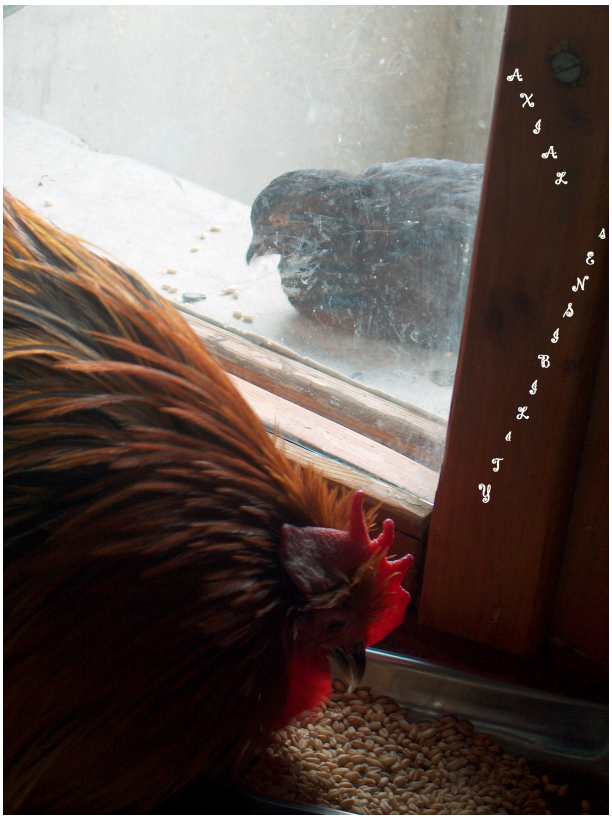
SYMMETRY IN QUANTUM NONRELATIVISTIC PHYSICS

M. Damnjanović



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INTRODUCTION

Powerful method of deduction, accurately extracting relevant characteristics of the studied object and allowing transparent interpretation of results, established the symmetry as one of the most important concepts in physics. Its techniques connect various fields of physics, offering a unified view to diverse phenomena. This distinguished status originates in the importance of symmetry as a *physical property* both of space-time and of physical systems. During the development of modern physics, this property has been more and more understood as the essential one. Nowadays, it is known that symmetry is the source of primary characteristics of physical systems, to mention only mass and spin, or various types of the fundamental interactions.

Symmetry based considerations require application of group theory, one of the leading fields of contemporary mathematics. Simultaneous rise of the concept of symmetry in physics and of the corresponding technique in mathematics reminds of a similar history of another great idea of physics: development of the mathematical analysis was indispensable for the precise formulation of the notion of *continuity* of the physical processes[1]. Mathematical analysis was necessary to understand the fundamental principles of mechanics, though the intuition of the physicists previously enabled to solve many related problems, even considerably complex ones. Without analysis, the natural notion of change, evolution, would not be operative. Investigating this notion, Newton opened a new epoch not only in physics, but in mathematics, too. Thus, both continuity and symmetry show mutual permeation of physics and mathematics, inherited from their common origin, antic geometry. Galileo's description of this relationship is: "The book of the nature is written in the language of mathematics".

The first considerations explicitly based on symmetry appeared during early research of minerals. Characteristic shapes of various crystals have always attracted attention of the scientists. Yet in 1611 Kepler thought about the cause of the invariant form of the snowflakes. Delisle in 1783 stated the precise relations among the angles and the edges of minerals. The end of the 18th and the beginning of the 19th century brought in early intimations of atomic physics; the classical idea about the elementary constituents of matter matured to the modern cognition by works of Dalton, Avogadro, Bercelius and others. The notion of the structure of matter got connotation of the arrangement of different atoms. In such a milieu the regular shapes of the minerals were no longer left to admiration of geologists, but became a

[1] In Greek, $\sigma\upsilon\mu\mu\varepsilon\tau\rho\iota\alpha$ denotes regularity, accordance; "continuity" comes from the notion $\kappa\omicron\iota\nu\omicron\varsigma$, for common acting (the older word is $\sigma\upsilon\nu\varepsilon\kappa\varsigma$).

challenge and milestone for new theory. Our predecessors in the dawn of atomistics unerringly conjectured that external visage reflected interior anatomy, arrangement of pieces of matter. Indeed, the laws observed in minerals were among the milestones in promoting atomistic ideas. After having realized the integral rates of the elements in molecules, Dalton learnt about the integral relations between the angles in crystals (attending the lectures on mineralogy), and this finally assured him in the atomistic hypothesis. The problem of determination of possible structures and their relation to observable shapes of minerals arose; a *method* was looked for to convert the *contents* of the observation, the regularity of the shapes, into conclusions on the structure, manifesting once again how far-reaching the new theory was.

And, the method was growing simultaneously but independently in the neighborhood — in mathematics, only articulation of the contents in the appropriate *form* was waited for. It was necessary to formalize the intuitive sense of the shape's regularity as a set of the symmetries — operations transforming the shape into itself. A succession of such operations is a new symmetry, and all of them form the algebraic structure of the group, being intensively studied by the mathematicians in these decades. In the works of Euler (1761), Lagrange and Vandermonde (1771) this structure is implicitly used, and Evariste Galois (1811-1832) called it *group* for the first time in 1830, while his last letter to Gauss and Jacobi (written in the evening before he was killed in a duel) contained many important results. Intense research during the 19. century (Gauss, Abel, Cartan, Klein, Jordan and other famous mathematicians) led to the contemporary axiomatization of the abstract group (Cayley, 1854) and group with analytic properties (Lie, 1895). At the very beginning of the 20. century Frobenius formulated the theory of representations of groups, which has proved to be the most important part for the physics.

Classification of crystal structures was reduced to classification of their symmetry groups. With help of the group theory only, in 1890, Fedorov and Schönfliess independently derived all of the 230 possible crystal lattices. Much before the first experimental technique capable to observe the crystal structure directly was invented (1912, X-ray diffraction, Laue, Friedrich and Knipping)!

Connection between symmetry and conservation laws shows profound penetration of the concept of symmetry into physics. More then 2000 years passed from the metaphysical inkling of the immutability of motion, to the precise formulations of the conservation laws of mass and energy (in the middle of the 19th century). Afterwards, the interplay between conservation laws and symmetry was rapidly revealing and in 1918 it obtained its present form in the work of E. Noether. Quantum theory, established itself in the same period by Planck, Einstein, Schrödinger, Pauli, Heisenberg, Eugen Wigner and many other physicists, as well as the mathematicians von Neumann and Weyl, additionally urged the development of the concept of symmetry, giving it the most suitable form — *representation of the symmetry group in the state space of the system*. This enabled a systematic use of conservation laws through good quantum numbers, which founded the forthcoming leading role of symmetry in the elementary particle physics in fifties of the last century: the experimental facts indicate some of the conservation laws, singling out the minimal symmetry group of the system; then the

groups containing this minimal one are looked for and used as a basis of various theoretical models. Closing one more circle in the evolution of knowledge, such a concept of symmetry recalls its origin: in the crowd of information on the elementary particles or minerals, the symmetry is the key for its classification and explanation. As always, a qualitative advance took place. In crystallography the symmetry operations had been known and transparent (rotations, translations, reflections); only their classification had to be performed. On the contrary, contemporary physics deals with symmetries having interpretation only within the theory; the essence of the problem is not to classify, but to define possible symmetries. Thus, from an unnoticed companion of the conservation laws, symmetry arose to be a cornerstone of the theories of elementary interactions.

The concept of continuity, introduced originally in physics, did induce development of mathematical analysis evolved into diverse contemporary branches. Many of them are far away from physics, but connection is firmly maintained by differential geometry, maybe the most important part of mathematics. Its development was permanently supported by physicist, both by concrete results and by bringing in new ideas. Even the phenomena characterized by discontinuity, singularities, being especially focused in modern physics, are described and treated in terms of differential geometry. This resembles a lot to the status of symmetry. Some of the symmetry based considerations can be performed without specific knowledge, but for profound insight the group theoretical techniques are necessary. Growing of this mathematical branch has been influenced from the very beginning by needs of physics. The group theory gives framework for studying symmetry breaking, the process of loosing symmetries. As a rule, such processes are abrupt, with discontinuities subdued to laws emphasizing profound relationship between continuity and symmetry. Therefore, intertwining of group theory and mathematical analysis within differential geometry is natural and symbolic: the great ideas of physics, continuity and symmetry, are joined in geometry, being the common origin both of physics and mathematics. One more circle of knowledge is closing, the great one perhaps.

Considerations involving symmetry are performed in all fields of physics, and in all stages of perceiving of physical problems. Technically, the application of symmetry gives significant simplifications of the task, and sometimes this is tacit, intuitive, with no explicit appeal to group theory. On the other hand, the primary postulate of physics, the principle of relativity (Galileo's or Einstein's), is essentially a statement on the space-time symmetry, and its meaning and far reaching consequences are most transparently and completely understood within a systematic group theoretical analysis. Therefore, one approach to the concept of symmetry is studying various aspects of its applications related to one system, i.e. within one discipline of physics (*e.g.* solid state, molecular or elementary particle physics). Contrariwise, there are attempts to extract common characteristics of the symmetry based analyses in various fields; such a view point requires formulation of physical problems in the standardized form, sublimating ingredients necessary for symmetry techniques.

Following the latter scheme, this text begins by introducing symmetry adapted bases and irreducible tensor operators, singling out the group projectors as the main tool of the symmetry based methods. After this follow general considerations of application of symmetry within

various approximate techniques. In the hierarchy of a physical theory, the contents (general physical principles and concrete facts which are involved in the formulation) and methods of solution are intertwined in many ways. Only exceptionally the answer is obtained directly from the first principles. Typically, a series of approximations is introduced and each of them effectively redefines the problem, introducing slightly different physical conditions with appropriate laws. The Art of Deduction in physics is to weave the way to a solvable problem, which, despite of various modifications, faithfully reflects the initial one, at least in the context of the studied properties. And this is the point where the symmetry is invaluable for its exactness. Approximations performed in standard techniques preserve symmetry, providing the exact treatment of the symmetry based characteristics. And, as these (characteristics) are sufficiently important and numerous to greatly determine the studied phenomenon, a qualitatively good description is insured. (For example, the assumption that the interaction of two particles is a function of their mutual distance only, implies that all rotations are symmetries of such a system; this suffices to obtain selection rules for quantum transitions of the system, independently of the concrete form of the interaction — Coulomb, harmonic or a more complex one. Also, the fact that the particles of the system are identical, *i.e.* that all their permutations are symmetries, yields a number of exact, surprisingly far reaching conclusions, independent on the other details of the system.)

In the second chapter the most important nonrelativistic symmetries are reviewed. There is no conceptual difference in the treatment of symmetries within relativistic and nonrelativistic theories; only different space-time groups of symmetry are involved, and this choice of the inertial transformations determines whether Galileo or Einstein relativity is proposed. The permutational symmetries of identical particles are also studied in this chapter, because of their specific relation to geometrical symmetries.

The third chapter deals with harmonic approximation, being the starting point of the most of the physical models. It is shown how symmetry simplifies calculations, giving at the same time classification of the degrees of freedom. The obtained picture, identifying the vibrations near the minimum of the potential energy with the elementary excitations of the system, underlies the fundamental notion of quasi-particles (including the particles themselves within quantum field theory), whose classification is governed by symmetry.

Within the concept of symmetry, the notion of symmetry breaking appeared. As well as normal vibrations, this phenomenon is observed in the various fields of physics: phase transitions in crystals, Jahn-Teller effect in molecules and the symmetry breaking in field theory, all of them are the same process of spontaneous symmetry breaking, described in the fourth chapter.

Finally, in the last chapter it is studied how the adiabatic approximation, yet one quite general theme of physics, is used to separate electronic and ionic subsystems in molecules and crystals. This approach offers some general symmetry based conclusions: the translational invariance suffices to understand the classification of crystals onto insulators and conductors; no crossing of the energy bands of the same symmetry is allowed.

The importance of group theory for understanding and applying symmetry in physics has

already been emphasized. To facilitate reading of the text, the most important notions and results of this theory are sketched in the appendices. These notions are simple, except the part related to the induction theory involving the projective representations. Therefore, an effort is made to avoid the projective representations in the main text: the alternative approach has been used whenever it was possible; otherwise, only a hint has been given. This task could be performed only at the cost of excluding a review of the Galileo group; consequently, symmetry treatment of mass and spin, and classification of the equations of motion in the nonrelativistic physics have been skipped. To justify this compromise, simply note that such considerations are really relevant only within relativistic physics, and in that case analogous study (of the Poincare group) is much simpler.

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Chapter 1

PRINCIPLES OF APPLICATION OF SYMMETRY

Numerous fields of physics, using immense bunch of methods, investigate different systems: atoms, molecules, crystals, elementary particles, etc. Still, the structure of all these theories is the same: object of investigation is analyzed to get formal description of its (studied) behavior in terms of relevant parameters. This introduces the notion of the *state* of the system, being a particular choice of values of these parameters. The set of all physical states is *state space*, $\mathcal{S}$. Essentially, the prediction expected from theory is *dynamics* of system, i.e. change, *evolution* of states during the time. More formally, initial state x evolves along curve $x(t)$ in $\mathcal{S}$, such that $x(0) = x$. Evolution is consequence of basic laws, usually expressed in the form of specific variational principle. As a result, there appears fundamental dynamical quantity H, which, sublimating all the information about the evolution, completely determines the dynamics. In this scheme, the physical system is identified with the pair $(\mathcal{S}, H)$.

In this sense quantum mechanics is a typical theory: the state space is postulated to be a *vector (Hilbert) space*, while the dynamics is governed by the *hamiltonian operator* H in this space [3, 17]. In other theories the nature of $\mathcal{S}$ i H may be different. For example, the classical mechanical state space, *the phase space*, may not be vector space; still, locally, in the vicinity of some point, the relevant entities are structured as in the quantum case[1]. Therefore, mathematical formalism developed for quantum mechanics is applicable, at least locally, to all physical theories.

