
Symmetries

We will suppose that the student has already completed an undergraduate course typically denominated *Introduction to Solid State Physics*, in which a substantial time is usually spent in describing *crystal structures* observed in common crystalline solids. We will just briefly summarize the most important concepts that were presented there, but we will go deeper into the underlying symmetries and their relevance to the theoretical description of such solids.

A crystal structure is a representation of how the positional ordering of the constituent atoms of a solid looks like. It consists in an underlying *lattice* of abstract points, and a set of atoms (called *basis*) that is associated to each lattice point. As mentioned in Text 1, *observation* of crystal structures of real solids is usually done via x-ray or neutron diffraction.

Apart from a scaling factor related to interatomic distances, there is a finite number of possible crystal structures. For three-dimensional (3D) solids, only 14 different lattices are needed, which are called *Bravais lattices*. They are divided in 7 *crystal systems*: cubic, tetragonal, orthorhombic, monoclinic, triclinic, hexagonal, and trigonal. Such a classification is heavily based on the concept of *symmetry*. Without going into details about the crystal systems, we will focus to some extent on the general relevance of symmetries to the properties of crystalline solids.

Let us begin by the formal definition of a Bravais lattice as a discrete but infinite set of vectors $\{\mathbf{R}\}$, which can be written as combinations of three (for space dimension $d = 3$) non coplanar *primitive vectors*, i.e.,

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 , \quad (1)$$

where n_1 , n_2 , and n_3 are integer numbers.

The set of lattice vectors also define a set of symmetry operations called *translations*, since a rigid displacement of the lattice by any of these vectors will take any lattice point to a place previously occupied by another one, thus leaving the lattice unchanged. We see that (discrete) translation symmetry is inherent to all Bravais lattices, and consequently to all crystal structures.

In addition to translations, there are other operations that leave a lattice (or a crystal structure) invariant: *rotations*, *reflections*, *inversion*, etc. It is easy to figure out that only translations are sure to be symmetry operations of both a crystal structure and its underlying Bravais lattice. Other symmetries of the lattice may not apply to the crystal

structure, depending on the local symmetries of the basis. We will mostly focus on lattice symmetries.

The symmetry operations of a system (or object) form a **group**, in the mathematical sense of the term: the group is closed with respect to **product** (meaning a sequential application of two operations), the product is associative, there exists an identity operation, and each operation has an inverse.

The set of all symmetry operations of a particular lattice (or crystal structure) is its **space group**. Lattice translations are a **subgroup** of the space group, i.e., a subset of the group operations that is a group in itself. The other operations mentioned above form another subgroup called the **point group**, defined as the set of all symmetry operations that leave at least one point **fixed** in space. There are 7 different point groups for the 3D Bravais lattices (which define the 7 crystal systems), and 14 space groups (corresponding to the 14 lattices). Just to mention, all possible 3D **crystal structures** are divided in 32 point groups and 230 space groups.

The consequences of symmetries to the properties of a system are more easily disclosed using **Group Theory** applied to the space group (or its subgroups). For this reason, we will review some principles of Group Theory. This review is not meant to be complete nor rigorous, but will seek to highlight the main points that will allow us to understand the effect of symmetry on physical properties of crystalline solids.

Elements of Group Theory (through an example)

Instead of using a realistic Bravais-lattice group (as, for example, the point group of cubic lattices, with 48 operations), we consider a simpler group, composed by only 6 operations: the 6 *permutations* of 3 *identical objects* or, equivalently, of the three coordinates of a vector (x, y, z) in three-dimensional space. This group is usually referred to as S_3 , which is a particular case of S_n , the group of permutations of n objects. We will write the group as

$$S_3 = \{\mathbb{1}, a, b, c, d, e\} . \quad (2)$$

- The operation denoted by $\mathbb{1}$ is the *identity*:

$$\mathbb{1}(x, y, z) = (x, y, z) . \quad (3)$$

- Operations a and b are *cyclic permutations*:

$$\begin{aligned} a(x, y, z) &= (z, x, y) , \\ b(x, y, z) &= (y, z, x) . \end{aligned} \quad (4)$$

- Operations c , d , and e are *pair permutations*:

$$\begin{aligned} c(x, y, z) &= (x, z, y) , \\ d(x, y, z) &= (z, y, x) , \\ e(x, y, z) &= (y, x, z) . \end{aligned} \quad (5)$$

It can be easily verified that any two operations in sequence are equivalent to another operation of the same set, i.e., the set of operations is closed to the product. For example,

$$(ab)(x, y, z) = a[b(x, y, z)] = a(y, z, x) = (x, y, z) = \mathbb{1}(x, y, z). \quad (6)$$

In addition to providing an example of product ($ab = \mathbb{1}$), the above equation shows that b is the inverse of a .

