# 6 Symmetry Properties of Electronic and Photonic Band Structures

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**Abstract.** Group theoretical investigations have a huge potential to simplify calculations in solid state theory. We will discuss the application of group theory to electronic and photonic band structures. The symmetry properties of the Schrödinger equation and Maxwell's equations as well will be investigated. We have developed methods to simplify group theoretical investigations based on the computer algebra system *Mathematica*.

## 6.1 Introduction

The majority of physical systems exhibit intrinsic symmetries which can be used to simplify the solution of the equations governing these systems. Group theory as a mathematical tool plays an important role to classify the solutions within the context of the underlying symmetries. Extensive use of group theory has been made to simplify the study of electronic structure or vibrational modes of solids or molecules. There exists a number of excellent books illustrating the use of group theory. [6.1–6.4]

Similarities between the solution of the Schrödinger equation, or the Kohn-Sham equations in the framework of density functional theory for a crystal, and the solution of Maxwell's equations have been already pointed out by Joannopoulos *et al.*. [6.5] Therefore, it is clear that the same group theoretical concepts like in the theory of electronic band structures including two-dimensional and three-dimensional structures, surfaces as well as defects should be applicable to photonic band structure calculations, if we take into account the vectorial nature of the electromagnetic field.

There are several publications about group theoretical investigations of photonic crystals in the literature. Sakoda has extensively studied the symmetry properties of two-dimensional and three-dimensional photonic crystals (cf. [6.6–6.9]), starting from a plane wave representation of the electromagnetic fields. Group theoretical investigations are done also by Ohtaka and Tanabe. [6.10] They investigate the symmetry properties of photonic crystals represented by an array of dielectric spheres. In this case a series expansion in terms of vector spherical harmonics is used.

The problem at the end for electronic and the photonic band structure calculations is: How to apply group theory in the actual research work, if one goes away from all the textbook examples. The aim of the paper is to show,

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that computer algebra tools are appropriate to simplify group theoretical discussions connected with the calculation of electronic and photonic band structures.

After a short discussion of the usefulness of computer algebra systems, we will introduce basic concepts of group theory. Representation theory will be discussed next, followed by the analysis of the symmetry properties of the Schrödinger equation and of Maxwell's equations. We want to solve the electronic and photonic problem for a lattice periodic situation. In the one case we have a periodic potential $V(\mathbf{r}) = V(\mathbf{r}+\mathbf{R})$ in the other case a periodic dielectric constant $\epsilon(\mathbf{r}) = \epsilon(\mathbf{r}+\mathbf{R})$. The consequences of that periodicity will be considered. A simplification of the solution of both kinds of problems is possible, if symmetry-adapted basis functions are used. This is discussed in more detail for the electronic problem. At the end we apply group theory to the calculation of photonic band structures.

## 6.2 Group Theory Packages for Computer Algebra Systems

Computer algebra (CA) systems like *Mathematica* or *Maple* have been developed to allow formal mathematical manipulations. Nowadays those systems are complete in such a sense, that formal manipulations, numerical calculations, as well as graphical representations are possible in an easy and intuitive way with the same software. Apart from such general purpose CA systems, there exist also systems developed for special applications in mathematics. Group theoretical considerations, although conceptionally easy, lead very often to time-consuming algebraic calculations, which are error-prone. Therefore group theory is an excellent field for the application of CA systems. Some systems for abstract group theory are available [6.11], but they are not very helpful for considerations in solid state theory. K. Shirai developed a *Mathematica* package for group theory in solid state physics [6.12]. We followed similar ideas but tried to make the package more easy to use.

We have constructed a package for the CA system *Mathematica* which allows to do group theoretical manipulations which occur in solid state theory. [6.13] The software allows basic considerations with point groups, contains tight-binding theory for the electronic structure of solids, but also special applications to photonic crystals. The package is accompanied by an on line help, which is integrated in *Mathematica*'s help system. All considerations discussed in this paper can be found in a *Mathematica* notebook which is part of our package. We will give references to the commands implemented in the package throughout the paper.

## 6.3 Basic Concepts in Group Theory

In this section we will introduce the basic concepts of group theory. We will focus on definitions which will be necessary for the following discussions. To illustrate the concepts, let us discuss the symmetry group of a square in two dimensions, i.e. we are interested in all transformations which transform the square into itself. (cf. Fig. 6.1) This example will be of later use for the discussion of photonic band structures.

A set $\mathcal{G}$ of elements A,B,C ... is called a *group* if the following four axioms are fulfilled: i) There exists an operation, often called multiplication, which associates every pair of elements of $\mathcal{G}$ with another element of $\mathcal{G}$: $A \in \mathcal{G}, B \in \mathcal{G} \rightarrow A \cdot B = C, C \in \mathcal{G}$, ii) The associative law is valid: $A, B, C \in \mathcal{G} \rightarrow (A \cdot B) \cdot C = A \cdot (B \cdot C) = A \cdot B \cdot C$, iii) in the set exists an identity element: $A, E \in \mathcal{G} \rightarrow A \cdot E = E \cdot A = A$, iv) for all $A \in \mathcal{G}$ exists an inverse element $A^{-1} \in \mathcal{G}$ with $A \cdot A^{-1} = A^{-1} \cdot A = E$.

The symmetry group of the square consists of rotations of $\pi/2$ around the z-axis and mirror operations. The normal vectors of the mirror planes are the x and y-axis, $\overrightarrow{Oa}$ and $\overrightarrow{Ob}$. A mirror symmetry may be expressed as a twofold rotation, followed by an inversion. All the symmetry operations of the group of the square, named $C_{4\mathrm{v}}$ are:

$$C_{4\mathrm{v}} = \left\{E, C_{2\mathrm{z}}, C_{4\mathrm{z}}, C_{4\mathrm{z}}^{-1}, IC_{2\mathrm{x}}, IC_{2\mathrm{y}}, IC_{2\mathrm{a}}, IC_{2\mathrm{b}}\right\} \tag{6.1}$$

If the group theory package is included in a *Mathematica* notebook by means of the command `Needs["GroupTheory`Master`"]`[1], the newly defined command `c4v=InstallGroup["C4v"]` will install the group in terms of the rotation matrices of the elements. The matrices are stored in the list `c4v`. The command `c4vs=GetSymbol[c4v]` will transform the elements of the group into symbolic form (cf.(6.1)). The symbols will be stored in the list `c4vs`. Operations on the group can be done in both representations of the group elements. The group multiplication is implemented in our *Mathematica* package by a redefinition of the infix-operator $\oplus$ (see [6.25]).

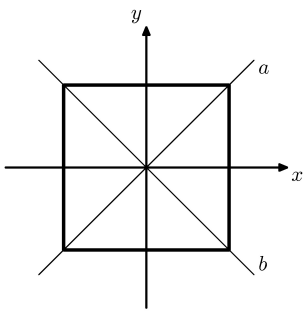


**Fig. 6.1.** Symmetry of a square.

[1] *Mathematica* commands are marked using this particular font.

For the graphical user interface of *Mathematica* we designed two additional palettes. The palette `SymmetryElements` contains all the symmetry elements of the 32 point groups. The palette `PointGroup` contains all the operations defined in the package.

The inspection of the multiplication table (`MultiplicationTable[c4v]`) of the group shows, that the table is not symmetric, indicating that the group multiplication is not commutative in this group. Therefore the group is not *abelian* (`AbelianQ[c4vs]` returns `False`.). All elements of the group can be also generated by successive multiplication of only two elements of the group, the so called *generators*. For our example we find the generators $C_{4z}, IC_{2x}$. (`Generators[group_]`) [2]

Any set of elements of a group which obeys all the group postulates is called a *subgroup* of the group. Examples for subgroups are: $\{E, C_{2z}, C_{4z}, C_{4z}^{-1}\}$ and $\{E, IC_{2y}\}$ (`SubGroupQ[group_,subgroup_]` performs a test).

Another structure of the group is introduced by the definition of *conjugate elements*. An element $B$ of the group $\mathcal{G}$ is said to be conjugate to $A$ if their exists a group element $X$ such that $B = XAX^{-1}$. A *class* (`Classes[c4vs]`) is a collection of mutually conjugate elements of a group. The classes of the group $C_{4v}$ are: $(E)$, $(C_{2z})$, $(C_{4z}, C_{4z}^{-1})$, $(IC_{2x}, IC_{2y})$, $(IC_{2a}, IC_{2b})$. It is easy to prove that: i) $E$ always forms a class on its own, ii) every group element in $\mathcal{G}$ is a member of some class of $\mathcal{G}$, iii) no element can be the member of two classes of $\mathcal{G}$, iv) if $\mathcal{G}$ is an abelian group, every element forms a class on its own.