1.1 Symmetry of system

Described (quantum like) formalism enables to introduce symmetry of the system by the language of the representations of the groups in the state space. This framework is empowered to formalize precisely intuitive notions and assumptions related to symmetry.

[1] E.g. phase space of a point particle moving along a circle is cylinder: for each point on the circle, momentum may be any real number. This is manifold, and locally it can be identified with $\mathbb{R}^2$, with evolution generated by some symmetric matrix.

Symmetries of the system are the transformations of the state space, bijections of $\mathcal{S}$ onto itself, which do not change dynamical law: if a symmetry maps the state x into the state y, than the evolution curve $x(t)$, starting at x, is also mapped into the evolution curve $y(t)$ starting at y, meaning that the same transformation maps at any instant t the state $x(t)$ to the corresponding state $y(t)$. The immediate consequence is that the set of symmetries is a *group* (§ A.1.1): successive action of symmetries is a symmetry (closeness), composition of mappings is associative, identical transformation is obviously symmetry of the system, as well as the inverse mapping of any symmetry.

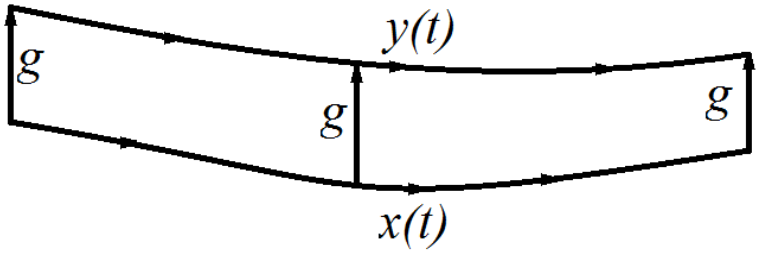

Figure 1.1: **Symmetry.** *The transformation g is symmetry if it commutes with the evolution of the system, i.e. if the diagram is commutative.*

In quantum mechanics ($\mathcal{S}$ is vector space, and H is the hamiltonian operator) the described invariance of the dynamics is expressed as the commuting of the operators *representing* symmetry transformations in $\mathcal{S}$ with H. Further, as the modules of the scalar products of the states are measurable transition probabilities, and the states are normalized vectors, transformations of symmetry must leave scalar product invariant. This implies that the operators representing symmetries are unitary or anti unitary, as the famous *Wigner's theorem* (§ B.2) shows. This is the point where the group of all unitary (and antiunitary) operators commuting with the hamiltonian appears[2]:

$$G_H = \{U \in \mathrm{U}(\mathcal{S}) \mid [U, H] = 0\}; \tag{1.1}$$

it is called the *the total symmetry group of the system* or the *symmetry group of the hamiltonian.*

The group G_H is not the group of symmetry which is directly used. In fact, it contains many unitary operators without any obvious physical interpretation. These cannot be noted *a priory*, without the formalism imposed by the quantum mechanics. Therefore, one usually starts with the subgroup G of G_H defined in more intuitive way. The physical context of the considered problem singles out some group of transformations, $\mathcal{G}$, and elements of this group only are the possible candidates for symmetries. For example, when the geometrical symmetries are looked for in non-relativistic mechanics, $\mathcal{G}$ is the Euclid's group (§ 2.1.3), while in elementary particle physics this role is taken by some orthogonal and unitary groups,

[2]With the exception of time reversal, only unitary operators are sufficient; this is tacitly assumed when the group $\mathrm{U}(\mathcal{S})$ of the unitary operators in $\mathcal{S}$ is used in the next expression.

combined with Poincare's group. However, these transformations do not act in in $\mathcal{S}$ (in the examples above the transformations are in Euclid's and Minkowski's space), and the group $\mathcal{G}$ is not group of the (anti) unitary operators in $\mathcal{S}$. To imbed it into the quantum formalism, it is *represented* by such operators: homomorphism D, mapping $g \in \mathcal{G}$ into the operator $D(g) \in \mathrm{U}(\mathcal{S})$, is established, providing linear action (§ A.1.4) of $\mathcal{G}$ in $\mathcal{S}$. Then G is the maximal subgroup of $\mathcal{G}$ containing only the elements commuting (when represented) with H, i.e. G is the intersection of $\mathcal{G}$ with the group of all the symmetries of the system $(\mathcal{S}, H)$:

$$G \stackrel{\text{def}}{=} \{g \in \mathcal{G} \mid D(g) \in G_H\} = \{g \in \mathcal{G} \mid [D(g), H] = 0\}. \tag{1.2}$$

Consequently, there may be some symmetries of H, which are not the elements of $\mathcal{G}$, and therefore they are not included in G. Most of these symmetries do not have any intuitive interpretation at the considered level of theory. Still, their complete discarding may have consequences to the scope and efficiency of theory (later on some of these questions will be elaborated), and sometimes they are *a posteriori* searched for. Note that introduction of $\mathcal{G}$ makes the definition of G is somewhat arbitrary, depending on the level and purpose of research, but exactly this restriction (to a familiar group $\mathcal{G}$) makes the relevant group G easy to determine.

To summarize this analysis, the triple $(\mathcal{S}, H, D(G))$ is suitable characterization of the physical system with symmetry group G acting in the state space by the representation D. Since each operator $D(g)$ is either unitary or anti unitary (Wigner's theorem), only unitary or anti unitary representations of groups in the state space are to be considered[3]. It turns out that only time reversal (§ 2.6.1) is represented by the anti unitary operator, while all other symmetries can be studied within the simplest framework of the unitary representations. As for the *Lie groups* (§ A.1.2), their generators, $\{l_1, \ldots, l_n\}$, are represented in $\mathcal{S}$ by hermitean operators, and interpreted as certain physical observables. These operators, $D(l_i)$, commute with H, since the operators representing the elements of group do.

A useful notion is the *group of symmetry of the state*, G_x, defined as the subgroup of G leaving invariant the state x, i.e. G_x is the little group or the stabilizer of x (§ A.1.4):

$$G_x \stackrel{\text{def}}{=} \{g \in G \mid D(g)\,|x\rangle = |x\rangle\}. \tag{1.3}$$

Note that different states of the same system may have different groups of symmetry.

Technically, utilization of symmetry can reduce the complexity of the problem. For example, the analysis can be performed only for some part of the state space, while the conclusions can be extended to other states, due to symmetry. Nevertheless, the best known applications and the most important phenomenological manifestations of symmetry, are the conservation laws. Commutation of the symmetries with hamiltonian implies that the properties of the system based on symmetries or their generators (in the case of Lie groups) are conserved during the evolution. E. g., if the state of the system is initially an eigenvector for the operator

[3]Since the collinear vectors after normalization give the vectors differing only by the phase factor, and all of them correspond to the same physical state, the *projective (anti)unitary representations* (§ A.2.7), and covering groups could be used, but this cumbersome approach proved to be inefficient.

$D(g)$, then during the evolution it remains the eigenvector for the same eigenvalue of this operator: $D(g)\,|x(t)\rangle = \alpha\,|x(t)\rangle$. The number of independent conservation laws is related to the structure of the symmetry group. Note that if G is not the maximal symmetry group of H, there can be some conservation laws which cannot be derived from G: just these "strange" conservation laws point out to the overlooked symmetries (in fact, contemporary physics uses some completely artificial new types of symmetries, without any obvious interpretation, which have been noticed only by such conservation laws.

1.2 Symmetry adapted eigenstates

Since the representation $D(G)$ is unitary, it is the orthogonal sum of its irreducible components, $D(G) = \oplus_{\mu=1}^{s} a_\mu D^{(\mu)}(G)$, and introduces the decomposition of the space $\mathcal{S}$ onto the irreducible subspaces: $\mathcal{S} = \oplus_\mu \mathcal{S}^{(\mu)} = \oplus_{\mu t_\mu} \mathcal{S}^{(\mu t_\mu)}$. In the *standard* or *symmetry adapted basis*, [8], $\{|\ \mu t_\mu m\ \rangle | \mu = 1, \ldots, s; t_\mu = 1, \ldots, a_\mu; m = 1, \ldots, |\mu|\}$ ($|\mu|$ is the dimension of the μ-th irreducible representation) of the space $\mathcal{S}$, the matrices representing the operators of $D(G)$ are block-diagonal, with the diagonal submatrices being irreducible matrix representations:

$$D(g)|\ \mu t_\mu m\ \rangle = \sum_{m'} D^{(\mu)}_{m'm}(g)\ |\mu t_\mu m'\rangle. \tag{1.4}$$

It will be assumed that the standard basis is orthonormalized.

It is well known from the linear algebra that if two operators commute, then the eigensubspaces of the first one are the invariant subspaces for the second one. This enables to use the symmetry to obtain the stationary states, *i.e.* the states which are not observably changed during the evolution. Indeed, these states are the eigenstates of H. Therefore, being invariant for $D(G)$, each eigensubspace of H can be decomposed to some irreducible subspaces. As a consequence, the symmetry adapted basis (1.4) can be chosen among the eigenvectors of H, and such basis will be called *stationary standard (or symmetry adapted) basis*. The same irreducible component may appear in the different eigenspaces of H, and therefore the eigenvalues of H can be labeled by the index of the irreducible representation and the index of its appearance: $H|\ \mu t_\mu m\ \rangle = E_{\mu t_\mu}|\ \mu t_\mu m\ \rangle$.

The previous conclusion is important for several reasons. The possibility to simplify the eigenvalue problem of H (by the breaking into many problems of the lower dimension) appears immediately. This is most efficiently performed by the *group projector* technique. The *group operators*

$$P^{(\mu)}_{mm'} \stackrel{\text{def}}{=} \frac{n_\mu}{|G|} \sum_{g\in G} d^{(\mu)*}_{mm'}(g) D(g) \tag{1.5}$$

commute with H. Especially, $P^{(\mu)}_{mm}$ are the projectors onto the a_μ-dimensional subspaces $\mathcal{S}^{(\mu)}_m \stackrel{\text{def}}{=} \text{spann}(\{|\,\mu t_\mu m\rangle | t_\mu = 1, \ldots, a_\mu\})$. Therefore, there exists a common eigen basis for H and $P^{(\mu)}_{11}$ in $\mathcal{S}^{(\mu)}_1$, *i.e.* the eigen basis for the reduced operator $P^{(\mu)}_{11}H$. These basis vectors are standard stationary vectors $\{|\ \mu t_\mu 1\rangle | t_\mu = 1, \ldots, a_\mu\}$, which should be mapped by the operators $P^{(\mu)}_{m1}$ to obtain the rest of the standard eigen basis (the same eigenvalue of H for

same t_μ): $|\mu t_\mu m\rangle = P^{(\mu)}_{m1}\,|\mu t_\mu 1\rangle$. In the presented algorithm, one a_μ-dimensional eigenproblem is solved for each μ, instead of the initial one in the whole space. Note that the group operators $P^{(\mu)}_{mm'}$ can understood as the $|D|\times|D|$ blocks of the $|\mu||D|$-dimensional *modified group projector* $G^\mu(D) = \frac{1}{|G|}\sum_{g\in G} d^{(\mu)^*}(g)\otimes D(g)$, projecting onto subspace of the (multiple) identity representation (i.e. on the fixed points) of the representation $d^{(\mu)^*}(G)\otimes D(G)$ in the space $\mathcal{S}^{\mu^*}\otimes\mathcal{S}$. This observation is the starting point of the modified group projector technique (Appendix C), as it is easier to deal with single projector $G^\mu(D)$ with convenient algebraic properties, especially when the $D(G)$ is induced representation.

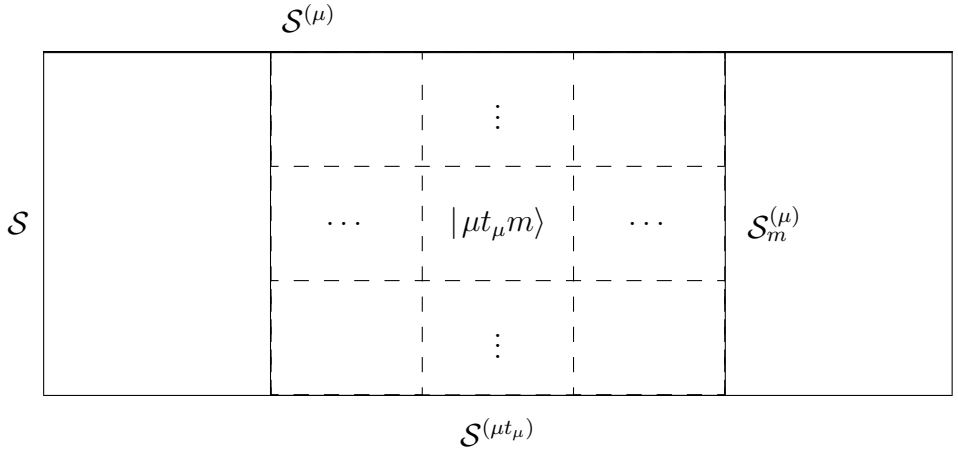

Figure 1.2: **Symmetry adapted basis.** *The state space $\mathcal{S}$ is decomposed onto the multiple irreducible subspaces $\mathcal{S}^{(\mu)}$. Each $\mathcal{S}^{(\mu)}$ is decomposed itself in two ways: either onto a_μ isomorphic n_μ-dimensional irreducible subspaces $\mathcal{S}^{(\mu t_\mu)}$, $t_\mu = 1,\ldots,a_\mu$ (vertical), or onto n_μ isomorphic a_μ-dimensional subspaces $\mathcal{S}^{(\mu)}_m$, $m = 1,\ldots,n_\mu$ (horizontal). The intersection of $\mathcal{S}^{(\mu t_\mu)}$ and $\mathcal{S}^{(\mu)}_m$ is one-dimensional, and spanned by the standard vector $|\mu t_\mu m\rangle$.*

The subspace $\mathcal{S}^{(\mu t_\mu)}$, spanned by the vectors $|\,\mu t_\mu m\,\rangle$ ($m = 1,\ldots,n_\mu$, t_μ fixed) is irreducible for the group action. All its vectors are eigenvectors of H, for the same eigen value $E_{\mu t_\mu}$. Thus, H acts in $\mathcal{S}^{(\mu t_\mu)}$ as the scalar operator. In other words, since $P^{(\mu t_\mu)} \stackrel{\text{def}}{=} \sum_m |\,\mu t_\mu m\,\rangle\langle\,\mu t_\mu m\,|$ is the projector onto this subspace, the action of H in $\mathcal{S}^{(\mu t_\mu)}$ is in fact $P^{(\mu t_\mu)}H = E_{\mu t_\mu}P^{(\mu t_\mu)}$. It is clear now that the dynamics of the system is reduced into the irreducible subspaces of the group: all the states from the same irreducible subspace evolve in the same way, remaining in that subspace. In fact, this is a form to express the conservation laws, giving the possibility to establish the dynamical equations on the symmetry ground. If G is the symmetry group of the system, each dynamical law must provide the decomposition of the state space onto the irreducible subspaces of the group G, to enable the evolution within these subspaces, in the described manner. In principle, this condition suffices to derive the equations of motion of the elementary systems (when the symmetry group is a priori equal to the group of relativity); this is especially important within the relativistic quantum field theory. In the same way the Bloch's theorem (§ 2.3.1) or the Schrödinger's equation of the free particle (§ 2.1.3) can be interpreted.