The results of all possible products of two elements can be organized in the group's **multiplication table**, shown below.

	$\mathbb{1}$	a	b	c	d	e	
$\mathbb{1}$	$\mathbb{1}$	a	b	c	d	e	
a	a	b	$\mathbb{1}$	e	c	d	
b	b	$\mathbb{1}$	a	d	e	c	
c	c	d	e	$\mathbb{1}$	a	b	
d	d	e	c	b	$\mathbb{1}$	a	
e	e	c	d	a	b	$\mathbb{1}$	

(7)

As we mentioned before, a subset of the group's operations forms a **subgroup** if the operations of this subset form a group. For example, $\{\mathbb{1}, a, b, \}$ is a subgroup of S_3 , as shown in the multiplication table below, extracted from the above table.

	$\mathbb{1}$	a	b	
$\mathbb{1}$	$\mathbb{1}$	a	b	
a	a	b	$\mathbb{1}$	
b	b	$\mathbb{1}$	a	

(8)

Operations and operators

Since we will be dealing with a quantum system, it is relevant to know what are the effects of symmetry operations on the states of the system, which are described by wave-functions in a Hilbert space. To any symmetry operation (acting on the space of coordinates) one can associate an *operator* acting on a space of functions.

We define the action of a symmetry operator A associated with the operation a by

$$A\psi(\mathbf{r}) = \psi(a^\dagger \mathbf{r}). \quad (9)$$

Given that symmetry operations are orthogonal transformations, a^\dagger is the inverse of a . We can understand why the inverse operation is used if we think of a rotation in space: rotating a “vector” (in this case, the wave function) in one sense is equivalent to rotating the coordinate system in the opposite sense.

Operators that perform transformations must be unitary in order to preserve the function's *norm*. Thus, symmetry operations are unitary transformations, i.e., $A^{-1} = A^\dagger$, in agreement with $a^{-1} = a^\dagger$.

In our example (group S_3), we define the group of operators

$$S_3 = \{I, A, B, C, D, E\}, \quad (10)$$

where I corresponds to the identity operation.

The groups S_3 and S_3 are said to be **isomorphic**, since there is a two-way correspondence between their elements, and both groups have the same multiplication table. This can be seen by the following example,

$$AC \psi(\mathbf{r}) = A \psi(c^\dagger \mathbf{r}) = \psi(c^\dagger [a^\dagger \mathbf{r}]) = \psi([ac]^\dagger \mathbf{r}) = \psi(e^\dagger \mathbf{r}) = E \psi(\mathbf{r}), \quad (11)$$

where it is evident that $AC = E$ in correspondence to $ac = e$.

Invariant manifolds

A set of n linearly independent functions defines a **manifold** to which these functions provide a basis, since any linear combination of functions of this set also belongs to the manifold.

To illustrate, let us choose

$$\begin{aligned} \psi_1(x, y, z) &= \frac{1}{(2\pi)^{3/2}} e^{i(-x+y+z)}, \\ \psi_2(x, y, z) &= \frac{1}{(2\pi)^{3/2}} e^{i(x-y+z)}, \\ \psi_3(x, y, z) &= \frac{1}{(2\pi)^{3/2}} e^{i(x+y-z)}. \end{aligned} \quad (12)$$

These functions are orthonormal in a cube of edge 2π , which means that

$$\int_0^{2\pi} dx \int_0^{2\pi} dy \int_0^{2\pi} dz \psi_i^*(x, y, z) \psi_j(x, y, z) = \delta_{ij}, \quad i, j = 1, 2, 3. \quad (13)$$

They define a three-dimensional manifold which we will call M .

The following table shows the results of operating with the elements of S_3 on the basis functions $\{\psi_1, \psi_2, \psi_3\}$ of M .