We have already seen, that the group in the example can be represented by the abstract symbols or the rotation matrices. The relation between groups is formulated more rigorously in terms of *homomorphism* and *isomorphism*. Two groups $\mathcal{G} = \{A, B, C, \dots\}$ and $\mathcal{G}' = \{A', B', C', \dots\}$ are called homomorphic, if i) to each element of $\mathcal{G}$ corresponds one and only one element of $\mathcal{G}'$ ii) for all elements holds $A \to A', B \to B' \hookrightarrow AB \to A'B'$. The set of elements which are mapped to $E' \in \mathcal{G}'$ in a homomorphism is called *kernel of the homomorphism* $\mathcal{N}_K$. In contrast to the homomorphism the mapping in the *isomorphism* is one-to-one. Whereas the mapping of the symbols on the rotation matrices constitutes an isomorphism, the following mapping $E, C_{2z}, C_{4z}, C_{4z}^{-1} \Rightarrow +1$ and $IC_{2x}, IC_{2y}, IC_{2a}, IC_{2b} \Rightarrow -1$ constitutes a homomorphism.

## 6.4 Representation Theory

### 6.4.1 Matrix Representations of Groups

*Matrix representations* of symmetry groups are the essential tools to investigate symmetry properties of solutions of field equations as Schrödinger's equation or Maxwell's equations.

[2] The formal arguments of the commands indicate, which type of information has to be plugged in. For more information use the help system or the example notebook.

A group of square matrices, with the matrix multiplication as relation between the elements, which is homomorphic to a group $\mathcal{G}$ is called a matrix representation of $\mathcal{G}$. Each element $A \in \mathcal{G}$ corresponds to a matrix $\Gamma(A)$:

$$\begin{aligned} \Gamma(A)\Gamma(B) &= \Gamma(C) \quad \forall \quad A, B, C \in \mathcal{G} \\ \Gamma(E) &= E \qquad (\text{identity matrix}) \\ \Gamma(A^{-1}) &= \Gamma(A)^{-1} \end{aligned} \tag{6.2}$$

It is obvious that an $l$-dimensional representation consisting of a set of $(l \times l)$-matrices can be transformed in another representation by means of a similarity transformation $\Gamma'(A) = S^{-1}\Gamma(A)S$ using a non-singular $(l \times l)$-matrix $S$.

The rotation matrices of a finite symmetry group form a three-dimensional matrix representation in that sense. The mapping of the group elements of $C_{4\mathrm{v}}$ onto the numbers $+1, -1$ represents also, in this case a one-dimensional, matrix representation of the group.

From two matrix representations $\Gamma^1$ and $\Gamma^2$ of $\mathcal{G}$ with the dimensions $l_1$ and $l_2$, a $(l_1 + l_2)$-dimensional representation $\Gamma$ can be built, forming the block matrices

$$\Gamma(A) = \left(\begin{array}{c|c} \Gamma^1(A) & 0 \\ \hline 0 & \Gamma^2(A) \end{array}\right). \tag{6.3}$$

The representation $\Gamma$ is called the *direct sum* of the representations $\Gamma^1$ and $\Gamma^2$ : $\Gamma = \Gamma^1 \oplus \Gamma^2$. Representations which can be transformed into direct sums by similarity transformations are called *reducible*. If such a transformation is not possible, the representation is called *irreducible*. The rotation matrices of the group $C_{4\mathrm{v}}$ are given by:

$$\Gamma(E) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \Gamma(C_{2\mathrm{z}}) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \Gamma(C_{4\mathrm{z}}) = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\Gamma(IC_{4\mathrm{z}}^{-1}) = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \Gamma(IC_{2\mathrm{x}}) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \Gamma(IC_{2\mathrm{y}}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\Gamma(IC_{2\mathrm{a}}) = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \Gamma(IC_{2\mathrm{b}}) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

The rotation matrices are block matrices and therefore reducible into a two-dimensional and a one-dimensional matrix representation of $C_{4\mathrm{v}}$.

An important quantity of a matrix representation which will not change under a similarity transformation is the trace of the rotation matrix. This trace is called the *character* $\chi$ of the representation matrix.

$$\chi(A) = \sum_{j=1}^{l} \Gamma(A)_{jj} \tag{6.4}$$

The character system of a group is called the character table. The character table can be generated automatically using `CharacterTable[c4vs]`. We will get:

| | $C_1$ | $C_2$ | 2 | $C_3$ | $2C_4$ | $2C_5$ |
|---|---|---|---|---|---|---|
| $\Gamma^1$ | 1 | 1 | 1 | 1 | 1 |
| $\Gamma^3$ | 1 | 1 | 1 | -1 | -1 |
| $\Gamma^4$ | 1 | 1 | -1 | 1 | -1 |
| $\Gamma^2$ | 1 | 1 | -1 | -1 | 1 |
| $\Gamma^5$ | 2 | -2 | 1 | 0 | 0 |

$C_1 = (E)$
$C_2 = (C_{2z})$
$C_3 = (C_{4z}, C_{4z}^{-1})$
$C_4 = (IC_{2x}, IC_{2x})$
$C_5 = (IC_{2a}, IC_{2b})$

The character table represents a series of character theorems, which are important for later use: i) the number of inequivalent irreducible representations of a group $\mathcal{G}$ is equal to the number of classes of $\mathcal{G}$, ii) the characters of the group elements in the same class are equal, iii) the sum of the squares of the dimensions of all irreducible representations is equal to the order of the group, iv) two representations are equivalent if their character systems are equivalent. Especially important are the following theorems:

– A representation $\Gamma$ is irreducible, if:

$$\sum_{T \in \mathcal{G}} \mid \chi(T) \mid^2 = g \; . \tag{6.5}$$

(The sum of the squares of the characters of the rotation matrices of $C_{4v}$ exceeds the group order $g = 8$, indicating that this representation cannot be irreducible.)

– The number $n$, how often an irreducible representation $\Gamma^i$, or a representation equivalent to $\Gamma^i$, is contained in the reduction of the reducible representation $\Gamma$, is given by:

$$n = \frac{1}{g} \sum_{T \in \mathcal{G}} \chi(T) \chi^i(T)^* \tag{6.6}$$

($g$- order of the group, $\chi(T), \chi^i(T)$ - character of the group element in the representation $\Gamma$ and $\Gamma^i$)

– Orthogonality theorems for characters

$$\sum_k \chi^i(\mathrm{C}_k)^* \chi^j(\mathrm{C}_k) N_k = g \, \delta_{ij} \tag{6.7}$$

$$\sum_i \chi^i(\mathrm{C}_k)^* \chi^i(\mathrm{C}_l) N_k = g \, \delta_{kl} \tag{6.8}$$

($\chi^i(\mathrm{C}_k), \chi^j(\mathrm{C}_k)$ characters of elements in class $\mathrm{C}_k$ in irreducible representations $\Gamma^i$ and $\Gamma^j$, $N_k$ - number of elements in $\mathrm{C}_k$. In the first relation the summation runs over all classes of the group. In the second relation it runs over all inequivalent irreducible representations of the group.)

The character theorems can be easily checked for all the point groups using *Mathematica*.

### 6.4.2 Basis Functions of Irreducible Representations

Our final goal is the investigation of the symmetry properties of the solutions of Maxwell's equation. Therefore we have to associate the symmetry expressed by the symmetry group, i.e. the point group $C_{4\mathrm{v}}$ in our example, with the symmetry properties of scalar and vector fields.

We define a transformation operator to a symmetry element $T$ as $\hat{P}(T)$. For a scalar function it holds:

$$\hat{P}(T)f(\boldsymbol{r}) = f(T^{-1}\boldsymbol{r}) \tag{6.9}$$

The operators $\hat{P}(T)$ form a group of linear unitary operators. If we discuss Maxwell's equations, we have to deal with vector fields in general. Instead of (6.9) the following transformation has to be applied to the vector field $\boldsymbol{F}$:

$$\hat{P}(T)\boldsymbol{F}(\boldsymbol{r}) = T\boldsymbol{F}(T^{-1}\boldsymbol{r}) \tag{6.10}$$

Now we define the *basis functions* of an irreducible representation (IR) and concentrate on scalar fields. If a set of $l$-dimensional matrices $\Gamma(T)$ forms a representation of the group $\mathcal{G}$ and $\phi_1(\boldsymbol{r}), \ldots, \phi_l(\boldsymbol{r})$ is a set of linear independent functions such that

$$\hat{P}(T)\phi_n(\boldsymbol{r}) = \sum_{m=1}^{l} \Gamma(T)_{mn}\phi_m(\boldsymbol{r}) \qquad n = 1, 2, \ldots, l \tag{6.11}$$

then functions $\phi_n(\boldsymbol{r})$ are called partners in a set of basis functions of the representation $\Gamma$. $\phi_n$ is said to transforms like the $n$th row of the representation. We can write any function $\phi(\boldsymbol{r})$, which can be normalized, as a sum of basis functions of the irreducible representations $\Gamma^p$ of the group.

$$\phi(\boldsymbol{r}) = \sum_{p} \sum_{n=1}^{l_p} \phi_n^p(\boldsymbol{r}) \tag{6.12}$$

Note, that this is not an expansion like the Fourier series. We don't expand a function with respect to an orthonormal complete set of functions here. The set of functions $\phi_n^p(\boldsymbol{r})$ depends on $\phi(\boldsymbol{r})$ itself. The functions $\phi_n^p(\boldsymbol{r})$ in (6.12) can be found by means of the so called *projection operators*.