The question if the eigen subspaces of H are irreducible for G, naturally arises in the context of the symmetry labels of the eigenvalues. The essential part of the problem is enlighten by the following

Teorem 1 *The eigen subspaces of H are irreducible subspaces for the group G_H of all the unitary operators in $\mathcal{S}$ commuting with H.*

Indeed, if $\mathcal{S}_i$ denotes the i-th eigen subspace of H, and $U(\mathcal{S}_i)$ is the set of the unitary operators in $\mathcal{S}$ acting as the identity in $\mathcal{S}_i^{\perp}$, then obviously $G_H = \otimes_i U(\mathcal{S}_i)$. The groups $U(\mathcal{S}_i)$ are the irreducible representations of themselves, and therefore, at the same time these are the irreducible representations of the group G_H (for each i the representation $D(U_1, \dots, U_i, \dots) = 1 \otimes \cdots \otimes 1 \otimes U_i \otimes 1 \cdots = U_i$ is irreducible representation of the group G_H).

The theorem explains the appearance of the *accidental degeneracy*, which is situation when the eigen subspaces of H are not irreducible for G. This means that there are unitary operators in $\mathcal{S}$ commuting with H, which represent no elements of G. Therefore these operators are not covered by the considered symmetry group, and G is not maximal; it can be supplemented by certain additional symmetries (maybe with no manifest physical interpretation), such that the eigen subspaces of H become irreducible for the extended group. Only in this sense can be introduced the *irreducibility postulate*, requiring the irreducibility of the eigen subspaces of H. There are famous examples of the accidental degeneracy, being consequence of the hidden symmetry of H: Kramers' degeneracy of fermions (§ 2.6.1), is caused by the time reversal; the degeneracy in the Coulomb's field is greater than it is required by the spherical symmetry, and *a posteriori* the additional symmetry isomorphic to the group $\mathrm{SO}(3, \mathbb{R})$ is revealed (§ 2.1.2).

1.3 Transformation of the operators

The operators in $\mathcal{S}$ form the vector space $\mathcal{S} \otimes \mathcal{S}^*$ (it is called the superspace). Also, it is well known that each operator in $\mathcal{S}$, determines a linear operator in the dual space $\mathcal{S}^*$, and, finally, in the $\mathcal{S} \otimes \mathcal{S}^*$. If the initial operator is unitary, the generated operator on $\mathcal{S} \otimes \mathcal{S}^*$ is unitary again (with respect to the scalar product $(A, B) \stackrel{\text{def}}{=} Tr(A^\dagger B)$). Therefore, the representation $D(G)$ of G in $\mathcal{S}$ determines the representation $\hat{D}(G)$ in $\mathcal{S} \otimes \mathcal{S}^*$ (homomorphism is easily verified) acting on the arbitrary operator A as: $\hat{D}(g)A \stackrel{\text{def}}{=} D(g)AD^{-1}(g)$. Obviously, the representation $\hat{D}(G)$ is equivalent to the direct product (§ A.2.5) $D(G) \otimes D^*(G)$.

The reduction of the representation $\hat{D}(G)$ can be performed in the standard way, giving the decomposition of the operator space onto the mutually orthogonal subspaces, invariant for $\hat{D}(G)$; this are called the *tensor subspaces*. The operators of the irreducible tensor subspaces are called the *irreducible tensors* (more precisely, the irreducible tensor operators). The components of the tensor operator are the operators of some basis in the tensor subspace. Clearly, the group projector technique can be used to determine the standard tensorial basis: if $\hat{D}(G) = \oplus_{\mu=1}^{s'} a'_\mu D^{(\mu)}(G)$, the standard components of the tensors in $\mathcal{S} \otimes \mathcal{S}^*$ are $\{A_m^{(\mu t_\mu)} | \mu = 1, \dots, s'; t_\mu = 1, \dots a'_\mu; m = 1, \dots n_\mu\}$, and for the given matrices of the irre-

ducible representations of the group G, these satisfy the relations analogous to (1.4):

$$\hat{D}(g)A_m^{(\mu t_\mu)} = D(g)A_m^{(\mu t_\mu)}D^{-1}(g) = \sum_{m'} D_{m'm}^{(\mu)}(g)A_{m'}^{(\mu t_\mu)}. \tag{1.6}$$

When the standard components of the tensors are known, the determination of the operators with given transformational properties is enabled. In fact, it is usual that the transformational properties of some physical quantity are known (*e.g.* it is invariant under the group action, or it is transformed according to some other representation). Then this quantity is in the state space represented by the linear combination of the standard tensor components with same characteristics, and the coefficients in the combination are related to the concrete physical problem. For example, the angular momentum and the magnetic field are transformed according to the same irreducible representation of the group $\mathrm{O}(3,\mathbb{R})$, but they are different combinations of the standard tensor components.

The product of two tensor components transforms as

$$D(g)A_m^{(\mu)}B_n^{(\nu)}D^{-1}(g) = \sum_{m'n'} D_{m'm}^{(\mu)}(g)D_{n'n}^{(\nu)}(g)A_{m'}^{(\mu)}B_{n'}^{(\nu)}.$$

Thus, the products for all m and n span the invariant subspace in $\mathcal{S}\otimes\mathcal{S}^*$, carrying the direct product of the representations, $D^{(\mu)}(G)\otimes D^{(\nu)}(G)$. This representation may not be irreducible, and its decomposition, the Clebsch-Gordan's series (§ A.2.5),

$$D^{(\mu)}(G)\otimes D^{(\nu)}(G) = \oplus_\lambda a_\lambda^{\mu\nu} D^{(\lambda)}(G), \tag{1.7}$$

shows the possible types of the transformational properties of the product of the tensor operators.

Frequently, the symmetry group G is obvious, while the exact form of the hamiltonian is unknown. This means that the available information about the system does not suffice to find the hamiltonian (*e.g.* the interaction potentials of some of the components of the systems are too complicated to be predicted from the experimental data). Then the theoretical model, *i.e.* the hamiltonian compatible to the observed physical evidence, should be proposed. Since the symmetry is known, and the operators $D(g)$ commute with the correct (but unknown) hamiltonian, the model hamiltonian has to be chosen among the operators transforming according to the identical representation of the group (such quantities are called *scalars* of the group). This significantly restricts the set of suitable candidates. If some physical arguments single out the quantities relevant for dynamics (*e.g.* the fields involved in the hamiltonian), the problem takes the known form: how to compose a scalar from the given quantities. The Clebsch-Gordan's series of the group show which products of these quantities can be used as the scalars. Thus, the symmetry condition that the potential must be scalar of the group, severely restricts possible models, and combined with some additional criteria (*e.g.* it is heuristic practice to choose the simplest one among the allowed models), it can even single out the optimal one. In such approach the assumption that the potentials are smooth functions is important, enabling to take the approximate polynomial of appropriate

order as a model. This polynomial must be invariant one, and the elaborated technique of the construction of the invariant polynomials can be employed (§ 4.1). The same type of application of symmetry appears in the approximate techniques, when, even known, the exact hamiltonian is too complicated, and the approximate one, still retaining the principal characteristics of the system, is proposed (§ 1.7).

1.4 Wigner-Eckart's theorem

Knowing the irreducible representations of the group G, and its action $D(G)$ in the state space $\mathcal{S}$, some relevant physical conclusions can be derived immediately, applying the mathematical formalism of the group theory. Probably the most frequently used analysis of this kind is related to the matrix elements of the tensor operators. As soon as it is realized that there is the standard basis in $\mathcal{S}$, while in the operator space there is the basis of the standard tensor components, it becomes clear that each matrix element of any operator (note that the measurable predictions of the quantum theory are essentially these quantities) can be expressed in terms of the matrix elements of the standard operators in the standard basis, *i.e.* in terms of the purely symmetry based entities.

The formulation of the results related to the matrix elements is especially simple when the group G is such that the coefficients $a_\lambda^{\mu\nu}$ in the Clebsch-Gordan's series (1.7) of its irreducible representations are either 0 or 1. This assumption has the following consequence (§ B.3):

Teorem 2 *The matrix element* $\langle\ \alpha t_\alpha a \mid A_m^{(\mu t_\mu)} \mid \beta t_\beta b\ \rangle$ *is product of the Clebsch-Gordan's coefficient* $\langle\ \mu\beta\alpha a \mid \mu m, \beta b\ \rangle$ *with the* reduced matrix element, $(\alpha t_\alpha \mid\mid A^{(\mu t_\mu)} \mid\mid \beta t_\beta)$, *being the same for all* a, b *and* m*:*

$$\langle\ \alpha t_\alpha a \mid A_m^{(\mu t_\mu)} \mid \beta t_\beta b\ \rangle = \langle\ \mu\beta\alpha a \mid \mu m, \beta b\ \rangle (\alpha t_\alpha \mid\mid A^{(\mu t_\mu)} \mid\mid \beta t_\beta).$$

Obviously the condition $a_\lambda^{\mu\nu} = 0, 1$ provides the uniqueness, up to a phase factor, of the Clebsch-Gordan's coefficients. In the case that group does not fulfill this condition, the Clebsch-Gordan's coefficients must be fixed by some additional convention.

The Wigner-Eckart's Theorem enables to calculate all of the $n_\alpha n_\mu n_\beta$ matrix elements $\langle\ \alpha t_\alpha a' \mid A_{m'}^{(\mu t_\mu)} \mid \beta t_\beta b'\ \rangle$, with same t_α, t_μ and t_β, when at list one of them, $\langle\ \alpha t_\alpha a \mid A_m^{(\mu t_\mu)} \mid \beta t_\beta b\ \rangle$, is known; only the appropriate change of the Clebsch-Gordan's coefficients is to be performed ($\langle\ \mu\beta\alpha a \mid \mu m, \beta b\ \rangle \neq 0$): $\langle\ \alpha t_\alpha a' \mid A_{m'}^{(\mu t_\mu)} \mid \beta t_\beta b'\ \rangle = \frac{\langle\ \mu\beta\alpha a' \mid \mu m', \beta b'\ \rangle}{\langle\ \mu\beta\alpha a \mid \mu m, \beta b\ \rangle} \langle\ \alpha t_\alpha a \mid A_m^{(\mu t_\mu)} \mid \beta t_\beta b\ \rangle$. The Clebsch-Gordan's coefficients are characteristics of the group itself: being independent on the actual physical context, they are tabulated or given as the numerical programs for many groups. Frequently only the rates of the matrix elements are looked for, being equal to the rates of Clebsch-Gordan's coefficients, and then these purely group theoretical data are sufficient. Even when the value of the matrix elements is necessary Wigner-Eckart's theorem is helpfull: some of them may be simple for calculation or even experimental estimation, and this suffices to determine all others with same t_α, t_μ and t_β. Especially, when A is scalar of the group (tensor operator of the identity representation) the Wigner-Eckart's theorem

reduces to the frequently used relation $\langle \alpha t_\alpha a \mid A \mid \beta t_\beta b \rangle = \delta_{\alpha\beta}\delta_{ab}(\alpha t_\alpha || A || \beta t_\beta)$, showing that the nonvanishing matrix elements of scalar operator connect the vectors of the same transformational properties.

1.5 Selection rules

The probabilities of the transition of the quantum system from one state to another, are expressed through the matrix elements of the relevant operator, and their calculation, being one of the typical tasks of the quantum physics, may serve as a useful illustration of the application of the Wigner-Eckart's theorem.

This is the most usual formulation of the problem: the system, being initially, at the instant $t = 0$, in the stationary state $|i\rangle$ (the eigen vector of the hamiltonian H_0 of the isolated system), is perturbed by the potential $V(t)$; the probability to find the system in the stationary state $|f\rangle$ of the hamiltonian H_0 at the later instant $t = \tau$ is looked for (*e.g.* the perturbation acts only during the interval $(0, \tau)$). All the approaches to this task (including the scattering theory) involve the matrix elements of the perturbation in the eigen basis of H_0. For example, in the simplest case of the time independent perturbation, $V(t) = V$, the transition probability is: $W_{if}(\tau) = 2\frac{1-\cos\frac{E_f-E_i}{\hbar}\tau}{|E_f-E_i|^2}|\langle\ f|V|i\ \rangle|^2$, where E denotes the corresponding eigen energies of the hamiltonian.

Once the symmetry of the system has been noticed, the prerequisites for application of the Wigner-Eckart's theorem, the standard stationary basis and standard components of the perturbation, become available. It is especially simple to determine when the probability transition is zero, *i.e.* when the transition is forbidden. Obviously, $W_{\beta b\mapsto\alpha a} = 0$ whenever the relevant Clebsch-Gordan's coefficient is zero (for all the tensor components of the perturbation). Thus, the *selection rules* are obtained. A less refined insight to selection rules gives the analysis of the Clebsch-Gordan's series: when the coefficient $a_\alpha^{\mu\beta}$ in (1.7) is 0, all the corresponding Clebsch-Gordan's coefficients vanish. Also, it should be noted that the transition may be forbidden by some other reasons, even when it is allowed by symmetry; in such case it can be concluded that G does not describe the real (meaning maximal) symmetry of system, *i.e.* that some of the symmetries are left aside.

