

2.2.9 Product of representations

Besides the *sums* of representations, one can also define their *products*. Consider two groups G and H and their direct product $G \times H$. If we have two representations D_1 and D_2 of G and H respectively, we may define their product as

$$D(g \cdot h) = D_1(g) \otimes D_2(h), \quad (1)$$

where \otimes is the tensor product of matrices: $(A \otimes B)_{ij,kl} = A_{ik}B_{jl}$. The dimension of such a representation equals the *product* of the dimensions of D_1 and D_2 , and its character is given by the *product* of the two characters.

Note that if both D_1 and D_2 are irreducible, then their product is also irreducible (as a representation of $G \times H$). In other words, if a group is a direct product of two groups, then its table of irreducible representations can be obtained as the product of the tables of irreducible representations of its factors.

One can also encounter a situation, where the two groups G and H are equal, and their product is also viewed as a representation of the same group:

$$D(g) = D_1(g) \otimes D_2(g). \quad (2)$$

In this case, the product of two irreducible representations is not generally irreducible. For example, the product of two spin-1/2 representations of the rotation group is decomposed into a singlet and a triplet (which can be symbolically written as $2 \otimes 2 = 1 \oplus 3$, if we mean by 1, 2, and 3 irreducible representations of $SU(2)$ with the corresponding dimensions).

2.3 Band structure and lattice symmetries: example of diamond

We now apply the general formalism developed in the last lecture to the example of the crystal structure of *diamond*. The first part of the discussion (about the Bloch waves) is general for any crystal structure, the rest is specific for the space group of diamond. Note that there is an additional complication for the diamond space group, since it is *non-symmorphic* (see definition below): we will remark this complication, but will not discuss it in detail. We will also not discuss the possibility of spin-orbit interactions. Please refer to literature for those details.

Recommended reading:

[BP] F. Bassani and G. Pastori Parravicini, *Electronic states and optical transitions in solids* (Pergamon Press, Oxford, 1975)

[DDJ] M. S. Dresselhaus, G. Dresselhaus, and A. Jorio, *Group theory: Applications to the physics of condensed matter* (Springer, Berlin, 2008)

2.3.1 Crystal symmetries

The full symmetry of the crystal structure is usually called *space group* or *crystallographic group*. It includes *translations* (in three noncollinear directions) as a subgroup. We may further define the *point group* as a factor of the space group modulo translations. The point group is a finite group of isometries preserving one fixed point. It may contain both *proper* (preserving the orientation) and *improper* (reversing the orientation) rotations.

Sometimes, the point group is a subgroup of the space group: in this case the space group is called *symmorphic*. Otherwise (if it is not possible to realize the point group as symmetries of the crystal with one common fixed point) it is called *non-symmorphic*.

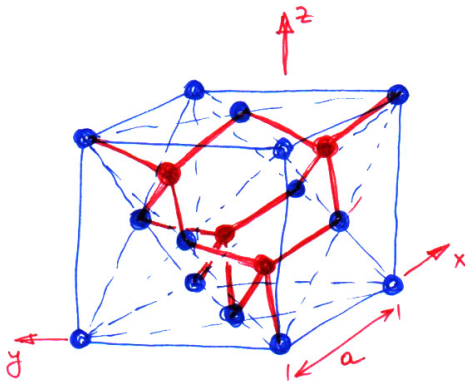


Figure 1: Diamond lattice.

2.3.2 Translational symmetries and Bloch waves

Consider first the classification of states with respect to translations. Pick the three *generating* translation vectors \mathbf{e}_1 , \mathbf{e}_2 , \mathbf{e}_3 . These translations commute, so the full translational part of the crystal symmetries is a direct product of the three one-dimensional translation groups. So it is sufficient to consider each of them separately, and then take the product of the three representations.

The group of one-dimensional lattice translations is abelian and is generated by an elementary translation T . The decomposition into irreducible representations is obtained by diagonalizing the matrix T . Each eigenstate of T (called a *Bloch wave*), is multiplied by a phase factor under such an elementary translation:

$$T\Psi = e^{i\phi}\Psi. \quad (3)$$

Note that the we only consider the case of phase factors and disregard the possibility of eigenstates $T\Psi = c\Psi$ with $|c| \neq 1$: such eigenstates would diverge at one of the two infinities and therefore do not belong to the space of physical states. In other words, only *unitary* representations appear in physical states.