$$\mathcal{P}^p_{mn} = \left(\frac{l_p}{g}\right) \sum_{T\in\mathcal{G}} \Gamma^p(T)^*_{mn} \hat{P}(T), \quad \mathcal{P}^p_{mn}\phi^q_i(\boldsymbol{r}) = \delta_{pq}\delta_{ni}\,\phi^p_m(\boldsymbol{r}) \tag{6.13}$$

$$\mathcal{P}^p = \left(\frac{l_p}{g}\right) \sum_{T\in\mathcal{G}} \chi^p(T)^* \hat{P}(T) \tag{6.14}$$

The projection operators are implemented in the package.
(cf. `CharacterProjectionOperator[classes_,chars_,func_]`.) As an example, we investigate the symmetry properties of a function $\phi(\boldsymbol{r}) = (a\,x + b\,y)g(r)$ (a and b are constants). We apply the projection operators connected to the group $C_{4v}$, to the function and get the following result

$$\begin{aligned} &\phi^5_1(\boldsymbol{r}) = \mathcal{P}^5_{11}\,\phi(\boldsymbol{r}) = a\,x\;g(r) \quad \mathcal{P}^5_{12}\,\phi(\boldsymbol{r}) = b\,x\;g(r) \\ &\mathcal{P}^5_{21}\,\phi(\boldsymbol{r}) = a\,y\;g(r) \qquad\qquad \phi^5_2(\boldsymbol{r}) = \mathcal{P}^5_{22}\,\phi(\boldsymbol{r}) = b\,y\;g(r) \end{aligned} \tag{6.15}$$

It is impossible to project out parts of $\phi(\boldsymbol{r})$ transforming like other IRs of $C_{4v}$. Therefore our trial function $\phi(\boldsymbol{r}) = (a\,x + b\,y)g(r)$ is a sum of functions, transforming like the representation $\Gamma^5$ $(E)$.

If we consider three-dimensional photonic crystals we cannot resort to scalar fields anymore. We have to take into account the full vectorial nature of the fields also in symmetry considerations. A more detailed discussion of the subject can be found in [6.14–6.16].

## 6.5 Symmetry Properties of Schrödinger's Equation and Maxwell's Equations

Here we want to investigate the symmetry properties of scalar or vector fields, which we get as solutions of Schrödinger's equation or Maxwell's equations. The operators $\hat{P}(T)$ form a group of linear unitary operators. This group is isomorphic to the group of symmetry elements $T$. The Hamilton-Operator $\hat{H}(\boldsymbol{r})$ of the time-independent Schrödinger equation $\hat{H}\psi(\boldsymbol{r}) = E\,\psi(\boldsymbol{r})$ is given by

$$\hat{H}(\boldsymbol{r}) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \boldsymbol{r}^2} + V(\boldsymbol{r})\ . \tag{6.16}$$

For an arbitrary transformation $T$ the transformation behavior of the Hamiltonian is given by

$$\hat{H}(\boldsymbol{r}) = \hat{P}(T)\hat{H}(T\boldsymbol{r})\hat{P}(T)^{-1}\ . \tag{6.17}$$

For transformations which leave $\hat{H}$ invariant, i.e. $\hat{H}(T\boldsymbol{r}) = \hat{H}(\boldsymbol{r})$ we get:

$$[\hat{H}, \hat{P}(T)] = 0\ . \tag{6.18}$$

All transformations, which let $\hat{H}$ invariant, form a group. The corresponding operators $\hat{P}(T)$ form an isomorphic group, the group of the Schrödinger equation. All elements of the group of the Schrödinger equation commute with $\hat{H}$. Because the operator of the kinetic energy is invariant under all rotations forming the group $O(3)$, the symmetry of the Hamiltonian is determined exclusively by the potential $V(\boldsymbol{r})$.

We want to consider photonic crystals. Therefore we have to extend the analysis to Maxwell's equations.

$$\begin{aligned} \nabla \boldsymbol{D}(\boldsymbol{r},t) &= 0 & \nabla \times \boldsymbol{E}(\boldsymbol{r},t) &= -\tfrac{\partial}{\partial t}\boldsymbol{B}(\boldsymbol{r},t) \\ \nabla \boldsymbol{B}(\boldsymbol{r},t) &= 0 & \nabla \times \boldsymbol{H}(\boldsymbol{r},t) &= \tfrac{\partial}{\partial t}\boldsymbol{D}(\boldsymbol{r},t) \end{aligned} \tag{6.19}$$

We assume that we have no free charges and currents. Using the materials equations $\boldsymbol{D} = \epsilon\epsilon_0\boldsymbol{E}, \boldsymbol{B} = \mu_0\boldsymbol{H}$ and a harmonic time dependence for the fields, i.e. $\boldsymbol{E}(\boldsymbol{r},t) = \boldsymbol{E}(\boldsymbol{r})\exp(i\omega t)$ the basic equations are given by

$$\hat{\Xi}_E \boldsymbol{E}(\boldsymbol{r}) = \frac{1}{\epsilon(\boldsymbol{r})}\nabla \times (\nabla \times \boldsymbol{E}(\boldsymbol{r})) = \left(\frac{\omega}{c}\right)^2 \boldsymbol{E}(\boldsymbol{r}) \tag{6.20}$$

$$\hat{\Xi}_H \boldsymbol{H}(\boldsymbol{r}) = \nabla \times \frac{1}{\epsilon(\boldsymbol{r})}\nabla \times \boldsymbol{H}(\boldsymbol{r}) = \left(\frac{\omega}{c}\right)^2 \boldsymbol{H}(\boldsymbol{r}) \tag{6.21}$$

If we assume a two-dimensional photonic crystal, i.e. the dielectric constant varies in the x-y-plane ($\boldsymbol{r}_{||}$) we can resort to the solution of scalar equations for the field components in z-direction.

$$\hat{\Xi}_E^{\mathrm{2D}} E_z(\boldsymbol{r}_{||}) = -\frac{1}{\epsilon(\boldsymbol{r}_{||})}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) E_z(\boldsymbol{r}_{||}) = \left(\frac{\omega}{c}\right)^2 E_z(\boldsymbol{r}_{||}) \tag{6.22}$$

$$\begin{aligned} \hat{\Xi}_H^{\mathrm{2D}} H_z(\boldsymbol{r}_{||}) &= -\left(\frac{\partial}{\partial x}\frac{1}{\epsilon(\boldsymbol{r}_{||})}\frac{\partial}{\partial x} + \frac{\partial}{\partial y}\frac{1}{\epsilon(\boldsymbol{r}_{||})}\frac{\partial}{\partial y}\right) H_z(\boldsymbol{r}_{||}) \\ &= \left(\frac{\omega}{c}\right)^2 H_z(\boldsymbol{r}_{||}) \end{aligned} \tag{6.23}$$

Corresponding to (6.18) we have to find all the transformations $T$ which leave the operators $\hat{\Xi}_E, \hat{\Xi}_H$ for the three-dimensional case or $\hat{\Xi}_E^{\mathrm{2D}}, \hat{\Xi}_H^{\mathrm{2D}}$ for the two-dimensional case invariant. It can be shown that the group of Maxwell's equations is formed by the space group of the photonic crystal, i.e. consists of all translations and rotations which transform $\epsilon(\boldsymbol{r})$ into itself.

## 6.6 Consequences of Lattice Periodicity

Here we want to illustrate the consequences of lattice periodicity to the solution of Schrödinger equation or Maxwell's equation. We consider crystals which have $d$-dimensional translational symmetry and can be represented as a set of points sitting on a Bravais-lattice (for convenience we do not take

into account a possible arrangement of basis atoms around the lattice points here). We want to denote the translation vectors which form the Bravais lattice $\{\mathbf{T}\}$ as

$$\mathbf{T} = \sum_{i=1}^{d} m_i \mathbf{a}_i, \qquad m_i = 0, \pm 1, \pm 2 \ldots \tag{6.24}$$

with $\mathbf{a}_i$ being a basic lattice vector. Associated with the set $\{\mathbf{T}\}$ is a set of symmetry transformations (translations), which leave the crystal invariant. It can easily established that this set forms a infinite, discrete group, denoted here as $\mathcal{T}$.

Associated with every lattice point might be a set of symmetry operations consisting of rotations, mirror reflections and so on, which leave the crystal and the point they are applied to also invariant. The group formed from this set is called a point group $\mathcal{G}_0$.

Let us introduce a new symbols to state the considerations made so far more clearly. The Seitz-operator $\{\mathbf{R}|\mathbf{t}\}$ takes some vector $\mathbf{r}$ to a new vector $\mathbf{r}'$ by first rotating and then translating it

$$\mathbf{r}' = \{\mathbf{R}|\mathbf{t}\}\mathbf{r} = \mathbf{R}\mathbf{r} + \mathbf{t}. \tag{6.25}$$

Here $\mathbf{R}$ denotes a rotation matrix and $\mathbf{t}$ is a vector. Then the translation group $\mathcal{T}$ can be characterised by the elements $\{\mathbf{E}|\mathbf{T}\}$ ($\mathbf{E}$ is the unity matrix) and the elements of the point group elements as $\{\mathbf{R}|\mathbf{0}\}$. The space group $\mathcal{G}$ of a crystal is defined as a group of operations $\{\mathbf{R}|\mathbf{t}\}$ which contains as a subgroup the set of all pure primitive translations of a lattice, $\mathcal{T}$, but which contains no other pure translations. Here we want to consider only symmorphic space groups whose symmetry operations consists of a rotation followed by a *primitive* translation $\mathbf{T}$ (this excludes the case of having for examples glide-planes and screw axis as symmetry elements of the crystal, where fractions of $\mathbf{T}$, $\mathbf{t} = \mathbf{T}/n$, $n \in \mathbb{N}$ are involved).