When the symmetry is described by a Lie's group, standard stationary basis is the basis of the weights (the common eigen basis for the operators representing the Cartan's subalgebra — the maximal set of the commuting generators), while the elements of the algebra are represented by the hermitean operators, usually having transparent physical interpretation (momenta, angular momenta, etc.). The weights give the eigen values of the operators of the Cartan's subalgebra, and the tensor operators are also labeled by these values. It is well known from the theory of the representations of the Lie's algebras, that the weights of the direct product of the representations are the sum of the weights of the factors; consequently, the selection rules are essentially the conservation laws for the associated physical quantities. The same contents of he selection rules can be observed for the finite groups, also (*e.g.*

conservation of the parity with respect to the inversion or the reflections, the conservation of the quasi momenta, quasi angular momenta, etc.).

1.6 Symmetry of the composed system

Within the described concept of the application of symmetry, the question of the symmetry of the subsystem can be discussed, which is relevant in the cases when the considered system is a part of some larger physical system. Two situations qualitatively differ. Firstly, it is possible that the rest of the system does not interact with the considered subsystem, when the transformations of one part do not influence the other one; then the total symmetry group is the direct product of the groups of symmetry of the subsystems (§ A.1.5). In the other case, when the subsystems interact, the total group is additionally restricted by the symmetry of the interaction, and it become the intersection of the symmetry group of the interaction with the direct product of the subsystem groups. This is one of the first symmetry based observations in physics, formulated by P. Curie more then the century ago, and known as the *Curie's principle*. Frequently, the interaction is invariant only under the coincident transformations common for the both subsystems, when the total symmetry is the intersection of the subsystem groups.

1.7 Methods of approximation

If the system is not isolated, but weakly interacts with the surrounding, the perturbative technique is suitable to correct the results obtained for the isolated system (with neglected influence of the surrounding). The same method is used also when the dynamics of the system is complex enough and prevent exact treatment: the approximation exactly encounters a chosen main part of the hamiltonian, and afterwards the results are corrected in accordance with the rest of the total hamiltonian. The formal treatment of these two situations is the same: the basic (unperturbed) part of the hamiltonian, H, and the perturbation, V, appear. Manifesting the Curie's principle, the total symmetry G' is the intersection of the symmetry group, G, of the unperturbed hamiltonian and the symmetry group of the perturbation. Therefore, G' is a subgroup of G (for the isolated system — the second case mentioned — it is important to chose H and V such that both of them posses the real symmetry of the total system; then G'=G, providing *a priory* the quality of the unperturbed and corrected results at least for the symmetry based results). Therefore, the many dimensional irreducible representations of G, related to the degeneracies of some eigen values of H, may not be irreducible for G' anymore. Indeed, in the corresponding irreducible subspace of the representation $D^{(\mu)}(G)$ the group G' acts by the subduced representation $D^{(\mu)}(G) \downarrow G'$, and it can be reducible according to the *compatibility relations* § A.2.6: $D^{(\mu)}(G) \downarrow G' = \oplus_{\lambda=1}^{s} a_\lambda^\mu D^{(\lambda)}(G')$. Since the vectors of the different irreducible representations of G' are necessary from the same eigen subspace of the operator $H + V$, the compatibility relations describe the splitting of the energy levels of the

unperturbed hamiltonian caused by the perturbation.

The amount of this splitting is estimated by the perturbation technique, [3, 16]: V is scalar operator of the group G', and for the standard basis $\{|\mu\lambda t_\lambda l\rangle|\lambda = 1,\dots,s; t_\lambda = 1,\dots,a^\mu_\lambda, l = 1,\dots,n_\lambda\}$ in the considered subspace of the representation $D^{(\mu t_\mu)}(G)$, the Wigner-Eckart's theorem yields $\langle \mu\lambda t_\lambda l \mid V \mid \mu\lambda' t'_{\lambda'} l'\rangle = \delta_{\lambda\lambda'}\delta_{ll'}(\mu\lambda t_\lambda||V||\mu\lambda t'_\lambda)$. Thus, in the matrix V the scalar submatrices appear in the blocks connecting the equivalent irreducible representations of the group G'. For example, if $D^{(\mu)}(G) \downarrow G' = 2D^{(\lambda)}(G') + D^{(\lambda')}(G')$, then the form of is $V = \begin{pmatrix} aI_\lambda & bI_\lambda & 0 \\ b^*I_\lambda & cI_\lambda & 0 \\ 0 & 0 & dI_{\lambda'} \end{pmatrix}$. The eigen values of this matrix are the corrections of the unperturbed states, and their differences express the splitting of the unperturbed level. In the case when the irreducible components of the subduced representation are different, the block-diagonal matrix is obtained, simplifying the eigen problem. The symmetry analysis can be performed for the higher order perturbations (since no novel symmetry technique is introduced they will not be considered in this text).

Another important approximation technique is the variational method, [3, 18]. It is based on the extreme properties of the eigen values; for example, the minimal eigen value of the operator H is also the minimal value of the functional $\varepsilon(|x\rangle) \stackrel{\text{def}}{=} \langle x|\ H\ |x\rangle$ (with the condition that $|\ x\rangle$ is normalized vector) on $\mathcal{S}$. Therefore, for any chosen subset $\mathcal{T} \subset \mathcal{S}$ of the *trial vectors* the minimal value of this functional on $\mathcal{T}$ is a majorant of the minimal eigen value of H (if $\mathcal{T}$ contains the ground state, the result is exact). Obviously, the validity of the method is based on the choice of the set $\mathcal{T}$. The symmetry can help already in this stage. For example, it is known that the ground state of the most of the physical systems is totally symmetric, *i.e.* invariant under the symmetry group. Therefore, the suitable candidates for the trial states are the vectors from the subspace of the identity representation in $\mathcal{S}$, that is the *fixed points* of the group action in $\mathcal{S}$. The analogous method is applicable for other states: when the ground state is determined, the remaining eigenstates of the hamiltonian are orthogonal, and the trial vectors can be chosen in accordance with this. If some other physical reasons points to certain transformational properties of these states, the selection is performed among the vectors of the subspace of the corresponding irreducible representation; unless further restriction are imposed, this subspace is a priory the set of the trial vectors, and the *Rayleigh-Ritz's method* emerges.

In fact, the main characteristics of the Rayleigh-Ritz's method is that the trial set is a subspace $\mathcal{T}$ in $\mathcal{S}$. The symmetry approach is especially straightforward if $\mathcal{T}$ is invariant subspace for the group action. This assumption, meaning that $D(G)$ commutes with the projector P onto $\mathcal{T}$, can be fulfilled always, by enlargening the initially chosen trial set. Then the group action is reduced in this subspace to the representation $D^{\mathcal{T}}(G) = PD(G)P$. The approximation is introduced when the operator H is substituted by the operator PHP in $\mathcal{T}$, (if $\mathcal{T}$ is invariant for H also, the obtained results are exact, and not approximate). Since $D(G)$ commutes both with P and H, then it commutes with PHP also, and the standard formulation of the problem, $(\mathcal{T}, PHP, D^{\mathcal{T}}(G))$, is obtained. This can be viewed as

a sort of approximate localization of the interaction to the trial subspace (tacitly performed when the matrix elements of the hamiltonian in this subspace are considered), yielding an approximate "isolation of the subsystem" described by the state space $\mathcal{T}$. Further steps are usual: diagonalization of PHP with help of the irreducible components $D^{\mathcal{T}}(G)$. The method of the approximation makes the possibility to introduce the group of symmetry of the "isolated" subsystem, being the maximal group of $\mathcal{T}$, and this is obviously the most efficient application of symmetry.

Nevertheless, for the traditional and experimental reasons, seemingly different, explicitly variational, point of view is usual . The set $\{|\, i\rangle | i = 1, \ldots, n\}$ of the linearly independent vectors is chosen, and $\mathcal{T}$ is defined as their linear span. Therefore, trial vectors are linear combinations $|\, x\rangle = \sum_i c_i \mid i\rangle$, while the coefficients c_i become variational parameters of the functional: $E(|\, x\rangle) = E(c_1, \ldots, c_n)$. The basis vectors $|\, i\rangle$ may not be orthonormal, and the Gram's matrix $S_{ij} = \langle i \mid \ j \,\rangle$ may not be the identity. Denoting by h the matrix $h_{ij} = \langle i|\, PHP \,|j\rangle$, the variational extreme (constrained by the normalization of the vectors) is found as the solution of the system of homogeneous linear equation over the coefficients c_i:

$$(h - \epsilon S)\,|x\rangle = 0 \quad \text{or} \quad \sum_j (h_{ij} - \epsilon S_{ij}) c_j = 0,\ i = 1. \ldots, n. \tag{1.8}$$

($|x\rangle$ is represented in the basis $|i\rangle$, becoming a column with the coefficients c_i). These equations are equivalent to the eigen problem of the operator PHP, since they are the projections of the equation $(PHP - \epsilon I) \mid x\rangle = 0$ onto the vectors of the initial basis; consequently, the subspaces of the variational extremes are simultaneously the eigen subspaces of PHP. Possible advantages of the variational point of view may be found in the explicit utilization of the representation of the group and choice of the suitable initial basis (usually reflecting some natural assumptions on the localization, frequently enabling to estimate "overlap integrals", S_{ij} and the matrix elements h_{ij}; *e.g.* Hückel's method of the molecular orbitals, § 5.3).

In the studies of complex systems, like molecules and crystals, significant simplification is introduced by the *adiabatic approximation*. The dynamics of the total system is decomposed onto the dynamics of two subsystems, the "light" and the "heavy" one. The underlying assumption is that the evolution of the "heavy" system is slow enough, providing the picture of the evolution of the "light" system in the field of the frozen "heavy" subsystem. This approach is suitable for very efficient application of symmetry. Due to the necessary specific techniques, it will be considered separately (§ 5.1). Analogously, very general *harmonic approximation*, is the starting point of the different perturbative techniques, and the essence of some important physical models (§ 3).

Chapter 2

NONRELATIVISTIC SYMMETRIES

The intuitive picture of the matter constituted of the elementary (within the assumed level of observation) parts, is closely related to the notion of locality. In fact, the ingredients of the structure are usually spatially separated, each of them occupying certain domain in the space. Within the quantum theory this picture is slightly changed, but its essential contents, the space-time based parametrization of the states, is preserved: the states are functions over the space-time coordinates, and the state space appears as the space of functions over the configurational space. The complete description of a real system requires such a space, and this is the form of *locality condition* in the quantum theories[1]. In this state space the group of symmetry acts by the *coordinate representation*: the geometrical transformation g, originally defined on the configurational space (§ A.1.4), is represented by the operator $D(g)$ acting on the state space vectors, i.e. on the coordinate functions $f(\boldsymbol{x})$, as $D(g)f(\boldsymbol{x}) \stackrel{\text{def}}{=} f(g^{-1}\boldsymbol{x})$. (It is often convenient to work with other spaces, but then some models, and not the real systems, are considered; for example, sometimes physical situation allows formal factorization of the system, such that study of the separate degrees of freedom, *e.g.* spin "subsystem", is possible.)

As any other representation, the coordinate one determines representation in the operator space (§ 1.3). It is suitable to describe the transformation of the operators under the action of the symmetries. The operators of the position, momentum, angular momentum and other physical quantities, being defined in the coordinate representation, must transform in accordance with the empirically well established transformation rules of the original quantities. For example, the rotation $R = (R_{ij})$ changes coordinates $\boldsymbol{x}$ to $\boldsymbol{x}' = R\boldsymbol{x}$, and in the coordinate representation the analogous law, $\hat{\boldsymbol{x}}' = D(R)\hat{\boldsymbol{x}}D^{\dagger}(R) = \sum_j R_{ji}\hat{\boldsymbol{x}}_j$ must be fulfilled. In this sense, the coordinate representation determines the transformation laws of the operators of the coordinates and other physical quantities.

On the other hand, the symmetry group of the elementary physical system, such as the point particle with no subsystems or the interactions, is the symmetry group of the space, *i.e.* the *group of relativity*. The state space of such system must be irreducible for this group, since

[1]Precisely, locality condition imposes the rigged space of the Hilbert's space $\mathcal{L}^2(\mathbb{R}^3)$ or $\mathcal{L}^2(\mathbb{R}^4)$, in order to include the description of the completely localized states by the Dirac's δ-function.

otherwise, as it has been explained in § 1.2, the larger symmetry group could be introduced, with the additional transformations of symmetry, which essentially reflects some unobserved structure of the system. Thus, the state space of the elementary system carries the irreducible, eventually projective, representation of the relativity group. Consequently, the locality condition requires that the representation of the symmetry group, suitable to describe elementary system acts in the space with defined observables corresponding to (and having transformation properties of) the coordinates. Such representation may be the irreducible component, $D^{(\mu)}(G)$, of the reducible coordinate representation. The condition establishing that the system (described by the state $|\,\psi\rangle$) belongs to some irreducible subspace, $P^{(\mu t_\mu)}\,|\,\psi\rangle = |\,\psi\rangle$, is the *equation of motion* of the free elementary system.

In the nonrelativistic physics, the Galileo's group is *postulated* as the group of relativity. Together with the spatial symmetries (translations and rotations), it contains the time translations and Galileo's boosts (the transformations describing transition to the system of reference moving uniformly with regard to the initial one; from the point of view of symmetry, the relativistic and the nonrelativistic physics differ just in these transformations). The construction of the irreducible representations of the Galileo's group is a complex task[2], [14], even more complicated then for the corresponding relativistic Poincare's group; since the notion and classification of the nonrelativistic elementary particles is not substantial for the contemporary physics, this construction will be avoided.