After we combine the translations along the three directions, we find for the full translation group the set of irreducible one-dimensional representations:

$$T_{n_1\mathbf{e}_1+n_2\mathbf{e}_2+n_3\mathbf{e}_3} = e^{i(n_1\phi_1+n_2\phi_2+n_3\phi_3)}\Psi. \quad (4)$$

The three phases ϕ_1 , ϕ_2 , and ϕ_3 parametrize the representation and define a point in the Brillouin zone. In other words, the Brillouin zone is the set of all irreducible representations of the translations of the crystal lattice.

If translations exhaust the symmetries of the lattice, this would be the end of the story. If, on the other hand, the point group is nontrivial, it mixes some of the points in the Brillouin zone and introduces degeneracies. Below we illustrate how it works in the example of the crystal lattice of diamond.

2.3.3 Diamond crystal lattice

The diamond crystal lattice (see Fig. 1) may be described in terms of positions of the carbon atoms. It contains two superimposed FCC (face-centered cubic) sublattices. The

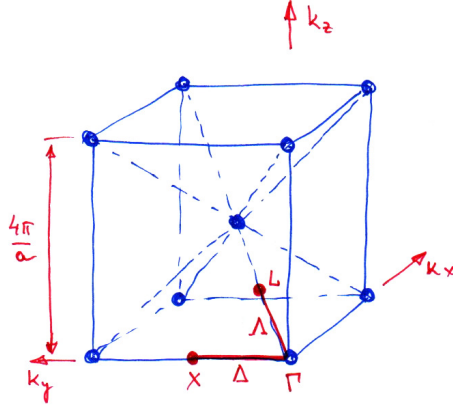


Figure 2: Dual lattice of k points and some points and lines of special symmetry.

positions of the points are:

$$\frac{a}{2}(n_1, n_2, n_3) \quad \text{and} \quad \frac{a}{2}\left(n_1 + \frac{1}{2}, n_2 + \frac{1}{2}, n_3 + \frac{1}{2}\right) \quad \text{with } (n_1 + n_2 + n_3) \text{ even.} \quad (5)$$

The lattice constant $a = 3.57 \text{ \AA}$ (at room temperature) is the length of the side of the cube in the FCC pattern.

The elementary lattice translations are

$$\mathbf{e}_1 = \frac{a}{2}(0, 1, 1), \quad \mathbf{e}_2 = \frac{a}{2}(1, 0, 1), \quad \mathbf{e}_3 = \frac{a}{2}(1, 1, 0). \quad (6)$$

The unit cell contains two atoms.

2.3.4 Diamond Brillouin zone

The dual lattice of k points is defined as lattice of k vectors which give trivial (multiple of 2π) phases under all translations of the lattice. From (6), we find the general formula for the lattice of k points:

$$\mathbf{k} = \frac{2\pi}{a}(-m_1 + m_2 + m_3, m_1 - m_2 + m_3, m_1 + m_2 - m_3), \quad (7)$$

where m_1 , m_2 , and m_3 run over all integer numbers. This defines the BCC (body-centered cubuc) lattice (Fig. 2).

One usually chooses the Brillouin zone (BZ) to be the set of k points that are closer to $k = 0$ than to any other k point of the lattice. This construction gives in our case the Brillouin zone in the shape of a truncated octahedron. We distinguish the points of special symmetry Γ (at $k = 0$), X [the center of a square face of the BZ, e.g., $k = (2, 0, 0)\pi/a$], and L [the center of a hexagonal face of the BZ, e.g., $k = (1, 1, 1)\pi/a$]. We also consider two lines of special symmetry: Δ (connecting Γ and X) and Λ (connecting Γ and L).

Our goal will be to find the level degeneracies at these points and on these lines.

2.3.5 Point group of the diamond lattice

If we look at the lattice of diamond (5), we find that the point group is the symmetry group of a cube (including both proper and improper rotations), but the full space group is *non-symmorphic*.

The total number of group elements of this symmetry group (denote it by O_h) is 48.

The simplest improper rotation is the inversion (the simultaneous change of sign of all the coordinates). Let us denote this transformation by I . It commutes with all the rotations, and therefore the full point group O_h can be decomposed into a *direct product* of the group of proper rotations (denoted by O , contains 24 elements) and the "inversion" group $\{0, I\}$. The latter has two irreducible representations (both are one-dimensional): the trivial one and the "parity" one. Therefore for constructing the irreducible representations of O_h , it will be sufficient to construct the representations of O and then multiply them by one of the two representations of $\{0, I\}$.