In what follows we want first use the properties of $\mathcal{T}$ to arrive at the Bloch-theorem which makes a statement about the form of the wavefunction in translational invariant systems. As stated above $\mathcal{T}$ is an infinite group behind of which the construct of an infinite crystal lies. To proceed we form a *finite* group[3] from $\mathcal{T}$ by imposing periodic boundary conditions in $d$ dimensions. We consider a building block of the crystal containing $N_1 \times \cdots \times N_d = N^d$ primitive cells.[4] This imposes the following condition on the wavefunction of the crystal

[3] This is done for convenience, because we then can use all statements for finite groups.

[4] This is an approximation which is not severe if we disregard surface effects. Note, that whereas imposing periodic boundary conditions in one dimension can be thought of forming a ring out of a chain of lattice points, in three dimensions this is topological not possible.

$$\psi(\mathbf{r}) = \psi(\{\mathbf{E}|N\mathbf{a_i}\}\mathbf{r}) \qquad i = 1, \ldots, d. \tag{6.26}$$

which can be mapped to a condition for function operators

$$\hat{P}(\{\mathbf{E}|N\mathbf{a_i}\}) = \hat{P}(\{\mathbf{E}|\mathbf{a_i}\})^N = \hat{P}(\{\mathbf{E}|0\}) \qquad i = 1, \ldots, d. \tag{6.27}$$

Therefore using (6.26) is equivalent to working with the finite group of function operators $P(\{\mathbf{E}|\sum_i^d m_i\mathbf{a_i}\})$ where $0 \leq m_i \leq N-1$ with dimension $N^d$. As two translations commute this group is abelian, *i.e.* all the irreducible representations are one dimensional. Using (6.27) one can work out a matrix representations for the IRs. Consider a one-dimensional IR $\Gamma$ of $\mathcal{T}$, and suppose that $\Gamma(\{\mathbf{E}|\mathbf{a_i}\})$ is the representation belonging to a translation by a basic vector $\mathbf{a_i}$.[5] Then from (6.27) it follows immediately that

$$(\Gamma(\{\mathbf{E}|\mathbf{a_i}\}))^N = 1 \tag{6.28}$$

which leads to the following condition for the matrix elements for the IRs

$$\Gamma(\{\mathbf{E}|\mathbf{a_i}\}) = e^{-2\pi i \frac{p_i}{N}}, \qquad p_i \in \mathbb{N}. \tag{6.29}$$

By (6.28) only $N$ values for $p_i$ are allowed and they may be taken to be $p_i = 1, \ldots, N-1$. If one now defines the basic vectors $\mathbf{b_j}$ of the reciprocal lattice by

$$\mathbf{a_i} \cdot \mathbf{b_j} = 2\pi\delta_{ij}, \qquad i, j = 1, \ldots, d \tag{6.30}$$

and allowed $\mathbf{k}$-vectors by

$$\mathbf{k} = \sum_{i=1}^{d} k_i \mathbf{b}_i \tag{6.31}$$

with $k_i = p_i/N$ one can express all IRs in terms of

$$\Gamma^{\mathbf{k}}(\{\mathbf{E}|\mathbf{T}\}) = e^{-i\mathbf{k}\cdot\mathbf{T}} \tag{6.32}$$

numerated by $N^d$ allowed $\mathbf{k}$-vectors. The character table is very simple and shown in Table 6.6.[6] The basis functions for the IR are then labelled by $\mathbf{k}$ and their transformation properties are given by

$$\hat{P}(\{\mathbf{E}|\mathbf{T}\})\phi_{\mathbf{k}}(\mathbf{r}) = e^{-i\mathbf{k}\cdot\mathbf{T}}\phi_{\mathbf{k}} = \phi_{\mathbf{k}}(\{\mathbf{E}|\mathbf{T}\}^{-1}\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r} - \mathbf{T}) \tag{6.33}$$

This leads to Bloch's theorem which states that the basis function of the IRs of the translation group $\mathcal{T}$ can be chosen as Bloch functions

[5] From now on we denote the *finite* group of translations as $\mathcal{T}$. No confusion with the infinite group mentioned before shall arise.

[6] As the IRs are one dimensional we obtain the character table immediately.

| | $\mathbf{T_1}$ | $\mathbf{T_2}$ | ... | $\mathbf{T}_{N^d}$ |
|---|---|---|---|---|
| $\Gamma^{\mathbf{k}_1}$ | $e^{-i\mathbf{k_1}\cdot\mathbf{T_1}}$ | $e^{-i\mathbf{k_1}\cdot\mathbf{T_2}}$ | ... | $e^{-i\mathbf{k_1}\cdot\mathbf{T_N}}$ |
| ... | | | | |
| $\Gamma^{\mathbf{k}_{N^d}}$ | $e^{-i\mathbf{k}_{N^d}\cdot\mathbf{T_1}}$ | $e^{-i\mathbf{k}_{N^d}\cdot\mathbf{T_2}}$ | ... | $e^{-i\mathbf{k}_{N^d}\cdot\mathbf{T}_{N^d}}$ |

$$\phi_{\mathbf{k}}(\mathbf{r}) = e^{i\theta}e^{-i\mathbf{k}\cdot\mathbf{T}}u_{\mathbf{k}}(\mathbf{r}), \tag{6.34}$$

where $u_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r}-\mathbf{T})$ has the periodicity of the lattice. The phase factor $e^{i\theta}$, $\theta \in \mathbb{R}$, is omitted in the following considerations. The label $\mathbf{k}$ for the wave function is called quantum number and in the limit $N \to \infty$, $\phi_{\mathbf{k}}$ is a smooth function of the wave vector $\mathbf{k}$.[7]

So far we have seen that the translational symmetry imposed certain conditions on the functional form of the wave-function. If now the space group $\mathcal{G}$ contains apart from the translational part point group symmetries we can find further IRs of $\mathcal{G}$ which are not necessarily one dimensional. Important here is the fact that the basis functions of these IRs can be constructed from the Bloch-functions (6.34) alone (this is not proven here). Before we can do this, we have to introduce some new concepts.

**Definition**: The point group $\mathcal{G}_0(\mathbf{k})$ of the wave-vector $\mathbf{k}$ is the subgroup of the point group $\mathcal{G}_0$ of the space group $\mathcal{G}$ that consists of all rotations $\{\mathbf{R}|\mathbf{0}\}$ that rotate $\mathbf{k}$ into itself or an equivalent vector $\mathbf{k}+\mathbf{G}$ where $\mathbf{G}$ is a vector of the reciprocal lattice given by: $\mathbf{G} = \sum_i n_i\mathbf{b_i}$, $\quad n_i = 0, \pm1, \pm2, \ldots, \quad i = 1, \ldots, d$.

Given a vector $\mathbf{k}' = \mathbf{k} + \mathbf{G}$ one realises that a IR $\Gamma^{\mathbf{k}}$ of $\mathcal{T}$ could also be labelled by $\mathbf{k}'$ because of $e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{T}} = e^{i\mathbf{k}\cdot\mathbf{T}}$; $\mathbf{k}$ and $\mathbf{k}'$ are said to be equivalent. This brings us to the concept of the Brillouinzone (BZ). The first BZ consists of the points of $\mathbf{k}$-space which lie closer to $\mathbf{k} = \mathbf{0}$ than any other reciprocal lattice points. The boundaries of the first BZ are given by the planes consisting of the points satisfying:

$$\mathbf{k}\cdot\mathbf{G} = \frac{1}{2}|\mathbf{G}|^2 \tag{6.35}$$

where here the $\mathbf{G}$'s are the nearer reciprocal lattice points. As an example in Fig. 6.2 the first BZ of an *fcc*-lattice is shown. In the BZ a high symmetry point is defined to have more members in $\mathcal{G}_0(\mathbf{k})$ than any neighbouring point $\mathbf{k}'$ in the BZ. Neighbouring points having the same $\mathcal{G}_0(\mathbf{k})$ are defined to form high symmetry lines and planes, respectively.

Working out the character table for a space group would be tedious, because of the vast number of IR that $\mathcal{G}$ possesses. However a fundamental theorem for symmorphic space groups exists (see *e.g.* [6.1]) which implies that any IR of $\mathcal{G}$ can be labelled by two quantities, namely the allowed $\mathbf{k}$-vector and a label $p$ specifying the IR of $\mathcal{G}_0(\mathbf{k})$. Therefore one can label the

[7] If the periodicity is lost in one spatial direction, say the $z$ direction perpendicular to a surface of a crystal , then $k_z$ cannot be used as quantum number to label the states.