Therefore, the main attention will be paid to the geometrical symmetries. These are the isometric transformations [5, 9] of the Euclid's 3-dimensional space (preserving the distance in $\mathbb{R}^3$), *i.e.* the elements of the extended Euclid's group $E_3 = T^3 \wedge \mathrm{O}(3,\mathbb{R})$. Each element of this semidirect product is uniquely factorized onto $R \in \mathrm{O}(3,\mathbb{R})$ and $\boldsymbol{t} \in T^3$ ($\boldsymbol{t}$ is the vector from $\mathbb{R}^3$ for which the translation is performed), and the transformations of the Euclid's group are given in the Koster-Seitz's form $(R|\boldsymbol{t})\boldsymbol{x} \stackrel{\text{def}}{=} R\boldsymbol{x} + \boldsymbol{t}$.

When the *isotropy* of the system is provided, the symmetry group is at least $\mathrm{SO}(3,\mathbb{R})$, and if the *homogeneity* is also the property of the system, the Euclid's group, $T^3 \wedge \mathrm{SO}(3,\mathbb{R})$, is found. Discrete many-particle systems cannot be neither isotropic nor invariant under continuous subgroup of the translational group T^3, and their geometrical symmetries are subgroups of the Euclid's group. Especially, only discrete subgroups of T^3 can be involved, and each such subgroup (except the trivial one, $\{(I|0)\}$) is infinite, manifesting the periodicity of the system in certain directions. Therefore, the discrete many particle systems are divided into the following classes:

(*i*) The systems with no translational periodicity (*e.g.* the molecules). Their symmetries form a subgroup of $\mathrm{O}(3,\mathbb{R})$. The transformations of such groups leave the point of the

[2]In fact, only the projective representations with the nontrivial factor system (§ A.2.7) satisfy the locality condition; the constant with the physical contents of mass appears in the factor-system (the covering group is nontrivial extension of the Galileo's group, and the new generator corresponds to the mass of the system). Therefore, for each mass the separate set of the representations is constructed, and in the nonrelativistic quantum theory, the superposition of the states with different masses is forbidden, due to their different transformation properties.

coordinate origin invariant, and therefore they are called *point groups*, [9, 20].

(*ii*) The systems periodical in one direction (polymers, quasi one dimensional subsystems of the crystals). Their symmetry group, besides the translations (generated by the single element), includes some of the orthogonal transformations leaving the axis of the periodicity invariant; thus they are called *line groups*, [24].

(*iii*) The symmetries of the system periodical in two directions (quasi 2-dimensional subsystems of the crystal, layers) are the translations (two generators with the independent vectors of translation) combined with the orthogonal transformations leaving the plain of the periodicity invariant. These groups are known as *diperiodic groups*, [10].

(*iv*) The systems with three directions of periodicity (crystals); their symmetries, besides the orthogonal ones, are the translations (generated by 3 independent vectors): *space groups* [23, 20].

The translational periodicity in one or two directions does not concern the dimensionality of the system. All these groups describe symmetries of 3-dimensional systems; lower dimensional system is treated as the special case, with symetry described also by some of these groups.

In what follows, the Euclid's group will be examined at first, to introduce the geometrical symmetries, and in the rest of chapter the more detailed analysis of the symmetries of the enumerated classes of the discrete systems. More attention is paid to the point and space groups, since they are well established in the physics of the discrete systems. The time reversal is traditionally studied together with the spatial symmetries, due to their mutual intertwining, which results in the Kramers's degeneracy and the construction of the magnetic groups. Similarly, the permutational symmetry of the systems of identical particles yields the classification of the physical systems onto the fermions and bosons; its deep connection with the geometrical symmetries is manifested through the relationship between the spin (the behavior of the system under the rotations) and the statistics (behavior with respect to the permutations), which is explained within the relativistic theories.

2.1 Geometrical symmetries

The Euclid's group is semidirect product of the translational and the group of the rotations in the space $\mathbb{R}^3$. Such structure enables simple construction of the irreducible representations, based on the representations of the subgroups. Besides, the study of the translational and the rotational groups gives a number of the physically relevant facts, and therefore these groups will be independently considered at first.

2.1.1 Translations

The group of the translations, T^3, is Abelian, being the direct product of three groups of the translations along the coordinate axes. Therefore, each vector $\boldsymbol{k} \in \mathbb{R}^3$ determines one unitary irreducible (one-dimensional) representation of T^3:

$$\Delta^{(\boldsymbol{k})}(I|\boldsymbol{t}) \stackrel{\text{def}}{=} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\boldsymbol{t}}. \tag{2.1}$$

In the coordinate representation, the translational operator acts on the function over $\mathbb{R}^3$ as $D(I|\boldsymbol{t})f(\boldsymbol{x}) \stackrel{\text{def}}{=} f(\boldsymbol{x}-\boldsymbol{t})$ (the passive picture is assumed: the operation is performed on the coordinate system). The subspace corresponding to the irreducible representation $\Delta^{(\boldsymbol{k})}(T^3)$ is given by the functional equation $D(I|\boldsymbol{t})f(\boldsymbol{x}) = \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\boldsymbol{t}}f(\boldsymbol{x})$, yielding the equation $f(\boldsymbol{x}-\boldsymbol{t}) = \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\boldsymbol{t}}f(\boldsymbol{x})$. The well known solutions of this equation are the *plane waves*, $f(\boldsymbol{x}) = C\mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{x}}$, and consequently, to each irreducible representation of the translational group there corresponds the one-dimensional subspace in the coordinate representation[3].

The generator of the translations along the x-axis is represented (§ A.2.1) by the operator $D(l_x)f(\boldsymbol{x}) = \frac{\partial f(x-t_x,y,z)}{\partial t_x}|_{t_x=0} = -\frac{\partial}{\partial x}f(\boldsymbol{x})$, and analogous relations hold for the other coordinates. Clearly, the generator of the translation, multiplied by $\mathrm{i}\hbar$, is identified to the momentum operator, $p_i = -\mathrm{i}\hbar\frac{\partial}{\partial x_i}$, and the translation itself is represented by the operator $D(I|\boldsymbol{t}) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\boldsymbol{t}\boldsymbol{p}}$. The condition that the function $f(\boldsymbol{x})$ is from $\boldsymbol{k}$-th irreducible subspace, becomes at the generator level the differential equation $\frac{\partial}{\partial x_i}f(\boldsymbol{x}) = \mathrm{i}k_i f(\boldsymbol{x})$, *i.e.* $p_i f(\boldsymbol{x}) = \hbar k_i f(\boldsymbol{x})$. Therefore, the plane wave is also the eigen state of the momenta, with the eigen value $\hbar\boldsymbol{k}$; thus the vector $\boldsymbol{k}$ defining the irreducible representation (multiplied by $\hbar$) is the momentum of the free particle in the state corresponding to the representation $\boldsymbol{k}$.

It should be emphasized that the performed procedure, determination of the irreducible representations of the group, and separation of the corresponding subspaces in the coordinate representation (yielding the functional equations at the level of the group, and the differential equations at the level of the generators of the Lie's group), is one of the most usual ways to apply the symmetry (§ 1.2; analogous equations, obtained for the total group of the relativity, are the equations of motion, such as the Schrödinger's or the Klein-Gordon's equation.)

2.1.2 Rotations and reflections

The group $\mathrm{O}(3,\mathbb{R})$ is the 3-dimensional compact, but unconnected Lie's group, [5, 13]. There are two connected components, and the component containing the identity is the subgroup $\mathrm{SO}(3,\mathbb{R})$, such that $\mathrm{O}(3,\mathbb{R}) = \mathrm{SO}(3,\mathbb{R}) \otimes \{e, P\}$, where $P = -I$ is the *spatial inversion*. Therefore the representations of $\mathrm{O}(3,\mathbb{R})$ are determined by the representations of the group $\mathrm{SO}(3,\mathbb{R})$.

Each rotation in $\mathbb{R}^3$ is determined by the angle α and the axis (given by the unit vector $\boldsymbol{a} = (a_1, a_2, a_3)$) around which the (right-handed) rotation is performed. This provides the

[3]The plane waves are normalized to the Dirac's δ-function, emphasizing both the necessity of the rigged Hilbert's space, and the importance of the locality condition.

bijective correspondence of the rotations and the 3-dimensional matrices from $\mathrm{SO}(3,\mathbb{R})$:

$$R(\alpha,\boldsymbol{a}) = \begin{pmatrix} \cos\alpha+a_1^2(1-\cos\alpha) & a_1a_2(1-\cos\alpha)-a_3\sin\alpha & a_1a_3(1-\cos\alpha)+a_2\sin\alpha \\ a_1a_2(1-\cos\alpha)+a_3\sin\alpha & \cos\alpha+a_2^2(1-\cos\alpha) & a_2a_3(1-\cos\alpha)-a_1\sin\alpha \\ a_1a_3(1-\cos\alpha)-a_2\sin\alpha & a_2a_3(1-\cos\alpha)+a_1\sin\alpha & \cos\alpha+a_3^2(1-\cos\alpha) \end{pmatrix}, \quad \alpha\in[0,\pi]; \tag{2.2a}$$

the interval of the angle α follows from the fact that for $\alpha>\pi$, $R(\alpha,\boldsymbol{a}) = R(2\pi-\alpha,-\boldsymbol{a})$. Also, it can be decomposed onto the three rotations for the *Euler's angles* $\varphi\in[0,2\pi]$, $\theta\in[0,\pi]$ and $\psi\in[0,\pi]$ around the coordinate axes z, x and z, respectively (this "z-x-z" convention is used throughout the text). This provides the bijective correspondence of the rotations and the 3-dimensional matrices from $\mathrm{SO}(3,\mathbb{R})$:

$$R(\varphi,\theta,\psi) = \begin{pmatrix} \cos\varphi\cos\psi-\cos\theta\sin\varphi\sin\psi & -\cos\varphi\sin\psi-\cos\theta\sin\varphi\cos\psi & \sin\varphi\sin\theta \\ \cos\psi\sin\varphi+\cos\theta\sin\psi\cos\varphi & \cos\theta\cos\varphi\cos\psi-\sin\varphi\sin\psi & -\cos\varphi\sin\theta \\ \sin\psi\sin\theta & \cos\psi\sin\theta & \cos\theta \end{pmatrix}. \tag{2.2b}$$

The correspondence between the two parameterisations is realized, noticing that if on the unit sphere $\boldsymbol{a}$ has spherical angles (φ,θ), then it can be got from the x-axis by rotations $R(\varphi,\theta,0)$, and then it is clear that $R(\varphi,\theta,\alpha) = R(\alpha,\boldsymbol{a})$; this also explains the used intervals for the Euler angles. The group $\mathrm{SO}(3,\mathbb{R})$ is nontrivially (double) connected, and its representations are found as the representations of the universal covering group[4] $\mathrm{SU}(2)$. To each element R of the group $\mathrm{SO}(3,\mathbb{R})$ two elements, U and $-U$, of the group $\mathrm{SU}(2)$ are associated. Namely, each element of $\mathrm{SU}(2)$ can be expressed in either of the angle-axis or Euler angles forms:

$$U(\alpha,\boldsymbol{a}) = \begin{pmatrix} \cos\frac{\alpha}{2}-\mathrm{i}a_3\sin\frac{\alpha}{2} & -(a_2+\mathrm{i}a_1)\sin\frac{\alpha}{2} \\ (a_2-\mathrm{i}a_1)\sin\frac{\alpha}{2} & \cos\frac{\alpha}{2}+\mathrm{i}a_3\sin\frac{\alpha}{2} \end{pmatrix}, \quad \alpha\in[0,2\pi] \tag{2.3a}$$

$$U(\varphi,\theta,\psi) = \begin{pmatrix} \mathrm{e}^{\frac{\mathrm{i}}{2}(\varphi+\psi)}\cos\frac{\theta}{2} & \mathrm{e}^{\frac{\mathrm{i}}{2}(\varphi-\psi)}\sin\frac{\theta}{2} \\ -\mathrm{e}^{\frac{\mathrm{i}}{2}(\psi-\varphi)}\sin\frac{\theta}{2} & \mathrm{e}^{-\frac{\mathrm{i}}{2}(\varphi+\psi)}\cos\frac{\theta}{2} \end{pmatrix}, \quad \varphi,\psi\in[0,2\pi],\ \theta\in[0,\pi]. \tag{2.3b}$$

Then, the mapping

$$h(U(\varphi,\theta,\psi)) \stackrel{\mathrm{def}}{=} R(\varphi,\theta,\psi) \tag{2.4}$$

is the (covering) homomorphism of $\mathrm{SU}(2)$ onto $\mathrm{SO}(3,\mathbb{R})$, which both $U(\alpha,\boldsymbol{a})$ and $-U(\alpha,\boldsymbol{a}) = U(\alpha+2\pi,\boldsymbol{a})$ maps to $R(\alpha,\boldsymbol{a})$ (especially, I_2 and $-I_2$ are mapped to I_3). In the space $\mathcal{S}$ with the representation $D(\mathrm{SU}(2))$, the operators $D(U)$ and $D(-U)$ (*i.e.* $D(h^{-1}(R))$ are associated to the element R. If these two operators are equal (then the D cannot be faithful representation of $\mathrm{SU}(2)$) the ordinary representation of the rotational group is obtained. On the contrary, if $D(U)$ and $D(-U)$ are different (*e.g.* the representation of the group $\mathrm{SU}(2)$ is faithful), the two valued representation of $\mathrm{SO}(3)$ is established: to each element R the pair of the operators correspond, and this is two valued correspondence. Rigorously this is not the representation, since the homomorphism condition is fulfilled only in the sense of the multiplication of the pairs: the product of any of the operators corresponding to R, with any operator corresponding to the rotation R', is one of the operators of the pair representing RR'. If only one operator from each pair is fixed, then the product satisfies $D(R)D(R') = f(R,R')D(RR')$, where $f(R,R')$ is 1 or -1, depending on the choice of the

[4] This is (§ A.2.7) simply connected group, homomorphically mapped onto $\mathrm{SO}(3,\mathbb{R})$.

pair representative; hence, this becomes the projective representation of the group $\mathrm{SO}(3,\mathbb{R})$, with the factor-system f (§ A.2.7).