2.3.6 Representations of O and O_h

To construct the table of characters for O , start with counting the classes of conjugate elements:

1 (1 element): unity;

6_{90° (6 elements): rotations by 90 degrees;

3_{180° (3 elements): rotations by 180 degrees about a face of the cube;

6_{180° (6 elements): rotations by 180 degrees about an edge center;

8_{120° (8 elements): rotations by 120 degrees about a cube diagonal.

Total 5 classes. Therefore there will be 5 irreducible representations in the character table.

The *trivial* representation is always there. We can also guess another one-dimensional representation (denote it by P): if we color the vertices of the cube in black and white in a checkerboard pattern, then the transformations can be classified into odd and even by whether they change the color of vertices. Finally, we also know a three-dimensional representation (by considering a cube in a 3D space), which is also obviously irreducible (can you explain why?). This three-dimensional representation may, in turn, be multiplied by P to produce yet another 3D representation. So we know already 4 out of 5 irreducible representations. The last one (or rather, its character) can be found from the orthogonality relations. As a result, we find the character table of O :

	1	6_{90°	3_{180°	6_{180°	8_{120°
1	1	1	1	1	1
P	1	-1	1	-1	1
2	2	0	2	0	-1
3	3	1	-1	-1	0
$3P$	3	-1	-1	1	0

Multiplying it by the character table of $\{0, I\}$,

	1	I
1	1	1
P_I	1	-1

we can write the character table of O_h (here we use the traditional crystallographic notation for the representations):

	1	6_{90°	3_{180°	6_{180°	8_{120°	I	$I6_{90^\circ}$	$I3_{180^\circ}$	$I6_{180^\circ}$	$I8_{120^\circ}$
Γ_1	1	1	1	1	1	1	1	1	1	1
Γ_2	1	-1	1	-1	1	1	-1	1	-1	1
Γ_{12}	2	0	2	0	-1	2	0	2	0	-1
Γ'_{15}	3	1	-1	-1	0	3	1	-1	-1	0
Γ'_{25}	3	-1	-1	1	0	3	-1	-1	1	0
Γ'_1	1	1	1	1	1	-1	-1	-1	-1	-1
Γ'_2	1	-1	1	-1	1	-1	1	-1	1	-1
Γ'_{12}	2	0	2	0	-1	-2	0	-2	0	1
Γ'_{15}	3	1	-1	-1	0	-3	-1	1	1	0
Γ'_{25}	3	-1	-1	1	0	-3	1	1	-1	0

2.3.7 Projective representations and non-symmorphic space groups

So far, we were assuming that we indeed had a linear representation of the symmetry group in the space of electron states. In fact, quantum states are defined up to a phase factor, and the group may also be represented only up to phase factors:

$$D(g_1)D(g_2) = e^{i\phi(g_1, g_2)} D(g_1 g_2). \quad (8)$$

In some situations, the phase factors $\phi(g_1, g_2)$ may be compensated by redefining $D(g)$:

$$D(g) \mapsto e^{i\alpha(g)} D(g), \quad (9)$$

and then the problem reduces to the conventional representation theory. In other situations, the phase factors $\phi(g_1, g_2)$ cannot be compensated, and we obtain a different type of representation, not included in the conventional character table.

The more general definition (8) of a representation is called a *projective representation*. The theory of projective representations may be reduced to the conventional theory of linear representations by extending the group (writing the phase factors as separate group elements commuting with the rest of the group) and then studying the conventional linear representations of the extended group (sometimes called the *double group* in the crystallographic context).

Examples of nontrivial projective representations include 3D rotations of a half-integer spin and translations of a charged particle in a magnetic field. In our example, we neglect the spin-orbit interaction, so no phase factors appear due to spin. However, one still needs to consider projective representations in order to classify the energy levels at some points at the boundary of the Brillouin zone in the case of a *non-symmorphic* space group. In our lecture, we will skip this part of the calculation.

2.3.8 Free-electron band structure

As a very crude approximation of the low-lying states, we may consider the band structure for a free electron by folding the parabolic spectrum centered at the lattice of k vectors (7) onto the BZ. This way we get the structure shown in Fig. 3. Note the very high degeneracies of levels. These degeneracies are reduced in a lattice potential down to the dimensions of the corresponding irreducible representations.

