2 Electronic band structure and lattice symmetries

In this section, we discuss how crystal symmetries can help in describing the electronic band structure (in particular, the level degeneracies at points of special symmetry in the Brillouin zone). In fact, the band structure itself (Bloch waves) may be viewed as a consequence of the translational symmetry of the crystal lattice.

2.1 Symmetries in quantum mechanics. Introductory remarks

Symetries play an important role in quantum mechanics. If a quantum problem has symmetries, then

- symmetries simplify the problem by providing good "quantum numbers"
- symmetries may be responsible for levels degeneracies

Namely, quantum levels may be classified according to the irreducible representations of the symmetry group. Then the Hamiltonian may be projected onto the states belonging to a specific type of irreducible representations, which reduces the dimension of the Hilbert space and thus simplifies the problem. If this irreducible representation is more than one-dimensional, then the corresponding levels are accordingly degenerate.

An example of such a reduction is known from a course of quantum mechanics: for a particle in a centrally symmetric potential, the states may be classified according to their angular momentum. In our course we will consider another example: how the *symmetries of the crystal lattice* may be used to classify electronic states.

The crystal symmetries involve two types of operations:

- Translations. These symmetries are responsible for the band structure: the states are classified according to their wave vectors ("Bloch theorem").
- Rotations and reflections. These symmetries are responsible for additional degeneracies occuring in the band structure.

Before discussing these symmetries in more detail, we briefly review the theory of group representations.

2.2 Groups and their representations: A crash course

Here I ony give a brief summary. Very helpful detailed notes on the representation theory may be found on the course web page of D. Vvedensky at the Imperial College London: `http://www.cmth.ph.ic.ac.uk/people/d.vvedensky/courses.html` [DV].

Please check the properites mentioned below against an example of your favorite group!

2.2.1 Definition of a group

A *group* is a set of elements with a multiplication operation. The multiplication must obey the following properties:

- $(ab)c = a(bc)$ — associativity
- $1 \cdot a = a \cdot 1 = a$ — the existence of unity (can you prove its uniqueness?)

- $aa^{-1} = a^{-1}a = 1$ — the existence of an inverse (one can further prove its uniqueness)

Groups often appear as symmetries of a geometric or physical object (atom, molecule, crystal). Think of examples of discrete and continuous groups.

2.2.2 Subgorups and direct product of groups

A *subgroup* is a group within a group (with the same multiplication operation). Think of interesting examples.

A *direct product* of two groups G and H is a set of pairs (g, h) with $g \in G$, $h \in H$, and a natural definition of multiplication: $(g_1, h_1) \cdot (g_2, h_2) = (g_1 g_2, h_1 h_2)$. Think of physical examples of this construction.

2.2.3 Abelian and nonabelian groups. Classes of conjugate elements

A group is said to be *abelian* if all its elements commute, $ab = ba$, and *nonabelian* otherwise. Example: rotations in 2D form an abelian group, rotations in 3D are nonabelian.

If we pick an element u in a group G, it defines a "similarity" (or *conjugation*) transformation $g \mapsto ugu^{-1}$ (for all elements $g \in G$). This similarity preserves the group multiplication: $(ug_1u^{-1})(ug_2u^{-1}) = u(g_1g_2)u^{-1}$. In other words, it is a symmetry of the group.

Abelian groups do not have nontrivial conjugations.

All elements related by conjugations form a *class of conjugate elements* (they are "similar" to each other). Example: in 3D, all rotation by a given angle (independently of the axis of rotation) are conjugate to each other.

2.2.4 Representations of groups

A (linear) *representation* of a group G is a set of $n \times n$ matrices which have the same multiplication table (with respect to the matrix product) as the group elements: to each group element g, there corresponds an *invertible* matrix $D(g)$ such that

$$D(g_1)D(g_2) = D(g_1g_2)\,. \tag{1}$$

The *dimension* of the representaiton is the size n of those matrices.

Example 1. If the group corresponds to spatial rotations of some object, than these spatial symmetries (written as coordinate transformations in space) realize its representation. The dimension of this representation equals the dimension of the physical space.

Example 2. For any group, there exists a one-dimensional trivial (identity) representation: matrices 1×1 (just numbers) with $D(g) \equiv 1$.

Example 3. For any group, there exists a so called *regular representation.* It is constructed in the following way. Consider group elements g as a basis of (quantum) states $|g\rangle$ and consider all possible superpositions

$$\psi = \sum_{g \in G} c_g \, |g\rangle \ . \tag{2}$$

Now if we define the action of a group element g_1 on the basis states by permuting them according to the group multiplication,

$$D(g_1) \, |g_2\rangle = |g_1 g_2\rangle \ , \tag{3}$$

then this action can be extended to a linear transformation on all the states ψ:

$$D(g) \sum_{g' \in G} c_{g'} \left| g' \right\rangle = \sum_{g' \in G} c_{g'} \left| g g' \right\rangle \tag{4}$$

and written as a matrix of the size equal to the number of elements in the group G. In the basis of the states $|g\rangle$, these matrices only contain zeros and ones. One can easily see that they form a representation of G.