The irreducible representations of the considered groups can be found by the standard method developed for the Lie's groups, based on the generators. The set of the rotations $R(\alpha,\boldsymbol{a})$, around the fixed unit vector $\boldsymbol{a}$, is the one-parameter subgroup (§ A.1.2). Therefore, the operators representing these rotations are

$$D(R_{\alpha\boldsymbol{a}}) = \mathrm{e}^{-\mathrm{i}\alpha S_{\boldsymbol{a}}}, \tag{2.5}$$

where $S_{\boldsymbol{a}} = -\mathrm{i}\hbar D(l_{\boldsymbol{a}}) = \boldsymbol{a}\cdot\boldsymbol{S} = \sum_i a_i S_i$ (S_i are coordinate angular momenta) is the hermitean operator of the $\boldsymbol{a}$-component of the angular momentum. Above exponential identity relating the angular momenta to the generators of the rotations is the well known property property of the Lie's groups (§ A.2.1), and analogous relation of the momenta and translations has been noted in the previous Subsection. However, this fact enables construction of the irreducible representations by the (standard in the theory of Lie's algebras) method based on the angular moments. The result is well known: the irreducible representations are completely characterized by the half integrals $l = 0, \frac{1}{2}, 1, \ldots$, each of them being $2l+1$-dimensional; in the corresponding irreducible subspaces the angular momenta are complete observables, with non degenerate eigen values $l, l-1, \ldots, -l+1, -l$. Usually, the eigen basis of the z-component, S_3, of the angular momentum is used, meaning that the matrix representing l_3 is diagonal with the mentioned eigenvalues on the diagonal. Also, the irreducible representations are uniquely characterized by the square of the angular momentum. Namely, the operator of the square of the angular moment (Kazimir's operator), $S^2 \stackrel{\mathrm{def}}{=} \sum_{i=1}^{3} S_i^2$, in the subspace of the l-th irreducible representation acts as the scalar operator $l(l+1)\hbar^2 I$.

The exponential form (2.5) provides more sophisticated point of view, free of vague notion of "two-valued representations": the actual group dealt with is SU(2), and its elements are spin-rotations around arbitrary axis $\boldsymbol{a}$ for angle $\alpha \in [0, 4\pi]$, obtained from (2.5) when coordinate angular momenta are spin matrices; with convention about choice of the rotational axis this gives (2.3a). In odd dimensional spaces it acts by its (integer) representation $D^{(j)}$ with kernel $\ker D^{(j)} = \{I_2, -I_2\}$, containing rotations for $\varphi = 0$ and $\varphi = 2\pi$ (around arbitrary axis), respectively. This action is not effective, as $\ker D^{(j)}$, represented by identity matrix, fixes any point of the space, and exactly this ineffective action in three-dimensional space ($j = 1$) is rotational group, while in higher dimensions (for j=2,3,...) faithfully represents it. On the other hand, in the even dimensional spaces (half-integer j) describing systems with odd number of fermions, the representations of SU(2) are faithful, and group acts effectively through spin-rotations on the spinors (vectors of these spaces; this explains why half-integer representations are also called spinor representations).

When the exponent of the diagonal form is found, it appears that the rotation for 2π is represented by the identity matrix only if l is integer, and only such representations are the representations of the group $\mathrm{SO}(3,\mathbb{R})$; the remaining half integral ones are two valued. Since the set of all the rotations for the same angle is exactly one conjugation class of the rotational group, the character of the irreducible representation can be found as the trace of

the exponent of the diagonal matrix l_3:

$$\chi^{(l)}(\varphi) = \frac{\sin\frac{2l+1}{2}\varphi}{\sin\frac{\varphi}{2}}.$$

Obviously, the characters are real, and there is no representations of the III kind (§ A.3); the character test (or direct examination) shows that the halfintegral representations are pseudoreal (II kind), while for the integral ones the real form exists (I kind).

In the coordinate representation, the rotations act as $D(R)f(\boldsymbol{x}) = f(R^{-1}\boldsymbol{x})$. Especially, for the rotations around the z-axis, $D(R_{\varphi\boldsymbol{e}_z})f(\boldsymbol{x}) = f(x_1\cos\varphi + x_2\sin\varphi, -x_1\sin\varphi + x_2\cos\varphi, x_3)$, and the corresponding generator satisfies $D(l_3)f(\boldsymbol{x}) = \frac{\partial}{\partial\varphi}(D(R_{\varphi\boldsymbol{e}_z})f(\boldsymbol{x}))|_{\varphi=0} = (x_1\frac{\partial}{\partial x_2} - x_2\frac{\partial}{\partial x_1})f(\boldsymbol{x})$. Analogous relations hold for the other generators: $D(l_i) = \sum_k \epsilon_{ijk}x_j\frac{\partial}{\partial x_k}$. The identification of these operators to the angular momenta is obvious: $S_{\boldsymbol{a}} = -\mathrm{i}\hbar D(l_{\boldsymbol{a}})$. The condition that the state $f(\boldsymbol{x})$ is in the l-th irreducible subspace, $D(R)f(\boldsymbol{x}) = D^{(l)}(R)f(\boldsymbol{x})$, is usually expressed at the level of the generators. Using the mentioned property of the square of the angular momentum, this condition becomes (in the spherical coordinates) $\sum_{i=1}^{3} D^2(l_i)f(\boldsymbol{x}) = (\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta})f(\boldsymbol{x}) = -l(l+1)f(\boldsymbol{x})$. The solutions of this differential equation are the spherical harmonics, $Y_l^m(\theta,\varphi)$, with the integral l (multiplied by the arbitrary function of the radial coordinate), which simultaneously satisfy the equation $S_3 f(\boldsymbol{x}) = m\hbar f(\boldsymbol{x}) = -\mathrm{i}\hbar\frac{\partial}{\partial\varphi}f(\boldsymbol{x})$, *i.e.* $D(R_{\varphi\boldsymbol{e}_z})f(\boldsymbol{x}) = \mathrm{e}^{-\mathrm{i}m\varphi}f(\boldsymbol{x})$.

The Clebsch-Gordan's series of the irreducible representations,

$$D^{(l)}(\mathrm{SU}(2)) \otimes D^{(l')}(\mathrm{SU}(2)) = \sum_{l''=|l-l'|}^{l+l'} D^{(l'')}(\mathrm{SU}(2)),$$

give the well known rule of the addition of the angular momenta, and in the associated selection rules the conservation of the angular momenta is easily recognized.

The irreducible representations of the group $\mathrm{O}(3,\mathbb{R})$ can be determined now. Each integral representation $D^{(l)}(\mathrm{SO}(3,\mathbb{R}))$ gives (§ A.2.8) two representations, $D^{(l,\pm)}(\mathrm{O}(3,\mathbb{R}))$: $D^{(l,\pm)}(R) = D^{(l)}(R)$ i $D^{(l,\pm)}(PR) = \pm D^{(l)}(R)$. Nevertheless, for the halfintegral (two-valued!) representations of the group $\mathrm{SO}(3,\mathbb{R})$, the same method shows that to the spatial inversion correspond both of the operators $\pm I_{2l+1}$, and only one two-valued representation of the group $\mathrm{O}(3,\mathbb{R})$ is obtained: the element PR is represented by the same pair of the operators as the element $R \in \mathrm{SO}(3,\mathbb{R})$.

2.1.3 Euclid's group

The irreducible representations of the Euclid's group are derived from the known representations of its subgroups of the rotations and the translations, by the inductive procedure (the Abel's subgroup T^3 is invariant). The representations of the extended Euclid's group are afterward found by the induction from Euclid's group, being subgroup of the index two.

Since $D^{(\boldsymbol{k})}((R^{-1}|0)(I|\boldsymbol{t})(R|0)) = D^{(\boldsymbol{k})}(I|R^{-1}\boldsymbol{t}) = \mathrm{e}^{-\mathrm{i}\boldsymbol{k}(R^{-1}\boldsymbol{t})} = \mathrm{e}^{-\mathrm{i}(R\boldsymbol{k})\boldsymbol{t}} = D^{(R\boldsymbol{k})}(I|\boldsymbol{t})$, the orbit of the irreducible representation $D^{(\boldsymbol{k})}(T^3)$ is the sphere with the radius $|\boldsymbol{k}| = k$. Taking

for the orbit representative the vector $k\boldsymbol{a}$ ($\boldsymbol{a}$ is an arbitrary unit vector), the stabilizer for $k > 0$ is the semidirect product of the group T^3 with the group of the all rotations around $\boldsymbol{a}$. The latter is $\boldsymbol{C}_\infty = \mathrm{SO}(2)$ (§ 2.2.1), with the irreducible representations $A_m(R_{\varphi \boldsymbol{e}_z}) = \mathrm{e}^{-\mathrm{i}m\varphi}$. In the case $k = 0$, the stabilizer is the complete Euclid's group, and the series of the representations is obtained from the known irreducible representations of the rotational group SO(3). Thus, the irreducible representations of the Euclid's group are characterized by the pair (k, m) for $k > 0$ and $m = 0, \pm 1, \ldots$, and for $|\boldsymbol{k}| = 0$, by the pair $(0, l)$, $l = 0, 1, \ldots$. If the covering group is considered, m and l take also the halfintegral values.

In the coordinate representation, as it has been shown already, the translations and the rotations are generated by the momenta and the angular momenta. Hence, $\boldsymbol{k}$ corresponds to the momentum of the system, and m to the projection of the angular moment onto the vector $\boldsymbol{k}$. Therefore the irreducible subspace ($k \neq 0, m$) of the Euclid's group distinguishes the states $|\,\boldsymbol{k}m\rangle$ with the same kinetic energy of the center of mass (i. e. the same absolute value of the total momentum $|\boldsymbol{P}| = k\hbar$) and the projection of the angular momentum in the direction $\boldsymbol{k}$ of the motion of the center of mass equal to $m\hbar$. For $k = 0$ the center of mass of the system is in rest, and the total angular momentum is reduced to the interior one, while its value is determined by the index l (within the classical theory, this is possible only for the many particle system).

For the single free particle, the angular momentum is zero, and the corresponding irreducible subspace is defined by the condition $\boldsymbol{P}^2 = k^2\hbar^2$. In the coordinate representation this is the Schrödinger's equation of the spinless free particle: $(\nabla^2 + k^2)f(\boldsymbol{x}) = 0$.

As for the extended Euclid's group, it should be noted that the spatial inversion changes the sign of the momentum, while the angular momentum remains the same. Thus the projection of the angular momentum on $\boldsymbol{k}$ changes its sign. This means that two representations of the group $T^3 \wedge \mathrm{SO}(3, \mathbb{R})$, with the same $k > 0$ and opposite $m \neq 0$ yield one representation of the Euclid's group; in the case $m = 0$, the representation $(k, 0)$ gives two representations of the Euclid's group. Finally, when $k = 0$, and the representation is essentially determined by the representation of the rotational group, the representations are classified by angular momentum and the parity, $(k = 0, l, \pm)$, as described in the previous subsection.

2.2 Molecules: point groups

The symmetry groups of the linear molecules are Lie's groups, to differ from all other discrete systems. Thus they will be studied separately.

2.2.1 Linear molecules

Any linear molecule is invariant under all rotations, $R(\phi)$, around its axis (z-axis, by default). These rotations form Lie's group $\mathrm{SO}(2, \mathbb{R})$, which is in the molecular physics [3] denoted by $\boldsymbol{C}_\infty$. The remaining symmetries must leave the z-axis invariant. Such transformations are vertical mirror planes, σ_v (planes containing z-axis), horizontal mirror plane (xy-plane), σ_h,

rotations U for π around horizontal axis, or their combinations with the rotations around z-axis. Since $\sigma_h\sigma_v = U$, if any two of these three symmetries are observed, the third one is present also. When σ_v is conjugated by the rotation $R(\phi)$, another vertical mirror plane, $R(\phi)\sigma R^{-1}(\phi)$, rotated for ϕ with respect to the initial one, is obtained. Therefore, if there is one vertical mirror plane in the symmetry group, there are all others too. The analogous result is easily verified for the horizontal U axes of symmetry.

In this way all the symmetry groups of the linear molecules are classified: $\boldsymbol{C}_\infty$, $\boldsymbol{C}_{\infty v} = \boldsymbol{C}_\infty \wedge \{e, \sigma_v\}$, $\boldsymbol{C}_{\infty h} = \boldsymbol{C}_\infty \otimes \{e, \sigma_h\}$, $\boldsymbol{D}_\infty = \boldsymbol{C}_\infty \wedge \{e, U\}$ and $\boldsymbol{D}_{\infty h} = \boldsymbol{C}_{\infty v} \otimes \{e, \sigma_h\}$. Their structure enables simple construction of the irreducible representations (the representations are unitary, since the groups are compact).

Since $\boldsymbol{C}_\infty$ is Abel's group, its irreducible representations are one-dimensional, and the homomorphism condition is $D(R(\phi)) = \mathrm{e}^{-\mathrm{i}m\phi}$; the periodicity, $R(2\pi) = e$, implies that m is integer. Thus, the irreducible representations of this group are $A_m(R(\phi)) = \mathrm{e}^{-\mathrm{i}m\phi}$, $\quad m = 0, \pm1, \pm2, \ldots$.