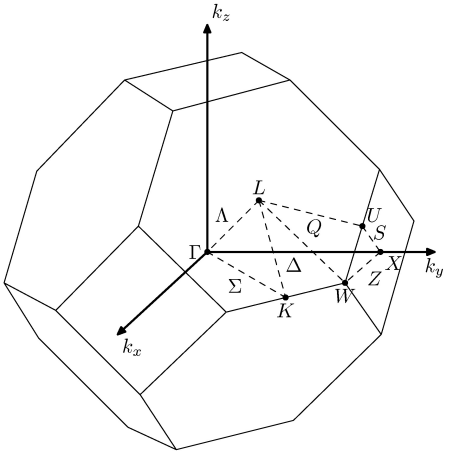


**Fig. 6.2.** Brillouin zone of the *fcc* structure. Symmetry points and symmetry lines are indicated.

IR's of $\mathcal{G}$ by $\Gamma^{\mathbf{k}p}$. Further basis functions transforming as the $i$th row of the $p$th IR of $\mathcal{G}_0(\mathbf{k})$ are labelled by $\phi^p_{\mathbf{k}i}(\mathbf{r})$.

The following matrix element theorem for Bloch-functions (see *e.g.* [6.1]) allows for considerable reduction of eigenvalue problems surfacing in the solution of the Schrödinger equation for crystals (see section 6.7). Given two Bloch functions $\phi^p_{\mathbf{k}i}$ and $\phi^{p'}_{\mathbf{k}'j}$ it states that the matrix elements $(\phi^p_{\mathbf{k}i}, \phi^{p'}_{\mathbf{k}'j})$ and $(\phi^p_{\mathbf{k}i}, \hat{H}\phi^{p'}_{\mathbf{k}'j})$ are both zero unless $\mathbf{k} = \mathbf{k}'$, $i = j$ and $p = p'$. Further $(\phi^p_{\mathbf{k}i}, \phi^p_{\mathbf{k}i})$ and $(\phi^p_{\mathbf{k}i}, \hat{H}\phi^p_{\mathbf{k}i})$ are independent of $i$.

## 6.7 Electronic Band Structure

We want to solve the following equation for an electron in an effective potential, which has lattice periodicity $V(\mathbf{r}) = V(\mathbf{r} + \mathbf{R})$.

$$\hat{H}\psi_{\mathbf{k}\nu}(\mathbf{r}) = E_\nu(\mathbf{k})\psi_{\mathbf{k}\nu}(\mathbf{r}) \tag{6.36}$$

The crystal wavefunction $\psi_{\mathbf{k}\nu}(\mathbf{r})$ is expanded with respect to a set of Bloch functions $\phi^n_{\mathbf{k}}(\mathbf{r})$.

$$\psi_{\mathbf{k}\nu}(\mathbf{r}) = \sum_n c^\nu_n(\mathbf{k})\phi^n_{\mathbf{k}}(\mathbf{r}) \tag{6.37}$$

Using this ansatz (6.36) can be transformed into an eigenvalue problem.

$$0 = \sum_n c^\nu_n(\mathbf{k}) \left[\hat{H}\phi^n_{\mathbf{k}}(\mathbf{r}) - E_\nu(\mathbf{k})\phi^n_{\mathbf{k}}(\mathbf{r})\right] \tag{6.38}$$

$$0 = \sum_n c^\nu_n(\mathbf{k}) \left[\left(\phi^m_{\mathbf{k}}, \hat{H}\phi^n_{\mathbf{k}}\right) - E_\nu(\mathbf{k})\left(\phi^m_{\mathbf{k}}, \phi^n_{\mathbf{k}}\right)\right] \tag{6.39}$$

A nontrivial solution requires of (6.39) requires:

$$0 = \det \left| \left( \phi^m_{\mathbf{k}}, \hat{H} \phi^n_{\mathbf{k}} \right) - E_\nu(\mathbf{k}) \left( \phi^m_{\mathbf{k}}, \phi^n_{\mathbf{k}} \right) \right| . \tag{6.40}$$

The dimension of the eigenvalue problem is given by the number of basis functions used in ansatz (6.37). If complex crystal structures have to be considered, the number of basis functions can be large. The problem can be simplified drastically at certain $\mathbf{k}$ points. This will be discussed later. If we plot the eigenvalues $E_\nu(\mathbf{k})$ along special lines in the Brillouin zone, we will get the so called band structure. The solutions are labelled with respect to the fundamental theorem by the allowed $\mathbf{k}$ vector and a label $p$ specifying the IR of $\mathcal{G}_0(\mathbf{k})$ as it can be seen in Fig. 6.3.

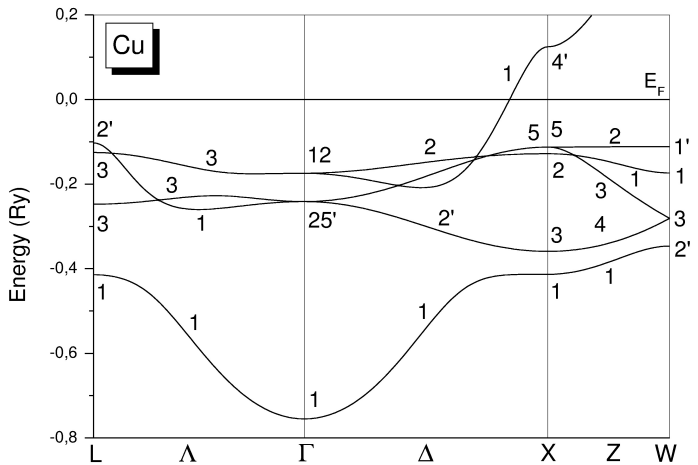


**Fig. 6.3.** Electronic band structure of Cu along the symmetry lines L-$\Gamma$-X-W

### 6.7.1 Compatibility Relations

The band structure of fcc Copper in Fig. 6.3 is shown between the high symmetry points $L$, $\Gamma$, $X$ and $W$. The lines between these symmetry points are usually labelled with $\Lambda$, $\Delta$ and $Z$. The question is, why are some bands crossing and others not or why are degeneracies at symmetry points are released along the symmetry lines? The reason for this are the different symmetry groups $\mathcal{G}_0(\mathbf{k})$ at the different $\boldsymbol{k}$-points. At $\Gamma$ ($\boldsymbol{k} = (0, 0, 0)$) there is the highest symmetry. For the fcc structure the pointgroup $\mathcal{G}_0(\Gamma)$ is $O_h$. The other $\boldsymbol{k}$-points have lower symmetries, but these groups are all subgroups of $O_h$. Let us concentrate on the representation $\Gamma_{12}$ at the $\Gamma$ point. We can read from the character table (Table 6.1) that the $\Gamma_{12}$ representation is twodimensional.

Therefore the corresponding energy value is twofold degenerate. The lower symmetry along $\Delta$ causes the split into two energy bands. The irreducible representations, corresponding to those bands, have to be compatible with the representation at $\Gamma$. This can be calculated with formula 6.6.

**Table 6.1.** Character table of the point group $O_\mathrm{h}$

| | | $E$ | $8C_3$ | $3C_2$ | $6C_4$ | $6C_2'$ | $i$ | $8S_6$ | $3\sigma_\mathrm{h}$ | $6S_4$ | $6\sigma_\mathrm{d}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $A_{1\mathrm{g}}$ | $\Gamma_1$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| $A_{2\mathrm{g}}$ | $\Gamma_2$ | 1 | 1 | 1 | -1 | -1 | 1 | 1 | 1 | -1 | -1 |
| $E_\mathrm{g}$ | $\Gamma_{12}$ | 2 | -1 | 2 | 0 | 0 | 2 | -1 | 2 | 0 | 0 |
| $T_{1\mathrm{g}}$ | $\Gamma_{15'}$ | 3 | 0 | -1 | 1 | -1 | 3 | 0 | -1 | 1 | -1 |
| $T_{2\mathrm{g}}$ | $\Gamma_{25'}$ | 3 | 0 | -1 | -1 | 1 | 3 | 0 | -1 | -1 | 1 |
| $A_{1\mathrm{u}}$ | $\Gamma_{1'}$ | 1 | 1 | 1 | 1 | 1 | -1 | -1 | -1 | -1 | -1 |
| $A_{2\mathrm{u}}$ | $\Gamma_{2'}$ | 1 | 1 | 1 | -1 | -1 | -1 | -1 | -1 | 1 | 1 |
| $E_\mathrm{u}$ | $\Gamma_{12'}$ | 2 | -1 | 2 | 0 | 0 | -2 | 1 | -2 | 0 | 0 |
| $T_{1\mathrm{u}}$ | $\Gamma_{15}$ | 3 | 0 | -1 | 1 | -1 | -3 | 0 | 1 | -1 | 1 |
| $T_{2\mathrm{u}}$ | $\Gamma_{25}$ | 3 | 0 | -1 | -1 | 1 | -3 | 0 | 1 | 1 | -1 |