This regular representation is useful in the represnetation theory, since it contains all the irreducible representations of the group (see below).

2.2.5 Reducible and irreducible representations

If some similarity transformation (change of basis)

$$D'(g) = U D(g) U^{-1} \tag{5}$$

with some matrix U (the same for all the elements g) brings a representation into a block-diagonal form

$$D'(g) = \begin{pmatrix} D'_1(g) & 0 \\ 0 & D'_2(g) \end{pmatrix} \tag{6}$$

(with some square matrices $D'_1(g)$ and $D'_2(g)$), then this representation is said to be *reducible* (and the representation $D(g)$ is decomposed into the *sum* of $D'_1(g)$ and $D'_2(g)$). Otherwise, it is called *irreducible.*

Note: if a representation is reducible, then there is a smaller subspace invariant with respect to all the elements of the group.

The reverse is true, if the representation is *unitary* (all $D(g)$ are unitary matrices).

- In general, any representation of a *finite* or, more generally, *compact* group can be brought to a unitary form by a suitable change of basis (5). For a counterexample (a representation of a non-compact group which cannot be brought to a unitary form), see the discussion of the translational symmetry of the lattice in the next lecture.
- In application to quantum mechanics, we always assume that our representations are unitary, since they correspond to physical symmetries of the Hilbert space of quantum states and hence are represented by unitary matrices.

Example. Consider the group of permutations of the three coordinate axes in the 3D space (6 permutations in total, this group is usually denoted S_3). Those permutations of the axes realize a three-dimensional representation of the group. The diagonal $x = y = z$ is invariant with respect to all those permutations. Therefore we immediately deduce that this representation is reducible.

2.2.6 Characters and character tables. Orthogonality relations

Our goal in this lecture is to learn how to

- classify all irreducible representations of a given group;

- for a given representation (physical symmetry acting in a physical Hilber space of quantum states), decompose it into a sum of irreducible representations.

This can be done with the help of characters.

A *character* of a representation $D(g)$ is a numerical function on the group elements defined as

$$\chi_D(g) = \mathrm{tr}\, D(g) \tag{7}$$

(trace of the matrix). It can be tought of as a fingerprint of a representation.

Some obvious properties of the character:

- $\chi_D(g)$ is basis independent;
- $\chi_D(g)$ is the same for all elements g in one class of conjugate elements. So the character is in fact a function on classes of conjugate elements;
- for any representation D, $\chi_D(1)$ gives the dimension of the representation (since 1 is always represented by the unit matrix);
- The character of a sum of representations (6) equals the sum of their characters.

For a finite group, the number of irreducible representations is also finite, and it is convenient to list the characters of all its irreducible representations in a table: the rows of the table correspond to the representations, the columns — to the classes of conjugate elements.

Example. The group S_3 of all the permutations of three elements. It has 6 group elements, which form three conjugate classes:

- identity element, 1, is always alone in its class
- three pairwise permutations, (12), (23) and (13). We denote this class $3_{(12)}$
- two cyclic permutations of the three elements, (123) and (132). We denote this class $2_{(123)}$

The representation table for S_3 looks as follows:

	1	$3_{(12)}$	$2_{(123)}$
Γ_1	1	1	1
Γ_2	1	-1	1
Γ_3	2	0	-1

For any group, its table of irreducible representations obeys the orthogonality relations (we don't prove them here, please refer to [DV] for proofs):

- **Orthogonality of rows:**

$$\sum_\alpha n_\alpha \chi_k(\alpha)\chi_{k'}(\alpha)^* = |G|\delta_{kk'}\,, \tag{8}$$

  where the sum is taken over classes of conjugate elements, n_α is the number of elements in each class, and $|G|$ is the total number of elements in the group. k and k' denote two (different or coinciding) irreducible representations. The star denotes complex conjugation (characters are sometimes complex!).

- **Orthogonality of columns:**

$$\sum_k \chi_k(\alpha)\chi_k(\alpha')^* = \frac{|G|}{n_\alpha}\delta_{\alpha\alpha'}\,, \tag{9}$$

  where the sum is now over irreducible representations.

Several useful properties follow from these general orthogonality relations (or can be deduced independently):

- The number of irreducible representations of the group equals the number of conjugacy classes of that group;

- The sum of squares of the dimensions of the irreducible representations equals the number of elements in the group:

$$\sum_k \dim(k)^2 = |G| \tag{10}$$

  Note that these two properties are usually sufficient to determine the dimensions of the irreducible representations for sufficiently small finite groups.

- Abelian (commutative) groups have only one-dimensional irreducible representations. Nonabelian (noncommutative) groups have at least one non-one-dimensional irreducible representation.

For sufficiently small finite groups, the character tables may be constructed "by hand": usually, one knows a priori some of the representations (e.g., the identity representation and other one-dimensional representations), and, together with the orthogonality relations, it is sufficient to complete the table. Formal algorithms also exist, but they are more suitable for computer programs and we will not study them.