The representations of the groups $\boldsymbol{C}_{\infty v}$ and $\boldsymbol{D}_\infty$ are found by induction from the halving subgroup $\boldsymbol{C}_\infty$. These groups are isomorphic, and their representations are equal (although differently denoted). Due to the relation $\sigma_v R(\phi)\sigma_v = R(-\phi)$, the σ_v-conjugated representation of $A_m(\boldsymbol{C}_\infty)$ is $A_{-m}(\boldsymbol{C}_\infty)$. Consequently, the representation $A_0(\boldsymbol{C}_\infty)$ is selfconjugated, giving two representations of the group $\boldsymbol{C}_{\infty v}$, namely $A_0(\boldsymbol{C}_{\infty v})$ and $B_0(\boldsymbol{C}_{\infty v})$. All other orbits contain two representations of $\boldsymbol{C}_\infty$, with opposite m, and each such pair gives one 2-dimensional representation, $E_m(\boldsymbol{C}_{\infty v})$ (as for the group $\boldsymbol{D}_\infty$, the one-dimensional representations are denoted by A_0^+ and A_0^-, instead of A_0 and B_0). The representations of the group $\boldsymbol{C}_{\infty h}$ are $A_m^\pm(\boldsymbol{C}_{\infty h})$ (this follows since $\boldsymbol{C}_{\infty h}$ is the direct product of $\boldsymbol{C}_\infty$ with the cyclic group $\{e, \sigma_h\}$). Similarly, using the direct product structure of the group $\boldsymbol{D}_{\infty h}$, the irreducible representations of this group are found: $A_0^\pm(\boldsymbol{D}_{\infty h})$, $B_0^\pm(\boldsymbol{D}_{\infty h})$ i $E_m^\pm(\boldsymbol{D}_{\infty h})$.

The representations are denoted in accordance with the physical contents of the good quantum numbers for the systems with the corresponding symmetries. Thus, m is the projection of the angular momentum on the z-axis, A and B shows the parity with respect to the vertical mirror plane, while $+$ and $-$ characterize the parity with respect to the reversal of the direction of the z-axis. The Clebsch-Gordan's series are easily found, and the selection rules following from the Wigner-Eckart's theorem manifest the conservation of the parities and of the z-component of the angular momentum. The greatest dimension of the obtained irreducible representations is 2, and this is the maximal degeneracy induced by symmetry.

2.2.2 Nonlinear molecules

The point groups of symmetry of nonlinear molecules are finite. There are 7 infinite series and 7 separated groups, [3].

Axial point groups are those leaving z-axis invariant, and they are classified into the 7 infinite families, with one group for positive integer n within each family: $\boldsymbol{C}_n$ (cyclic group generated by $C_n = R(\frac{2\pi}{n})$) of the order n, $\boldsymbol{S}_{2n} = \boldsymbol{C}_n + C_{2n}\sigma_h\boldsymbol{C}_n$ (cyclic group with the

generator $C_{2n}\sigma_h$) of the order $2n$, $\boldsymbol{C}_{nv} = \boldsymbol{C}_n \wedge \{e, \sigma_v\}$ of the order $2n$, $\boldsymbol{D}_n = \boldsymbol{C}_n \wedge \{e, U\}$ of the order $2n$, $\boldsymbol{C}_{nh} = \boldsymbol{C}_n \otimes \{e, \sigma_h\}$ of the order $2n$, $\boldsymbol{D}_{nh} = \boldsymbol{C}_{nv} \otimes \{e, \sigma_h\}$ of the order $4n$ and $\boldsymbol{D}_{nd} = \boldsymbol{C}_{nv} + U'\boldsymbol{C}_{nv}$ (U' is the horizontal axis bisecting the angle between the adjacent vertical mirror planes of $\boldsymbol{C}_{nv}$) of the order $4n$.

The remaining groups are: $\boldsymbol{T}$, the group of the rotations leaving the tetrahedron invariant (of the order 12), $\boldsymbol{T}_d$ the group of all the symmetries of the tetrahedron (of the order 24), $\boldsymbol{T}_h = \boldsymbol{T} \otimes \{e, P\}$ (of the order 24), $\boldsymbol{O}$ the group of the rotational symmetries of the cube (of the order 24), $\boldsymbol{O}_h = \boldsymbol{O} \otimes \{e, P\}$ the group of the all symmetries of the cube (of the order 48), $\boldsymbol{Y}$ the group of the rotational symmetries of the icosahedra (of the order 60) i $\boldsymbol{Y}_h = \boldsymbol{Y} \otimes \{e, P\}$ group of the all symmetries of the icosahedron (of the order 120). In the above relations P denotes the spatial inversion.

The representations can be obtained by the standard inductive methods. For the axial groups it suffices to note their hierarchy: $\boldsymbol{C}_n$ and $\boldsymbol{S}_{2n}$ are cyclic, $\boldsymbol{C}_{nv}$, $\boldsymbol{D}_n$ and $\boldsymbol{C}_{nh}$ have $\boldsymbol{C}_n$ as the halving subgroup, and $\boldsymbol{C}_{nv}$ is halving subgroup in $\boldsymbol{D}_{nh}$ and $\boldsymbol{D}_{nd}$. Therefore their representations can be derived directly or by the induction (§ A.2.8) from the halving subgroup in the two steps at most. Analogous, but slightly more complicated structural analysis yields the representations of $\boldsymbol{T}$, $\boldsymbol{O}$ and $\boldsymbol{Y}$, and then the representations of the remaining groups are easily found.

In all these cases the selection rules express conservation of the z-component of the angular momentum. Due to the finite order of the rotational axis, the representations with the quantum number m differing by the multiple of the order of the principle axis, n, are same. This is manifested in the form of the conservation law: the quantum numbers are added modulo n, and the selection rule is $m + m' \doteq m''$, meaning that $m'' = m + m' + zn$ (z is an integer). Such rule is called the conservation of the *quasi angular momentum*. As for other rotational axis as well as for the parities (mirror planes, inversion and rotations for π), the analogous conservation laws are easily established.

2.3 Crystals: space groups

The common property of the crystals, [4], is their discrete translational symmetry, described by the translational group T. The additional orthogonal symmetry, depends on the concrete compound, and therefore in the solid state physics the translational invariance is always considered, while only in the study of some specific crystall its whole space group is involved.

2.3.1 Translational group and lattices

The translational group is discrete Abelian group, generated by three independent vectors in $\mathbb{R}^3$. These vectors, $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ i $\boldsymbol{a}_3$, define the *primitive translations*, $(I \,|\boldsymbol{a}_i)$, which generate infinite cyclic groups $T_i = \{(I \,|z_i\boldsymbol{a}_i) \mid z_i \in \mathbb{Z}\}$. The whole translational group is the direct product $T = \otimes_{i=1}^{3} T_i$, and each element of T is product $(I \,|\boldsymbol{z}) = (I \,|z_1\boldsymbol{a}_1 + z_2\boldsymbol{a}_2 + z_3\boldsymbol{a}_3)$ given by triple of integers (z_1, z_2, z_3).

Acting on any point of $\mathbb{R}^3$ (*e.g.* $(0,0,0)$), the translations of T generate periodically arranged set of points in $\mathbb{R}^3$. This is an orbit of T, called the *lattice* with the *periods* $\boldsymbol{a}_i$, and the *elementary cell* being the box with the edges $\boldsymbol{a}_i$.

The choice of the periods of the given lattice is not unique. Let the $(\boldsymbol{a})_{[\boldsymbol{x}]}$ be matrix with columns being the vectors of the periods $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ i $\boldsymbol{a}_3$ represented in the basis $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3\}$ of the space $\mathbb{R}^3$. If S is the operator mapping original periods to another ones, $\boldsymbol{a}'$, i.e. $\boldsymbol{a}'_i = S\boldsymbol{a}_i$, then $(\boldsymbol{a}')_{[\boldsymbol{x}]} = S_{[\boldsymbol{x}]}(\boldsymbol{a})_{[\boldsymbol{x}]}$ (here $S_{[\boldsymbol{x}]}$ is the matrix representing the operator S in the basis $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3\}$). Especially, if $\boldsymbol{x}_i = \boldsymbol{a}_i$, then $(\boldsymbol{a})_{[\boldsymbol{a}]}$ is 3-dimensional identity matrix, and $(\boldsymbol{a}')_{[\boldsymbol{a}]} = S_{[\boldsymbol{a}]}$. Since primed basis is also a basis of periods, $\boldsymbol{a}'_i$ is an integral linear combination of the vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ and $\boldsymbol{a}_3$, and matrices $(\boldsymbol{a}')_{[\boldsymbol{a}]}$ and $S_{[\boldsymbol{a}]}$ are with integral elements. Further, starting from the periods $\boldsymbol{a}'_i$, the same argument shows that the elements of $(\boldsymbol{a})_{[\boldsymbol{a}']} = S^{-1}_{[\boldsymbol{a}']}$ and $S^{-1}_{[\boldsymbol{a}']}$ are integral. But it is known that the operator S is represented by the same matrices in both bases it connects, i.e. $S^{-1}_{[\boldsymbol{a}']} = S^{-1}_{[\boldsymbol{a}]}$; hence, both of the matrices $S_{[\boldsymbol{a}]}$ and $S^{-1}_{[\boldsymbol{a}]}$ are integral. This means that the group $\mathrm{GL}(3,\mathbb{Z})$ describes the different choices of the periods of the given lattice ($\mathrm{GL}(3,\mathbb{Z}) < \mathrm{GL}(3,\mathbb{R})$).

As the determinant of the integral matrix is integer itself, and the determinant of the of the inverse is inverse of the determinant, it follows that elements of $\mathrm{GL}(3,\mathbb{Z})$ satisfy $\det S = \pm 1$. Moreover, a determinant is independent of the representative basis, and the last equation is valid in any basis (although the matrix S is not necessarily integral in any basis). Especially, in the Descartes's basis, $\boldsymbol{e}_i$, determinant $\det(\boldsymbol{a})_{[\boldsymbol{e}]} = [\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3]$ (mixed vector product) is volume of the original elementary cell, while $\det(\boldsymbol{a}')_{[\boldsymbol{e}]} = \det S_{[\boldsymbol{e}]} \det(\boldsymbol{a})_{[\boldsymbol{e}]}$ is volume of the final one. Thus, for any choice of the periods elementary cell is of the same volume.

The irreducible representations of the translational group are easily found, since T is the direct product of the cyclic groups. In fact, for the cyclic group T_i, generated by the elementary translation $(I|\boldsymbol{a}_i)$, the irreducible representations are $D^{(k_i)}(\ I \mid z_i\boldsymbol{a}_i\ ) = \mathrm{e}^{-\mathrm{i}k_i z_i \boldsymbol{a}_i}$, where k_i is any complex number. Among them, unitary representations are distinguished by real values of k_i. The representations $D^{(k_i)}(T_i)$ and $D^{(k_i+K_i z)}(T_i)$ are the same for $K_i = \frac{2\pi}{a_i}$ and any $z \in \mathbb{Z}$, meaning that nonequivalent representations are found for $k_i \in (-\frac{\pi}{\boldsymbol{a}_i}, \frac{\pi}{\boldsymbol{a}_i}]$. Hence, irreducible representations of the whole translational group T are $D^{(\boldsymbol{k})}(\ I\ |\boldsymbol{z}\ ) = \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\boldsymbol{z}}$, with $\boldsymbol{k} = k_1\boldsymbol{b}_1 + k_2\boldsymbol{b}_2 + k_3\boldsymbol{b}_3$, and

$$\boldsymbol{b}_1 = 2\pi\frac{\boldsymbol{a}_2 \times \boldsymbol{a}_3}{[\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3]}, \quad \boldsymbol{b}_2 = 2\pi\frac{\boldsymbol{a}_3 \times \boldsymbol{a}_1}{[\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3]}, \quad \boldsymbol{b}_3 = 2\pi\frac{\boldsymbol{a}_1 \times \boldsymbol{a}_2}{[\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3]}.$$

Vectors $\boldsymbol{b}_i$ form a basis of the *inverse lattice*, and the corresponding elementary cell includes the nonequivalent unitary representations of T: $\boldsymbol{k} + \boldsymbol{K}$ and $\boldsymbol{k}$ give the same representation if and only if $\boldsymbol{K} = z_1\boldsymbol{b}_1 + z_2\boldsymbol{b}_2 + z_3\boldsymbol{b}_3$ is the vector of the inverse lattice.

Usually, instead of the elementary cell of the lattice the *Wigner-Seitz's cell* is used: this is the domain including all the points of $\mathbb{R}^3$ which are closer to the origin of the lattice ($\boldsymbol{z} = 0$) than to any other point $\boldsymbol{z} \neq 0$ of the lattice. Obviously, this domain is bounded by the planes perpendicular to the vectors connecting the adjacent points of the lattice and halving these vectors. It has the same volume as the elementary cell, but its shape has the orthogonal symmetry of the crystal. Analogous construction in the inverse lattice is known as the *Brillouin's*

zone, and its symmetry is very important in the construction of the irreducible representations of the space groups. Therefore, it is assumed that the vector $\boldsymbol{k}$, labeling the irreducible representations of T, takes on the values from the Brillouin's zone. According to the general principles of the applications of symmetry, § 1.2, the eigenvalues of the hamiltonians related to the various properties of crystal are labeled by good quantum number $\boldsymbol{k}$. Therefore, the eigen energies are functions (hyper surfaces), $E_{\boldsymbol{k},t_{\boldsymbol{k}}}$, over the Brillouin's zone: these *energy bands* are one of the general characteristics of the physics of the crystals.

In order to simplify some calculations, the *Born-von Karman's periodical conditions* are frequently mentioned in theoretical studies of crystals: the requirement $(I \mid z_i\boldsymbol{a}_i)^{N_i} = (I \mid N_i z_i \boldsymbol{a}_i) = (I \mid 0)$ is introduced, meaning that the groups T_i are substituted by finite cyclic groups of order N_i. To provide physical justification for this simplification, loose arguments about physically equal conditions at the boundaries of the crystal, or finiteness of real crystals, are usually invoked. Nevertheless, Born-von Karman's conditions describe the lattice on a 3-dimensional torus, which topologically differs from the real crystal; this can lead to some problems and artifacts of theory. On the other hand, finiteness of real crystals makes results obtained with use of infinite translational groups approximate, though for many properties difference between N periods and infinite structures are negligible for N of order 10. Especially, when effects related to the boundaries of real crystal are studied, none of the approaches offers reliable predictions.