The use of group theory proceeds as follows:
Let $\mathcal{G}_0(\Gamma)$ and $\mathcal{G}_0(\Delta) = C_{4\mathrm{v}}$ be the pointgroup $\mathcal{G}_0(\boldsymbol{k})$ for $\boldsymbol{k}$ at $\Gamma$ and $\Delta$. Then $\mathcal{G}_0(\Delta)$ is a subgroup of $\mathcal{G}_0(\Gamma)$ and so the irreducible representations (IRs) of $\mathcal{G}_0(\Gamma)$ are in general reducible representations of $\mathcal{G}_0(\Delta)$. The number $n_p$, how often an irreducible representation $\Gamma^{p\Delta}$ of $\mathcal{G}_0(\Delta)$ is contained in the reduction of the reducible representation $\Gamma^\Gamma$, wich is irreducible with respect to $\mathcal{G}_0(\Gamma)$is given by

$$n_p = \frac{1}{g} \sum_{T \in \mathcal{G}_0(\Delta)} \chi^{p\,\Delta}(T)\, \chi^{\Gamma}(T)^* \tag{6.41}$$

where $g$ is the order of the group $\mathcal{G}_0(\Delta)$. The evaluation of 6.41 for $\Gamma_{12}$ along $\Delta$ shows, using the character tables 6.1 and 6.4, that the representation $\Gamma_{12}$ can be written as direct sum of $\Delta_1$ and $\Delta_2$

$$\Gamma_{12} = \Delta_1 \oplus \Delta_2. \tag{6.42}$$

because only the numbers of $n_{\Delta_1}$ and $n_{\Delta_2}$ are one, the other are all zero. Working out all the relations for the different symmetry points and lines, we get the so called *compatibility relations*, given in Table 6.2.

It can be seen from the band structure, that bands of the same symmetry never cross. This can be understood by the following argumentation. Lets assume two bands corresponding to the same onedimensional irreducible representation will cross. At the crossing point the degeneracy is twofold corresponding to a twodimensional irreducible representation. This is a contradiction.

**Table 6.2.** Compatibility relations between the high symmetry points $\Gamma$, $X$, $L$ and $W$ and the symmetry axes $\Lambda$, $\Delta$ and $Z$ for the face-centered cubic space group $O_{\mathrm{h}}^{5}$. (see picture 6.3)

| $\Gamma_1$ | $\Gamma_2$ | $\Gamma_{12}$ | $\Gamma_{15}$ | $\Gamma_{25}$ | $\Gamma_{1'}$ | $\Gamma_{2'}$ | $\Gamma_{12'}$ | $\Gamma_{15'}$ | $\Gamma_{25'}$ |
|---|---|---|---|---|---|---|---|---|---|
| $\Delta_1$ | $\Delta_2$ | $\Delta_1\ \Delta_2$ | $\Delta_1\ \Delta_5$ | $\Delta_2\ \Delta_5$ | $\Delta_{1'}$ | $\Delta_{2'}$ | $\Delta_{1'}\Delta_{2'}$ | $\Delta_{1'}\ \Delta_{5'}$ | $\Delta_{2'}\ \Delta_5$ |
| $\Lambda_1$ | $\Lambda_2$ | $\Lambda_3$ | $\Lambda_1\ \Lambda_3$ | $\Lambda_2\Lambda_3$ | $\Lambda_2$ | $\Lambda_1$ | $\Lambda_3$ | $\Lambda_2\Lambda_3$ | $\Lambda_1\Lambda_3$ |

| $X_1$ | $X_2$ | $X_3$ | $X_4$ | $X_5$ | $X_{1'}$ | $X_{2'}$ | $X_{3'}$ | $X_{4'}$ | $X_{5'}$ |
|---|---|---|---|---|---|---|---|---|---|
| $\Delta_1$ | $\Delta_2$ | $\Delta_{2'}$ | $\Delta_{1'}$ | $\Delta_5$ | $\Delta_{1'}$ | $\Delta_{2'}$ | $\Delta_2$ | $\Delta_1$ | $\Delta_5$ |
| $Z_1$ | $Z_1$ | $Z_4$ | $Z_4$ | $Z_2Z_3$ | $Z_2$ | $Z_2$ | $Z_3$ | $Z_3$ | $Z_1Z_4$ |

| $W_1$ | $W_2$ | $W_{1'}$ | $W_{2'}$ | $W_3$ |
|---|---|---|---|---|
| $Z_1$ | $Z_2$ | $Z_2$ | $Z_1$ | $Z_3Z_4$ |

| $L_1$ | $L_2$ | $L_3$ | $L_{1'}$ | $L_{2'}$ | $L_{3'}$ |
|---|---|---|---|---|---|
| $\Lambda_1$ | $\Lambda_2$ | $\Lambda_3$ | $\Lambda_2$ | $\Lambda_1$ | $\Lambda_3$ |

### 6.7.2 Symmetry-Adapted Basis Functions

Making use of the symmetry in the solution of the eigenvalue problem (6.40) is now quite simple. Suppose the Schrödinger equation is $\hat{H}\psi(\mathbf{r}) = E\psi(\mathbf{r})$. The group of the Schrödinger equation is $\mathcal{G}$. The function $\psi(\mathbf{r})$ can be expressed as

$$\psi(\mathbf{r}) = \sum_{i=1}^{\infty} \sum_{p} \sum_{m} C_{ip}^{m} \phi_{im}^{p}(\mathbf{r}) \tag{6.43}$$

The transformation to the eigenvalue problem leads therefore to:

$$det \left| \left( \phi_{jn}^{q}, \hat{H} \phi_{im}^{p} \right) - E \left( \phi_{jn}^{q}, \phi_{im}^{p} \right) \right| = 0 \tag{6.44}$$

Corresponding to the matrix element theorems the determinant takes a block form, i.e. the large eigenvalue problem splits in a set of smaller ones. To use such properties, we have to construct symmetry-adapted basis functions. Projection operators can be used to generate the symmetry-adapted basis functions.

**Symmetry-adapted plane waves.** A plane wave

$$\phi_{\mathbf{k}m}(\mathbf{r}) = e^{i(\mathbf{k}+\mathbf{K}_m)\cdot\mathbf{r}} \tag{6.45}$$

is a Bloch function. The vector $\mathbf{K}_m$ is a reciprocal lattice vector. Therefore the crystal wave function can be expanded in a set of such plane waves. An expansion of such a form converges normally too slowly. A better choice at the point $\mathbf{k}$ of the Brillouin zone will be a function that transforms according to the $s$th row of the irreducible representation $\Gamma^p$ of $\mathcal{G}_0(\mathbf{k})$. Such a function is obtained by operating on $\phi_{\mathbf{k}m}(\mathbf{r})$ with the projection operator $\mathcal{P}_{ss}^{p}$. (cf. 6.13). The application of $\hat{P}(T)$ to the plane wave gives

$$\hat{P}(T)\phi_{\mathbf{k}m}(\mathbf{r}) = e^{i\mathbf{R}(\mathbf{k}+\mathbf{K}_m)\cdot\mathbf{r}} \tag{6.46}$$

whereas $\mathbf{R}$ denotes the rotation matrix connected with the symmetry element $T$. Because $T = \{\mathbf{R} \mid 0\} \in \mathcal{G}_0(\mathbf{k})$, $\mathbf{R}\cdot\mathbf{k}$ is equivalent to $\mathbf{k}$. Because $\mathbf{R}\cdot\mathbf{K}_m$ is also a lattice vector of the reciprocal lattice, there exists a lattice vector $\mathbf{K}_n$ such, that

$$\mathbf{R}(\mathbf{k}+\mathbf{K}_m) = \mathbf{k}+\mathbf{K}_n \quad , \quad \mid \mathbf{R}(\mathbf{k}+\mathbf{K}_m) \mid = \mid \mathbf{k}+\mathbf{K}_m \mid \tag{6.47}$$

The second equation holds because of the orthogonality of $\mathbf{R}$. Let us consider an example for the face centered cubic space group $O_{\mathrm{h}}^5$. The point group of the point L ( $\mathbf{k_L} = \frac{\pi}{a}(1,1,1)$ ) is $\mathrm{D_{3d}}$. If we use the plane wave $\phi_{\mathbf{k_L}0}(\mathbf{r}) = e^{i\mathbf{k_L}\cdot\mathbf{r}}$ and apply the character projection operator to all irreducible representations of $\mathrm{D_{3d}}$ we get:

$$\begin{aligned}
L_1 &: \frac{1}{2}\left(e^{-i\pi(x+y+z)} + e^{-i\pi(x+y+z)}\right) \\
L_{2'} &: \frac{1}{2}\left(-e^{-i\pi(x+y+z)} + e^{-i\pi(x+y+z)}\right) \\
L_3 &: \frac{1}{4}\left(e^{-i\pi(3x+y+z)} - e^{-i\pi(x+3y+z)} + e^{i\pi(3x+y+z)} - e^{i\pi(x+3y+z)}\right) \\
&: \frac{1}{12}\Big(e^{-i\pi(3x+y+z)} + e^{-i\pi(x+3y+z)} + e^{i\pi(3x+y+z)} + e^{i\pi(x+3y+z)} \\
&\quad -2e^{-i\pi(x+y+3z)} - 2e^{i\pi(x+y+3z)}\Big)
\end{aligned}$$

To all the other IRs no symmetrized basis function can be projected out. One has to choose reciprocal lattice vectors different from zero to project basis functions corresponding to the other IRs out ouf a plane wave.