$I \psi_1 = \psi_1$	$A \psi_1 = \psi_2$	$B \psi_1 = \psi_3$	$C \psi_1 = \psi_1$	$D \psi_1 = \psi_3$	$E \psi_1 = \psi_2$
$I \psi_2 = \psi_2$	$A \psi_2 = \psi_3$	$B \psi_2 = \psi_1$	$C \psi_2 = \psi_3$	$D \psi_2 = \psi_2$	$E \psi_2 = \psi_1$
$I \psi_3 = \psi_3$	$A \psi_3 = \psi_1$	$B \psi_3 = \psi_2$	$C \psi_3 = \psi_2$	$D \psi_3 = \psi_1$	$E \psi_3 = \psi_3$

(14)

Note that the application of any operator of S_3 on any function of M results in another function belonging to M . It is then said that M is an **invariant manifold** of S_3 .

Manifold decomposition

In many cases a manifold can be *decomposed* into smaller manifolds. If this is possible, the original manifold is said to be **reducible**. The decomposition is performed by choosing an appropriate new basis.

For our manifold M , we can define, for example, the following combinations of the functions given in Eq. (12):

$$\begin{aligned}\chi_1 &= \frac{1}{\sqrt{3}}(\psi_1 + \psi_2 + \psi_3) , \\ \chi_2 &= \frac{1}{\sqrt{2}}(\psi_2 - \psi_3) , \\ \chi_3 &= \frac{1}{\sqrt{6}}(2\psi_1 - \psi_2 - \psi_3) .\end{aligned}\tag{15}$$

It is easy to show that

- (1) the set $\{\chi_1, \chi_2, \chi_3\}$ is also orthonormal on a cube of edge 2π (**EXERCISE 1**);
- (2) χ_1 defines a **one-dimensional** invariant manifold of S_3 (**EXERCISE 2**);
- (3) $\{\chi_2, \chi_3\}$ defines a **two-dimensional** invariant manifold of S_3 (**EXERCISE 3**).

Thus, it was possible to **decompose** the three-dimensional invariant manifold M into two other invariant manifolds (of lower dimensions) by the basis change $\{\psi_i\} \rightarrow \{\chi_i\}$.

Matrix representations

If A is an operator belonging to a (generic) group G , one can construct a matrix representation of A by choosing a basis $\{\psi_i\}$ in an invariant manifold of G , and evaluating the matrix elements

$$A_{ij} \equiv \langle \psi_i | A | \psi_j \rangle .\tag{16}$$

Suppose that three operators of G obey the product rule $C = AB$. Taking into account that the basis $\{\psi_i\}$ is orthonormal and *complete*, i.e.,

$$\sum_{i=1}^n |\psi_i\rangle \langle \psi_i| = 1 ,\tag{17}$$

we have

$$C_{ij} = \langle \psi_i | C | \psi_j \rangle = \langle \psi_i | AB | \psi_j \rangle = \sum_l \langle \psi_i | A | \psi_l \rangle \langle \psi_l | B | \psi_j \rangle = \sum_l A_{il} B_{lj} ,\tag{18}$$

which is the usual rule of matrix product ($\mathbf{C} = \mathbf{AB}$). Therefore, the set of matrices representing operators belonging to G **forms a group**, which we will call \mathcal{G} , with the same product rule of the group G , thus being a *matrix representation* of this group.

If there is a one-to-one correspondence between the group of operators and the group of matrices that represent them, we say that these groups are **isomorphic**. If the number of operators of G associated with the same matrix of \mathcal{G} is greater than one, we say that G is **homomorphic** to \mathcal{G} . In the case of isomorphism, the group representation is said to be *faithful*. To each representation there are associated *basis functions*, which are nothing but a set of functions defining a basis for the corresponding invariant manifold.

From the above definition of matrix representation, it is easy to see that any group has a **one-dimensional** representation in which **all** group members are represented by the number **1**. It is called the *identity representation* (or *trivial representation*). Any function that is invariant under all operations of the group may be a basis function for this representation.

If an invariant manifold M of a group G is **reducible**, the matrices of a representation of G in this manifold can be brought to a **block-diagonal form**, each block corresponding to an **irreducible representation** (often shortened to *irrep*).

