G , try the command.

```
gap> RepresentativeAction(G,x,y);
```

- ²⁶ In fact, the splitting field of the polynomial $x_1^4+6x_1^3-4x_1^2-54x_1-29$ is not $\mathbb{Q}_{15}$ (of the extension of eight degrees to $\mathbb{Q}$), but $\mathbb{Q}(a)$ (of the extension of four degrees to $\mathbb{Q}$), the latter of which is obtained by adding one of the solution “ a ” of this polynomial to $\mathbb{Q}$. It is equal to $\mathbb{Q}(E(15)+E(15)^{14})$ (denoted as $NF(15,[1,14])$ in GAP). To be exact, one should discuss in this field.

- ²⁷ The Galois group of this polynomial is computed by GAP.

```
gap> ge[8];
x_1^4+6*x_1^3-4*x_1^2-54*x_1-29
gap> GaloisType(ge[8]);
1
gap> TransitiveGroup(4,1);
C(4) = 4
```

The command `GaloisType(f)` computes the Galois Group of the polynomial f , and returns an integer i if the Galois group is isomorphic to `TransitiveGroup(n,i)`, where n is the degree of f .

- ²⁸ The semi-direct product of a group N with a group G is composed by the Cartesian product $G \times N$ with the multiplication $(g, n) \cdot (h, m) = (g \cdot h, \alpha^h(n) \cdot m)$, where α^h is an automorphism on N determined by the element h in G . (In fact another definition is also possible: $(g, n) \cdot (h, m) = (g \cdot h, n \cdot \alpha^g(m))$). The familiar example for physicists is the crystallographic group, in which the multiplication is defined as $\{G|n\} \cdot \{H|m\} = \{G \cdot H|n + G \cdot m\}$.)
- ²⁹ The expressions such as 0 and 0*x signify different objects. The former is the zero as a number, and the latter the zero monomial. If one promiscuously uses 0 and 0*x, it might cause some errors.
- ³⁰ In this definition, the projectors of the matrix group G are composed through the isomorphism from the permutation group R to G , not directly from G . This is a precaution to avoid a possible confusion, since the character tables of R and G , computed by GAP, might be presented in the slightly different orders, even if these two groups are isomorphic.
- ³¹ In the basis vectors of the vibrational mode computed hereafter, those which belong to the fourth irreducible representation, include the elements such as

$$\begin{pmatrix} I_i & 0 & 0 & \cdots \\ 0 & I_i & 0 & \cdots \\ 0 & 0 & I_i & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \cdot v$$

where v are the basis vector in the trivial irreducible representation (invariant by the symmetry operation), and $I_i (i = 1, 2, 3)$ are

$$I_1 = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, I_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, I_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}.$$

These vectors represent the degrees of freedoms of the rotation. They are set of 60 of three-dimensional vectors, defined on each vertex, and located in the tangent plane to the sphere where the 60 vertex are placed.

- ³² One might demand numerical basis as well as symbolic one. The latter can be easily modified into quasi-fortran form. For example, by replacements of strings, a formula such as

$$f := -1/5 * E(5) + 1/5 * E(5)^2 + 1/5 * E(5)^3 - 1/5 * E(5)^4;$$

is rewritten as

```

FUNCTION E(I)
  INTEGER I
  COMPLEX*16 E
  REAL*8 TWOPI
  TWOPI=8.0D0*ATAN(1.0D0)
  E=DCMPLX(COS(TWOPI/I),SIN(TWOPI/I))
  RETURN
END

SUBROUTINE(f)
  COMPLEX*16 f,E
  f=-1./5*E(5)+1./5*E(5)**2+1./5*E(5)**3-1./5*E(5)**4
  RETURN
END
```

- ³³ The basis vectors generated in this way are “vertex-wise” orthogonal to those in the trivial representation: the basis vectors are the set of 60 small three-dimensional vectors, and the small vectors of the former and the latter are orthogonal at each vertex. The vectors, “vertex-wise” orthogonal to those in the trivial representation, form the

subspace that includes several copies of the proper irreducible space.