**Symmetry-adapted spherical harmonics.** The spherical harmonics $Y_{l,m}(\theta,\phi)$ are basis functions of irreducible representations of dimension $(2l+1)$ of the rotation group $O(3)$. The group $C_{4\mathrm{v}}$ is a subgroup of $O(3)$, therefore the representations of $O(3)$ will be reducible with respect to $C_{4\mathrm{v}}$, in general. On the other hand we can construct linear combinations of spherical harmonics, which are basis function of the IRs of $C_{4\mathrm{v}}$.

It is obvious, that all the spherical harmonics to $m = 0$ are basis function of $\Gamma^1$, because they are independent of the azimuthal angle $\phi$. For higher angular momentum $l \geq 4$ we can built linear combinations which transform like $\Gamma^1$ from the functions $Y_{l\pm4}$ because they correspond to the fourfold rotation axis. *Lattice Harmonics* in general are symmetry-adapted spherical harmonics which are given as linear combinations of those. Lattice harmonics are tabulated in the literature [6.26, 6.27] or can be generated automatically using our projection operator technique.

**Table 6.3.** Linear combinations of spherical harmonics as basis functions of the point group $C_{4v}$. ($S^+_{lm} = (Y_{lm} + Y_{l,-m})/\sqrt{2}$, $S^-_{lm} = (Y_{lm} - Y_{l,-m})/(\sqrt{2}i)$

| $l =$ | 0 | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| $\Gamma^1(A_1)$ | $Y_{00}$ | $Y_{10}$ | $Y_{20}$ | $Y_{30}$ | $Y_{40}$ $S^+_{44}$ | ... |
| $\Gamma^2(A_2)$ | – | – | – | – | $S^-_{44}$ | ... |
| $\Gamma^3(B_1)$ | – | – | $S^+_{22}$ | $S^+_{32}$ | $S^+_{42}$ | ... |
| $\Gamma^4(B_2)$ | – | – | $S^-_{22}$ | $S^-_{32}$ | $S^-_{42}$ | ... |
| $\Gamma^5(E)$ | – | $S^+_{11}$ | $S^+_{21}$ | $S^+_{31}$ $S^+_{33}$ | $S^+_{41}$ $S^+_{43}$ | ... |
| | – | $S^-_{11}$ | $S^-_{21}$ | $S^-_{31}$ $S^-_{33}$ | $S^-_{41}$ $S^-_{43}$ | ... |

## 6.8 Discussion of Photonic Band Structures

To calculate the photonic band structures, we will use the program developed by Johnson *et al.* [6.28] The fully-vectorial eigenmodes of Maxwell's equations with periodic boundary conditions are computed by preconditioned conjugate-gradient minimization of the block Rayleigh quotient in a plane wave basis in this package. The program itself calculates the bands, but will not directly assign the irreducible representation which belongs to a certain band at a special $\boldsymbol{k}$. First we will demonstrate how this can be done easily by an investigation of the fields.

### 6.8.1 Assignment of the IRs to the Photonic Band Structure

As an example we will discuss a simple two-dimensional photonic crystal. Therefore we have to deal with scalar fields which are solutions of (6.22). Our example consists of circular air-pores in a dielectric medium of $\epsilon = 2.1$ arranged in a square lattice. Fig. 6.4 shows the first Brillouin zone of the square lattice. The point groups $\mathcal{G}_0(\boldsymbol{k})$ for the points $\Gamma$, X and $\Delta$ are $C_{4v}, C_{2v}$ and $C_{1h}$. The character tables are given in Table 6.4.

At $\Gamma$ we have a higher symmetry than along the line $\Delta$. This implicates that the IRs of the group $C_{4v}$ will be reducible representations of the group $C_{1h}$. From (6.6) we know how to calculate how often an IR occurs in a representation. The result of such considerations are the so called *compatibility relations*. In our case we find easily the following: The group $C_{4v}$ contains only one two-dimensional representation. Therefore the two-fold degenerate eigenvalues at $\Gamma$ have to be labeled $E$. We can calculate the compatibility of $E$ with the IRS of $C_{1h}$ using (6.6) and get: $E = A \oplus B$, i.e. $E$ is a direct sum of the IRs $A$ and $B$ of $C_{1h}$.

Figure 6.5 presents the band structure for TM polarization, respectively. The irreducible representations with respect to the groups $\mathcal{G}_0(\boldsymbol{k})$ at the differ-

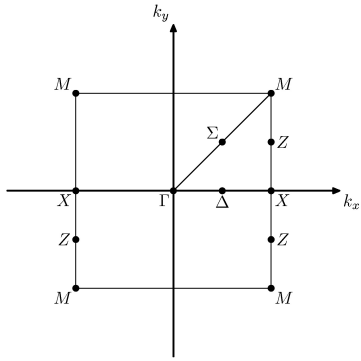


**Fig. 6.4.** Brillouin zone of the square lattice.

**Table 6.4.** Character tables of the point groups $C_{4v}$, $C_{2v}$ and $C_{1h}$

| $C_{4v}$ | $E$ | $2C_4$ | $C_2$ | $2\sigma_v$ | $2\sigma_d$ |
|---|---|---|---|---|---|
| $A_1$ $\Delta_1$ | 1 | 1 | 1 | 1 | 1 |
| $A_2$ $\Delta_{1'}$ | 1 | 1 | 1 | -1 | -1 |
| $B_1$ $\Delta_2$ | 1 | -1 | 1 | 1 | -1 |
| $B_2$ $\Delta_{2'}$ | 1 | -1 | 1 | -1 | 1 |
| E $\Delta_5$ | 2 | 0 | -2 | 0 | 0 |

| $C_{2v}$ | $E$ | $C_2$ | $\sigma_y$ | $\sigma_x$ |
|---|---|---|---|---|
| $A_1$ | 1 | 1 | 1 | 1 |
| $A_2$ | 1 | 1 | -1 | -1 |
| $B_1$ | 1 | -1 | 1 | -1 |
| $B_2$ | 1 | -1 | -1 | 1 |

| $C_{1h}$ | $E$ | $\sigma$ |
|---|---|---|
| A | 1 | 1 |
| B | 1 | -1 |

ent symmetry points and lines are already indicated. It is not possible to find all IRs without doubt at all symmetry points and lines indicated in Fig. 6.5 only by the inspection of the band structure. In the TM-mode picture of Fig. 6.5 three special areas are indicated. **1** and **3** show, that bands of the same symmetry will not cross each other. The reason is of course the same like in the electronic case. A is a one-dimensional representation of $C_{1h}$. If two A representations would cross along $\Sigma$, the dimension of the representation would have to bee two-dimensional in the crossing point. This is a contradiction and therefore crossing of bands of the same symmetry is forbidden. In **2** the representations are not indicated. We will dicuss now, how to get quickly information about the symmetry. First we calculate the fields. In case of TM-polarization this will be the z-component of the $\boldsymbol{E}$-field at the point $\Gamma$ of the Brillouin zone. Now we apply the character projection operator, defined in (6.14) to the fields pixel by pixel with respect to all IRs of the corresponding group $\mathcal{G}_0(\Gamma) = C_{4v}$. If we get the same figure after transformation, we have found the correct IR. Figure 6.6 shows the result of such an analysis for the bands 2-5 at the $\Gamma$ point and TM-polarization for our example.

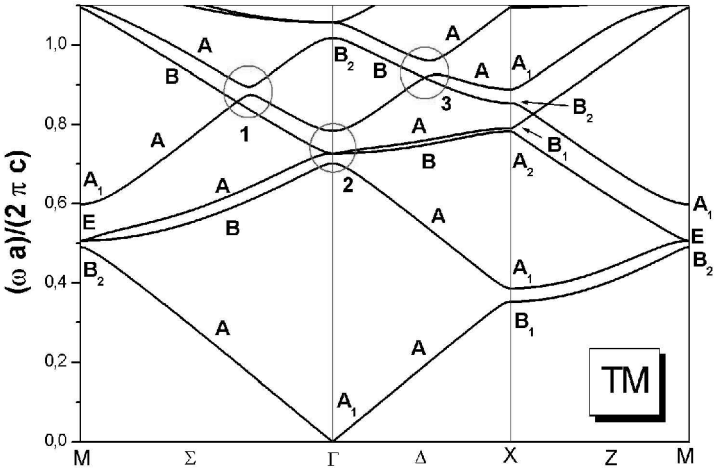


**Fig. 6.5.** Band structure of a 2D photonic crystal. Circular air-pores are arranged in a square lattice. The filling factor of the structure is f=0.5. The dielectric constant of the material is $\epsilon = 2.1$