Classes

If three operators, A , B and X , of a group G satisfy the relation

$$B = XAX^\dagger, \quad (19)$$

then A and B belong to the same **class**. Note that, by this definition, the identity element constitutes a class by itself.

As the **trace** of a matrix is invariant under a unitary transformation, all elements of the same class have identical traces in a given representation. In Group Theory, traces are called *characters*. So, the character is a property of a class (not of a single element), but depends on representation.

Some theorems (for finite groups)

We present the following theorems as tools to analyze groups that we might study. Formal demonstrations can be found in textbooks of Group Theory.

Theorem 1 - The number of irreducible representations of a group is equal to the number of classes.

Theorem 2 - The dimensions (n_α) of all the irreducible representations (α) of a group with N elements satisfy the sum rule

$$\sum_{\alpha} n_{\alpha}^2 = N . \quad (20)$$

Theorem 3 - The following *orthogonality relations* hold for the characters (χ) of the irreducible representations of a group:

$$\sum_A N_A \chi_{\alpha}^*(A) \chi_{\beta}(A) = N \delta_{\alpha\beta} , \quad (21a)$$

$$\sum_{\alpha} \chi_{\alpha}^*(A) \chi_{\alpha}(A') = \frac{N}{N_A} \delta_{A,A'} , \quad (21b)$$

where N_A is the number of elements belonging to class A .

In fact, Eq. (20) is contained in Eq. (21b) when $A = A' = E$, where E is the usual notation for the identity class (we did not follow this usage in our S_3 example!).

If we know the elements of a group and which classes they define, these theorems allow to determine the number of *irrep*'s, and the *character* of each class in each *irrep*. Usually, these characters are arranged in a *character table*, with columns labeled by class and rows by *irrep*. It is usual to add an extra column containing some simple possible basis functions for each *irrep*.

Relationship with energy eigenfunctions

Given a physical system described by a Hamiltonian \mathcal{H} , the system's symmetry group (G) is composed by all the independent unitary operators that leave the Hamiltonian invariant. Therefore, for any $A \in G$,

$$A\mathcal{H}A^{\dagger} = \mathcal{H} \quad \Rightarrow \quad [A, \mathcal{H}] = 0 . \quad (22)$$

If ψ is an energy eigenfunction corresponding to the eigenvalue E , i.e., $\mathcal{H}\psi = E\psi$, then

$$A\mathcal{H}\psi = EA\psi \quad \Rightarrow \quad \mathcal{H}(A\psi) = E(A\psi) . \quad (23)$$

Therefore, $A\psi$ is also an energy eigenfunction corresponding to the same eigenvalue.

We can define a manifold M whose basis consists of a set $\{\psi_1, \psi_2, \dots, \psi_n\}$ of linearly independent energy eigenfunctions corresponding to an eigenvalue E , n times degenerate. Any linear combination

$$\phi = \sum_{i=1}^n c_i \psi_i \quad (24)$$

is an eigenfunction of \mathcal{H} corresponding to the same eigenvalue. This also holds for a function $A\phi$, where A is any operator of the symmetry group, since

$$\mathcal{H}(A\phi) = A\mathcal{H}\phi = AE\phi = E(A\phi) . \quad (25)$$

So, M is an *invariant manifold* of G .

In summary, the eigenfunctions of the Hamiltonian \mathcal{H} of **any** quantum system can be chosen to belong to *irreducible* invariant manifolds of the system's symmetry group, therefore providing basis functions for its *irreps*.

As matrix elements of the Hamiltonian between eigenfunctions belonging to distinct *irreps* are null, the matrix representation of the Hamiltonian in the whole Hilbert space can be made *block diagonal*, each block corresponding to an *irrep*. The same applies to matrix representations of any operators that commute with the Hamiltonian (including the operators of the symmetry group).

The **dimension** of a given *irrep* determines the degree of ***essential degeneracy*** of the corresponding energy eigenvalue. **Essential** means that the degeneracy is **mandatory**, being a consequence of symmetry properties. In contrast, equality between eigenvalues corresponding to distinct irreducible representations characterizes an ***accidental degeneracy***. It must be due to a special choice of parameter values in the Hamiltonian that effectively changes its symmetry group.

In Text 3 we will use the generic concepts reviewed here to analyze electron states in crystalline solids in the *independent electron approximation*.