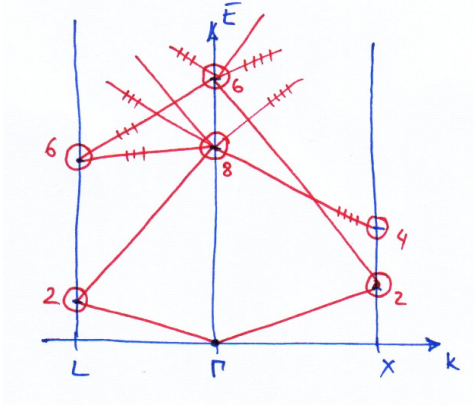


Figure 3: Sketch of the free-electron band structure of the diamond. Level degeneracies are marked.

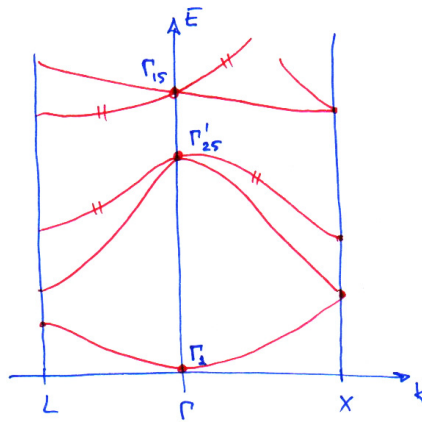


Figure 4: Sketch of the actual band structure of diamond, as calculated numerically in Bassani and Yoshimine, Phys. Rev. **130**, 20 (1963).

2.3.9 Numerically calculated band structure

The band structure calculated with a numerical method (orthogonalized plane wave) is schematically shown in Fig. 4. The degeneracies can be understood in terms of irreducible representations as discussed below.

2.3.10 Classification of states at the point Γ

The symmetry operations of the space group may be written as

$$g : x \mapsto Rx + L, \quad (10)$$

where R is an element of the point group (with respect to some center) and L is a translation. At the point Γ , translations do not produce extra phase factors (since $k = 0$), and therefore we have a conventional linear representation of the point group O_h . This representation may be decomposed into a sum of irreducible representations from the table above. Numerics shows that the three representations with the lowest energy are Γ_1 , Γ'_{25} (in the valence band), and Γ_{15} (in the conduction band).

2.3.11 Classification of states at the line $\Gamma - X$

At this line, the point group is reduced to those operations preserving the wave vector k (the so called *small point group*), i.e., preserving the direction along one of the crystallographic axes (e.g., $(1, 0, 0)$).

One can check that, since the direction is preserved, the translation in (10) contributes a phase factor, which may be compensated by putting $\alpha(g) = -\mathbf{k} \Delta \mathbf{x}$, where $\Delta \mathbf{x}$ is the vector of the translation L . Therefore it is again sufficient to consider the conventional representations without phase factors.

The small point group consists of only those group elements of O_h which preserve one of the faces of the cube. There are 8 such elements which fall into five classes of conjugate elements. The character table is

	1	2_{90°	1_{180°	2_+	2_\times
Δ_1	1	1	1	1	1
Δ_2	1	-1	1	-1	1
Δ'_1	1	1	1	-1	-1
Δ'_2	1	-1	1	1	-1
Δ_5	2	0	-2	0	0

2.3.12 Classification of states at the line $\Gamma - L$

The same argument is valid for the line $\Gamma - L$, except that now the small group only contains elements preserving the diagonal $(1, 1, 1)$. In terms of the symmetries of a cube, this group corresponds to fixing one corner of the cube.

The group has three elements and is equivalent to the group S_3 considered in the previous lecture. There are 6 elements, 3 conjugacy classes, and the representations have dimensions 1, 1, and 2.

2.3.13 Classifications of states at the points X and L

At these points, the phase factors cannot be compensated, since now the direction of the k vector may also be reversed. The classification of the states in this case requires the use of projective representations (or, equivalently, doubling the group). We do not discuss it in the lecture, but those interested may find details in the literature.

Problem Set 3

Problem 3.1

In the numerical calculation, the valence band at point Γ is three-fold degenerate and belongs to the representation Γ'_{25} . How does this three-fold degeneracy split along the lines $\Gamma - X$ and $\Gamma - L$? Calculate the result by treating Γ'_{25} as a representation of the small point group and by decomposing it into irreducible representations.

Problem 3.2

If one adds a potential to the free-electron band structure in Fig. 3, how would the 8-point degenerate level at the Γ point split? Hint: this degenerate level comes from the eight nearest-neighbor k points of the dual lattice in Fig. 2. They transform into each other under the O_h group as eight vertices of the cube.