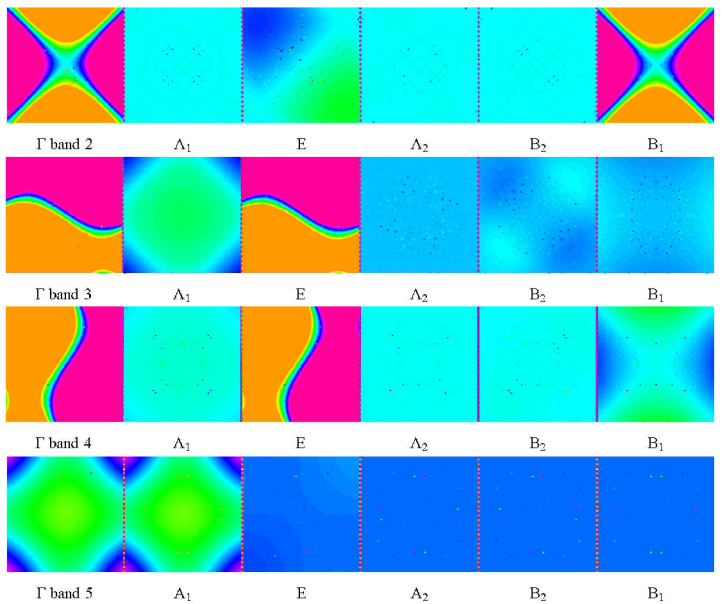


**Fig. 6.6.** z-component of the E-field at point $\Gamma$ for bands 2 to 5 of the band structure of Fig. 6.5 for TM-polarization

Another possibility to investigate the symmetry properties in our example is the discussion of symmetrized plane waves. An extensive study of the symmetrized plane waves was given by Luehrmann. [6.29] To solve (6.22) we

expand the solution in terms of plane waves:

$$E_z(\boldsymbol{r}_{||}) = \sum_{\boldsymbol{G}_{||}} C_{\boldsymbol{k}_{||}}(\boldsymbol{G}_{||}) e^{i(\boldsymbol{k}_{||}+\boldsymbol{G}_{||})\cdot\boldsymbol{r}_{||}} \tag{6.48}$$

The projection operator technique can be used to construct symmetrized plane waves. Basis functions constructed from a plane wave

$$\phi_{\boldsymbol{k}_{||},\boldsymbol{G}_{||}}(\boldsymbol{r}_{||}) = e^{i(\boldsymbol{k}_{||}+\boldsymbol{G}_{||})\cdot\boldsymbol{r}_{||}} \tag{6.49}$$

that transform like the $s$th row of the irreducible representation $\Gamma^p$ of $\mathcal{G}_0(\boldsymbol{k})$ are obtained by simply operating on $\phi_{\boldsymbol{k}_{||},\boldsymbol{G}_{||}}(\boldsymbol{r}_{||})$ with the projection operator $\mathcal{P}^p_{ss}$. If we want to construct symmetrized plane waves at the $\Gamma$ point ($\boldsymbol{k}_{||} = 0$) from the reciprocal lattice vectors with $\mid \boldsymbol{G}_{||} \mid = 2\pi/a$ we get the following symmetrized linear combinations with respect to IRs of $C_{4\mathrm{v}}$ belonging to $\mathrm{A}_1$ and $\mathrm{A}_2$ and E:

$$\begin{aligned}
A_1 &: \frac{1}{4}\left(e^{-2\pi x/a} + e^{-2\pi x/a} + e^{-2\pi y/a} + e^{-2\pi y/a}\right) \\
A_2 &: \frac{1}{4}\left(e^{-2\pi x/a} + e^{-2\pi x/a} - e^{-2\pi y/a} - e^{-2\pi y/a}\right) \\
E &: \frac{1}{2}\left(-e^{-2\pi x/a} + e^{-2\pi x/a}\right) \\
E &: \frac{1}{2}\left(-e^{-2\pi y/a} + e^{-2\pi y/a}\right)
\end{aligned}$$

Symmetrized linear combinations of plane waves to the IRs $\mathrm{B}_1$ and $\mathrm{B}_2$ have to be constructed from different reciprocal lattice vectors.

The *Mathematica* package allows to calculate the photonic band structure for two-dimensional photonic crystals. We get the IRs for a given eigenfrequency $\omega(\boldsymbol{k})$ by comparison of the signs of the plane wave components in the series expansion (6.48) with the symmetrized plane waves which belong to $\mathcal{G}_0(\boldsymbol{k})$.

The methods, explained in this chapter can be extended to the three-dimensional case in a straightforward manner.

## 6.9 Conclusions

In summary, we have introduced the group theoretical treatment of photonic band structures. We have demonstrated that computer algebra systems like *Mathematica* can be used to investigate in an effective way the symmetry properties of two- and three-dimensional photonic band structures. The symmetry properties of the fields can be investigated directly by the projection operator technique. The properties of symmetrized basis functions like vector

spherical harmonics can be considered easily. We believe that such tools will be helpful for detailed analysis of photonic band structure calculations or the interpretation of experimental results.

## References


[6.1] J.F. Cornwell, Group Theory and Electronic Energy Bands in Solids, Selected Topics in Solid State Physics Vol. 10 (North Holland, Amsterdam, 1969).

[6.2] J.F. Cornwell, Group Theory in Physics, Techniques in Physics Vol.7 (Academic Press, London 1984)

[6.3] W. Ludwig and C. Falter, Symmetry in Physics, Springer Series in Solid State Sciences 64 (Springer, Berlin, 1988).

[6.4] B.S. Tsukerblat, Group Theory in Chemistry and Spectroscopy - A simple guide to advanced usage (Academic Press, London, 1994).

[6.5] J.D. Joannopoulos, R.D. Meade, J.N. Winn, Photonic Crystals (Princeton University Press, Princeton 1995).

[6.6] K. Sakoda, Phys. Rev. B **52**, 7982 (1995).

[6.7] K. Sakoda, Phys. Rev. B **55**, 15345 (1997).

[6.8] T. Ochiai and K. Sakoda, Phys. Rev. B **64**, 045108 (2001).

[6.9] K. Sakoda, Optical Properties of Photonic Crystals, Springer Series in Optical Sciences Vol.80 (Springer, Berlin, 2001).

[6.10] K. Ohtaka and Y. Tanabe, J. Phys. Soc. Japan **65**, 2670 (1996).

[6.11] Computeralgebra in Deutschland, Bestandsaufnahme, Möglichkeiten, Perspektiven, Fachgruppe Computeralgebra der GI, DMV und GAMM, Passau und Heidelberg 1993

[6.12] K. Shirai, Theories of point group in solid state physics, package available from the *Mathematica* resource library `http://library.wolfram.com/database/`.

[6.13] The package can be found at
`http://www.physik.uni-halle.de/Heraeus/Summer/f_main.htm`.
The software is still under development. Critical comments and hints are welcome.

[6.14] C.F. Bohren, D.R. Huffman, Absorption and Scattering of Light by Small Particles, (John Wiley & Sons, New York ).

[6.15] G.B. Arfken, H.J. Weber, Mathematical Methods for Physicists (Academic Press, San Diego 1995)

[6.16] J.A. Stratton, Electromagnetic Theory (McGraw-Hill, New York 1941).

[6.17] R.F. Egorov, B.I. Reser, V.P. Shirkovskii, phys. stat. sol. **26**, 391 (1968).

[6.18] E. Lidorikis, M.M. Sigalas, E.N. Economou, and C.M. Soukoulis, Phys. Rev. Lett. **81**, 1405 (1998).

[6.19] J.P. Albert, C. Jouanin, D. Cassagne, and D. Monge, Opt. and Quantum Electronics **34**, 251 (2002).

[6.20] M. Le Vassor d'Yerville, D. Monge, D. Cassange, and J.P. Albert, Opt. and Quantum Electronics **34**, 445 (2002).

[6.21] J.P. Albert, C. Jouanin, D. Cassagne, and D. Bertho, Phys. Rev. B **61**, 4381 (2000).

[6.22] M. Bayindir, B. Temelkuran, and E. Ozbay, Phys. Rev. B **61**, R11855 (2000).

[6.23] M. Bayindir, B. Temelkuran, and E. Ozbay, Phys. Rev. Lett. **84**, 2140 (2000).
[6.24] M. Bayindir and E. Ozbay, Phys. Rev. B **62**, R2247 (2000).
[6.25] S. Wolfram, Das *Mathematica*-Buch, Die offizielle Dokumentation (Addison-Wesley-Longman, Bonn 1997).
[6.26] S.L. Altmann and A.P. Cracknell, Rev. Mod. Phys. **37**, 19 (1965).
[6.27] S.L. Altmann and C.J. Bradley, Rev. Mod. Phys. **37**, 33 (1965).
[6.28] S.G. Johnson and J.D. Joannopoulos, Optics Express **8**, 173 (2001).
[6.29] A.W. Luehrmann, Adv. in Physics, **17**, 3 (1968).
[6.30] W.M. Robertson, G. Arjavalingam, R.D. Meade, K.D. Brommer, A.M. Rappe, and J.D. Joannopoulos, Phys. Rev. Lett. **68**, 2023 (1992).
[6.31] W.M. Robertson, G. Arjavalingam, R.D. Meade, K.D. Brommer, A.M. Rappe, and J.D. Joannopoulos, J. Opt. Soc. Am B **10**, 322 (1993).
[6.32] F. López-Tejeira, T. Ochiai, K. Sakoda, and J. Sánchez-Dehesa, Phys. Rev. B **65**, 195110 (2002).