Furthermore, the orthogonality relations help in decomposing a given representation into a sum of irreducible representations. This can be done by *projecting* onto each irreducibe representation using (8):

$$N_k = \frac{1}{|G|}\sum_\alpha n_\alpha \chi(\alpha)\chi_k(\alpha)^*\,. \tag{11}$$

In particular, if we apply this formula to the *regular representation* (whose character is $\chi(1) = |G|$ and $\chi(\alpha) = 0$ for all other conjugacy classes), we find that the fundamental representation contains all the irreducible representations with multiplicities equal to their dimensions [cf. Eq. (10)].

2.2.7 Irreducible representations in quantum mechanics

Suppose now that G is the group of symmetries of a quantum Hamiltonian H. Then it is represented by linear (unitary) operators in the Hilbert space of quantum states.

Usually, this representation is reducible. The symmetry of the Hamiltonain implies $D(g)HD(g)^{-1} = H$ for all group elements g.[1]

Suppose, Ψ is an eigenstate of H at energy E. Then, for any group element g, its action on Ψ produces again an eigenstate at the same energy E. Formally, we may write this as

$$HD(g)\Psi = D(g)H\Psi = D(g)E\Psi = ED(g)\Psi\,. \tag{12}$$

If we diagonalize the Hamiltonian, then the eigenvectors corresponding to the same energy transform into each other by the group G and therefore form a representation of G.

Thus the diagonalization of the Hamiltonian simultaneously decomposes the representation of G in the full Hilbert space into a sum of smaller representation. If those smaller representations are reducible, we may decompose them further, until we reach a decomposition into irreducible representations. Each of the irreducible representations is an eigenspace of the Hamiltonian corresponding to some energy E.

In the most general situation, all those energies E are different, and we find that the degeneracies of levels are given by the dimensions of the irreducible representations. Sometimes, some of those energies may coincide, and then the degeneracy is given by the sum of the dimensions of several irreducible representations. Usually, this coincidence happens either as a result of a fine-tuning of some parameters (*accidental degeneracy*) or as a consequence of a larger symmetry not taken into account.

We can also reverse this procedure and first decompose the full representation of G into a sum of irreducible representations, and then it will be sufficient to diagonalize the Hamiltonian separately within each class of irreducible representations. This classification into irreducible representations provides a good set of "quantum numbers" and considerably simplifies the problem (by reducing the dimension of the Hamiltonian).

Example: For a quantum particle in a symmetric potential $U(x) = U(-x)$, we may require that the eigenstates are either even or odd in x: $\Psi(x) = \pm\Psi(-x)$. Those even (odd) wave functions belong to the even (odd) representation of the reflection symmetry group (transforming $x \mapsto -x$).

2.2.8 Concluding remarks

For understanding general properties of groups and their representations, it is always helpful to keep in mind some simple examples (cyclic groups, 3D rotations, etc.).

We have discussed mainly representations of *finite* groups: in this case, there is only a finite number of irreducible representations, and the character table is finite. However, many of the properties of representations of infinite groups (e.g., orthogonality relations) are very similar to the finite case, with the only difference that the number of irreducible representations becomes infinite, and the finite sums get replaced either by infinite sums or by integrals.

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[1] Rigorously speaking, since quantum states are defined up to a phase factor, the group G is also represented up to arbitrary phase factors in Eq. (1). In this way, the notion of a linear representation is generalized to a *projective representation* (in the context of electronic structure, also sometimes called a *representation of the double group*). The examples of nontrivial projective representations are 3D rotations of a half-integer spin and translations of a charged particle in a magnetic field. In our lecture, we will discuss the band structure in the absence of magnetic field and neglecting the spin-orbit interaction. Under these assumptions, the geometric symmetries of the crystal lattice form a linear representation without phase factors. See however the discussion of *non-symmorphic* crystallographic groups in the next section.

Problem Set 2

Problem 2.1

(a) Construct the character table for the group D_4 of all the symmetries of a square, including rotations and reflections. How many irreducible representations are there? Can you also construct those representations explicitly?

(b) Consider a sinlge quantum particle hopping between the four corners of a square. The hopping amplitude along each side of the square is $-t_1$ and along each of the two diagonals $-t_2$. The Hamiltonian of the particle can be written as the matrix

$$H = \begin{pmatrix} 0 & -t_1 & -t_2 & -t_1 \\ -t_1 & 0 & -t_1 & -t_2 \\ -t_2 & -t_1 & 0 & -t_1 \\ -t_1 & -t_2 & -t_1 & 0 \end{pmatrix} . \tag{13}$$

Find the spectrum of this Hamiltonian and classify the levels according to the representations of D_4.

(c) Suppose now that the square is stretched along the axis parallel to a pair of sides (so that the hopping coefficients t_1' along this direction and t_1'' along the perpendicular direction become different). How will the energy levels split?

(d) The same question if the square is stretched along one of the diagonals (so that the two coefficients along the two diagonals t_2' and t_2'' become different).