- ³⁴ Since the tenth irreducible matrix representation is a real representation, the generated basis are real and we can work in the real number. Meanwhile the four-dimensional irreducible matrix representations (computed by GAP) are complex and the generated basis are complex. However, the complex irreducible representation in this case can be remade into real one. The complex-valued matrix representation of a generator (M_i) can be replaced by a real matrix:

$$\begin{pmatrix} \text{Re}(M_i) & -\text{Im}(M_i) \\ \text{Im}(M_i) & \text{Re}(M_i) \end{pmatrix}.$$

This representation is reducible, including two copies of the irreducible representation, but as the matrix group, it is isomorphic to the original group. We extract the basis set from the columns of the projector of this matrix group and divide it into two independent irreducible vector spaces by means of the procedure explained hereafter in the article. Each of the separated vector space provides us the real valued basis set and the real valued matrix representation. One set of such real matrix representations (for the generators r1 and r2) is given as follows:

```
r1:=[[1,
      3/2*E(5)+1/2*E(5)^2+1/2*E(5)^3+3/2*E(5)^4,
      -3*E(5)-7*E(5)^2-7*E(5)^3-3*E(5)^4,
      -1081/2131*E(5)-1797/2131*E(5)^2-1797/2131*E(5)^3-1081/2131*E(5)^4],
     [0,
      -1/2*E(5)-E(5)^2-E(5)^3-1/2*E(5)^4,
      -5*E(5)-14*E(5)^2-14*E(5)^3-5*E(5)^4,
      -1681/2131*E(5)-3510/2131*E(5)^2-3510/2131*E(5)^3-1681/2131*E(5)^4],
     [0,
```

$$\begin{aligned}
& -2*E(5)-3/2*E(5)^2-3/2*E(5)^3-2*E(5)^4, \\
& -2*E(5)-7*E(5)^2-7*E(5)^3-2*E(5)^4, \\
& -600/2131*E(5)-1713/2131*E(5)^2-1713/2131*E(5)^3-600/2131*E(5)^4], \\
& [0, \\
& 113/44*E(5)+92/11*E(5)^2+92/11*E(5)^3+113/44*E(5)^4, \\
& 623/22*E(5)+807/11*E(5)^2+807/11*E(5)^3+623/22*E(5)^4, \\
& 5/2*E(5)+8*E(5)^2+8*E(5)^3+5/2*E(5)^4]]];
\end{aligned}$$

$$\begin{aligned}
r2:=& [[-4/11*E(5)-3/11*E(5)^2-3/11*E(5)^3-4/11*E(5)^4, \\
& 7/22*E(5)+19/22*E(5)^2+19/22*E(5)^3+7/22*E(5)^4, \\
& 36/11*E(5)+104/11*E(5)^2+104/11*E(5)^3+36/11*E(5)^4, \\
& 383/2131*E(5)+2127/2131*E(5)^2+2127/2131*E(5)^3+383/2131*E(5)^4], \\
& [12/11*E(5)-2/11*E(5)^2-2/11*E(5)^3+12/11*E(5)^4, \\
& -16/11*E(5)-1/11*E(5)^2-1/11*E(5)^3-16/11*E(5)^4, \\
& 57/11*E(5)+128/11*E(5)^2+128/11*E(5)^3+57/11*E(5)^4, \\
& -1516/2131*E(5)+1596/2131*E(5)^2+1596/2131*E(5)^3-1516/2131*E(5)^4], \\
& [32/11*E(5)+13/11*E(5)^2+13/11*E(5)^3+32/11*E(5)^4, \\
& -39/11*E(5)-31/22*E(5)^2-31/22*E(5)^3-39/11*E(5)^4, \\
& 53/11*E(5)+92/11*E(5)^2+92/11*E(5)^3+53/11*E(5)^4, \\
& -1784/2131*E(5)+703/2131*E(5)^2+703/2131*E(5)^3-1784/2131*E(5)^4], \\
& [0,0, \\
& -623/22*E(5)-807/11*E(5)^2-807/11*E(5)^3-623/22*E(5)^4, \\
& -2*E(5)-7*E(5)^2-7*E(5)^3-2*E(5)^4]]];
\end{aligned}$$

We can use them in common in the two four-dimensional representations, with $r3 := \pm I$ (the four dimensional unit matrix).

- ³⁵ G. Polya, “Kombinatorische Anzahlbestimmungen für Gruppen, Graphen und chemische Verbindungen”, *Acta Mathematica* **68**(1): 145–254(1937), doi:10.1007/BF02546665.
- ³⁶ R. Schmied, K. K. Lehmann, “Computer-generated character tables and nuclear spin statistical weights: Application to benzene dimer and methane dimer”, *Journal of Molecular Spectroscopy* **226** 201–202 (2004), DOI:10.1016/j.jms.2004.04.003.
- ³⁷ D. M. Jonas, “Spin statistics: An error in Landau and Lifschitz’ Quantum Mechanics”, *J.Chem.Phys.***90**(10),5563–5565 (1989).
- ³⁸ L. D. Landau and E. M. Lifschitz, *Quantum Mechanics*, 3rd ed.(Pergamon,1977), Sec.105.
- ³⁹ A. Kikuchi, *QScience Connect* 2013:14 (2013), <http://dx.doi.org/10.5339/connect.2013.14>.
- ⁴⁰ R. Courant and D. Hilbert, *Method of mathematical physics*, Vol.1–2,(Wiley-VCH,1989).