If $D(T)$ is a representation of translational group, the group projector (§ A.2.4) of the irreducible representation $D^{(\boldsymbol{k})}(T)$ is $P^{(\boldsymbol{k})} = \frac{1}{|T|}\sum_{\boldsymbol{z}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{z}} D(I|\boldsymbol{z})$. In the coordinate representation, the component of the function from the subspace $\mathcal{S}^{(\boldsymbol{k})}$ of $D^{(\boldsymbol{k})}(T)$ is found as the projection $\psi^{(\boldsymbol{k})}(\boldsymbol{x}) = P^{(\boldsymbol{k})} f(\boldsymbol{x}) = \frac{1}{|T|}\sum_{\boldsymbol{z}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{z}} f(\boldsymbol{x}-\boldsymbol{z}) = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{x}} u^{(0)}_{\boldsymbol{k}}(\boldsymbol{x})$, where $u^{(0)}_{\boldsymbol{k}}(\boldsymbol{x}) = \sum_{\boldsymbol{z}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}(\boldsymbol{z}-\boldsymbol{x})} f(\boldsymbol{x}-\boldsymbol{z})$. The functions $u^{(0)}_{\boldsymbol{k}}(\boldsymbol{x})$ are invariant under translations (translations simply permute terms in the sum). This result is known as the *Bloch's theorem* [31]: each function transforming according to representation $\boldsymbol{k}$ (*i.e.* $D(I \mid \boldsymbol{z})\psi^{(\boldsymbol{k})}(\boldsymbol{x}) = \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\boldsymbol{z}}\psi^{(\boldsymbol{k})}(\boldsymbol{x})$) is plane wave $\mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{x}}$ ($\boldsymbol{k}$ from the Brillouin's zone) multiplied by a periodical function $u^{(0)}_{\boldsymbol{k}}$.

This conclusion enables to consider only the translationally invariant factors instead of the whole functions, leading to the specific form of the dynamical law. The reduction of the hamiltonian operator into the multiple irreducible subspace $\mathcal{S}^{(\boldsymbol{k})}$ of the translational group, gives, for each $\boldsymbol{k}$ in the Brillouin's zone, the Schrödinger's equation for the periodical functions $u^{(0)}_{\boldsymbol{k}}$; therefore, the eigenvalues are the functions of $\boldsymbol{k}$, realizing the mentioned scheme of the energy bands of the crystal. Moreover, the periodicity of the functions $u^{(0)}_{\boldsymbol{k}}$ enables their expansion in the Fourier's series, $u^{(0)}_{\boldsymbol{k}}(\boldsymbol{x}) = \sum_{\boldsymbol{K}} f_{\boldsymbol{k},\boldsymbol{K}} \mathrm{e}^{\mathrm{i}\boldsymbol{K}\boldsymbol{x}}$ (the sum is over the vectors of the inverse lattice), and the functions can be found or modeled through the coefficients $f_{\boldsymbol{k},\boldsymbol{K}}$. Hence, typical solid state theoretical approach to consider various quantities through their Fourier's coefficients originates in the translational symmetry. Later on, § 3.3 and § 5.4, all these consequences will be illustrated during the study of the phonons and electrons in crystals.

Clebsch-Gordan series of the irreducible representations are easily calculated, since they are one-dimensional: $D^{(\boldsymbol{k})}(T) \otimes D^{(\boldsymbol{k}')}(T) = D^{(\boldsymbol{k}'')}(T)$, where $\boldsymbol{k}'' \doteq \boldsymbol{k} + \boldsymbol{k}' = \boldsymbol{k} + \boldsymbol{k}' +$

$\boldsymbol{K}$ (equality modulo vector of the inverse lattice). The Wigner-Eckart's theorem implies $\langle\ \boldsymbol{k}''\lambda_{\boldsymbol{k}''}|V^{\boldsymbol{k}'\lambda_{\boldsymbol{k}'}}|\boldsymbol{k}\lambda_{\boldsymbol{k}}\ \rangle = 0$, if the condition $\boldsymbol{k}'' \doteq \boldsymbol{k} + \boldsymbol{k}'$ is not fulfilled. In the condensed matter physics, $\hbar\boldsymbol{k}$ is interpreted as the *quasi momentum* of the considered subsystem in the crystal, and the last selection rule becomes conservation law of the quasi momentum; the fact that this quantity is defined up to the vector of the inverse lattice is manifested by the non vanishing $\boldsymbol{K}$ in some processes (these are called *indirect* or *Umklapp* processes to distinguish from the *direct* ones with $\boldsymbol{K} = 0$ ares).

2.3.2 Crystal systems

All orthogonal transformations leaving a lattice invariant form a group called *holohedry* or the *singony*, P_H. This is a finite point group, being the maximal subgroup of the full orthogonal group O(3) with elements permuting the lattice points. Periodicity of the lattice restricts the set of holohedries. In fact, if the rotation for ϕ leaves the lattice invariant, its representative matrix in the basis of the periods must be integral, and thus its trace, $1 + 2\cos\phi$, too. It follows that the angle of rotation (assumed to be less or equal to π) can take the values $\frac{2\pi}{n}$ for $n = 1, 2, 3, 4, 6$ ($R(2\pi) = R(0)$ for $n = 1$). Only the point groups (listed in § 2.2.2) with these values of n may be symmetries of the lattice. There are 32 such groups and they are called *crystallographic point groups*:
$\boldsymbol{C}_1$, $\boldsymbol{C}_2$, $\boldsymbol{C}_3$, $\boldsymbol{C}_4$, $\boldsymbol{C}_6$, $\boldsymbol{C}_{2v}$, $\boldsymbol{C}_{3v}$, $\boldsymbol{C}_{4v}$, $\boldsymbol{C}_{6v}$, $\boldsymbol{S}_2 \stackrel{\text{def}}{=} \boldsymbol{C}_i$, $\boldsymbol{S}_4$, $\boldsymbol{S}_6$, $\boldsymbol{C}_{1h} \stackrel{\text{def}}{=} \boldsymbol{C}_s$, $\boldsymbol{C}_{2h}$, $\boldsymbol{C}_{3h}$, $\boldsymbol{C}_{4h}$, $\boldsymbol{C}_{6h}$, $\boldsymbol{D}_2$, $\boldsymbol{D}_3$, $\boldsymbol{D}_4$, $\boldsymbol{D}_6$, $\boldsymbol{D}_{2h}$, $\boldsymbol{D}_{3h}$, $\boldsymbol{D}_{4h}$, $\boldsymbol{D}_{6h}$, $\boldsymbol{D}_{2d}$, $\boldsymbol{D}_{3d}$, $\boldsymbol{T}$, $\boldsymbol{T}_h$, $\boldsymbol{T}_d$, $\boldsymbol{O}$ i $\boldsymbol{O}_h$(the groups with same geometrical contents are encountered only once: $\boldsymbol{D}_1 = \boldsymbol{C}_2$, $\boldsymbol{C}_{1h} = \boldsymbol{C}_{1v}$, $\boldsymbol{D}_{1h} = \boldsymbol{C}_{2v}$ and $\boldsymbol{D}_{1d} = \boldsymbol{C}_{2h}$; these are the mutually conjugated subgroups of $\mathrm{O}(3, \mathbb{R})$).

The space inversion is obviously symmetry of the lattice: if $\boldsymbol{a}$ is lattice vector, then $-\boldsymbol{a}$ also belong to the lattice; this implies that the candidates for the holohedries are only the groups containing the inversion. Also, it is obvious that invariance of the lattice under $\boldsymbol{C}_3$ yields also invariance under $\boldsymbol{C}_{3v}$; similar results are obtained for $\boldsymbol{C}_4$ and $\boldsymbol{C}_{4v}$, and $\boldsymbol{C}_6$ and $\boldsymbol{C}_{6v}$. Consequently, the invariance under the transformations from $\boldsymbol{S}_6$, $\boldsymbol{C}_{4h}$ and $\boldsymbol{C}_{6h}$ implies the symmetry of the groups $\boldsymbol{D}_{3d}$, $\boldsymbol{D}_{4h}$ and $\boldsymbol{D}_{6h}$, respectively. Thus, altogether there are 7 holohedries: $\boldsymbol{S}_2$, $\boldsymbol{C}_{2h}$, $\boldsymbol{D}_{2h}$, $\boldsymbol{D}_{4h}$, $\boldsymbol{D}_{6h}$, $\boldsymbol{D}_{3d}$ and $\boldsymbol{O}_h$. Holohedries form partially ordered set, [4, 8], with respect to the subgroup relation, $A < B$:

$$\begin{array}{ccccccc} & & & & \boldsymbol{D}_{6h} & > & \boldsymbol{D}_{3d} \\ & & & & \vee & & \vee \\ \boldsymbol{O}_h & > & \boldsymbol{D}_{4h} & > & \boldsymbol{D}_{2h} & > & \boldsymbol{C}_{2h} > \boldsymbol{S}_2 \end{array}$$

Given the holohedry, P_H, different lattices can be formed, suitably choosing periods of T. The set of all such lattices is called the *crystal system* (of the holohedry P_H). Two lattices of the same holohedry P_H are considered as equivalent if they can be continuously transformed one to another such that the holohedry of the lattice in any of the intermediate position is at least P_H. This means that, after some homotetical mapping, two equivalent lattices can be identified by the action of the transformation from $\mathrm{O}(3, \mathbb{R})$. It appears that there are at all

14 nonequivalent lattices, called *Bravais's lattices*, distributed over 7 crystal systems (Table 2.1).

Successive action of the elements of P_H and T leaves lattice invariant. The intersection of P_H and T is the identity element only. Finally, when a lattice translation is conjugated by an element from P_H, another lattice translation is obtained, meaning that T is invariant subgroup of the total lattice symmetry group. It follows that the total group of symmetry of the lattice with holohedry P_H (for any of the associated Bravais's lattices) is $S_H = T \wedge P_H$.

2.3.3 Space groups

Having considered orthogonal symmetry of the translational lattices only, the crystal systems and the Bravais's lattices are obtained, with the symmetry groups $S_H = T \wedge P_H$. Nevertheless, these are not all symmetry groups of real crystals. In fact, when real crystals are studied, besides the geometrical arrangement, the symmetry of the atomic physical properties must be encountered. Also, atoms in crystals are not positioned only in the lattice sites: translational invariance allows crystals containing several equal but slightly mutually translated Bravais's lattices occupied by (different or same) atoms. Thus, certain atoms appear in the interior of elementary cell. In this sense, Bravais's lattices are also called "empty" lattices. Obviously, the total symmetry group of a crystal contains all the translations of the lattice, but the orthogonal subgroup is less than that of the lattice, while some of the orthogonal elements may become the symmetries of the crystal only when combined with the translations.

Each real crystal uniquely defines its translational symmetry group T, defining afterward the crystal lattice and its symmetry, P_H. On the other hand, real crystal determines its group of geometrical symmetries, the *space group* of the crystal, S. Clearly, S contains all pure translations, i.e. T is its subgroup. Also, if $(R|\boldsymbol{x})$ is an arbitrary element of the group S, and $(I|\boldsymbol{z})$ is an element from the subgroup T, the conjugated element, $(R|\boldsymbol{x})(I|\boldsymbol{z})(R|\boldsymbol{x})^{-1} = (I \,|\, R\boldsymbol{z})$ is pure translation, thus belonging to T. This shows that translational subgroup is invariant in S; also, it follows that the orthogonal factor R of any element of the group S leaves lattice invariant, i.e. R is an element of P_H. Also, it can be easily verified that group is the set of such orthogonal elements which combined with certain translations give symmetry transformations of the crystal. This group is called the *isogonal* point group, P_I, and it is obviously a subgroup in P_H. However, note that the elements of P_H and P_I may not be symmetries of the crystal (i.e. these groups may not be subgroups of S).

Still, for each element R of P_I there exists vector $\boldsymbol{r}$ such that $(R \,|\, \boldsymbol{r})$ is in S. This determines uniquely the coset $(R \,|\, \boldsymbol{r})T = \{(R \,|\, \boldsymbol{r} + \boldsymbol{z})\}$ of the translational subgroup in S. Further, this coset contains exactly one element, $(R \,|\, \boldsymbol{f}_R)$, with vector $\boldsymbol{f}_R$ from the interior of the elementary cell of the crystal (there is $\boldsymbol{z}$ such that $\boldsymbol{f}_R = \boldsymbol{r} + \boldsymbol{z}$). If $\boldsymbol{f}_R \neq 0$, then R is not symmetry of the crystal, and $\boldsymbol{f}_R$ is called the *fractional translation*; in this way the *screw axes*, $(C_n \,|\, \boldsymbol{f})$ and the *glide planes*, $(\sigma \,|\, \boldsymbol{f})$, are obtained (Fig. 2.1).

On the other hand, since T is invariant subgroup, the coset multiplication is well defined: $(R \,|\, \boldsymbol{f}_R)T(R' \,|\, \boldsymbol{f}_{R'})T = (RR' \,|\, \boldsymbol{f}_R + R\boldsymbol{f}_{R'})T = (RR' \,|\, \boldsymbol{f}_{RR'})T$. The orthogonal factors are

multiplied as in P_I, enabling to identify P_I to the corresponding factor group: $P_I = S/T$.

Since $P_I < P_H$, all of the 32 crystallographic point groups can be distributed over the holohedries, such that each is uniquely (due to the introduced partial ordering on the set of the holohedries) associated to the minimal holohedry containing it. This procedure provides total of 32 *crystal classes* distributed among 7 systems. The definition of the isogonal group (its elements are obtained by forgetting for the translational parts of the transformations of the space group), shows that, even when P_I is not subgroup of S, some characteristics of the crystals will be preserved after the transformations by the elements of this group: these are the properties determined by the directions in the crystal only, independent on the details of the arrangements of the atoms along these directions. In fact, all the directions along which the arrangement of the atoms is equal up to some translation (including fractional ones), are equivalent for such properties, and P_I appears as the group of the symmetry of the directions, connecting the mutually equivalent directions. It is commonly considered that the *macroscopic properties* depend on the directions in the crystal only, and in this context P_I is taken as the group describing the macroscopic symmetries [4].

Table 2.1: Space groups: for each crystal system, the number of the Bravais's lattices (BL), the holohedry (P_H), and the corresponding crystal classes (represented by the associated isogonal point groups, P_I), with the number of the spaces groups within each class, are presented.

	System	BL	P_H	P_I
1	Triclinic	1	$\boldsymbol{S}_2$	$\boldsymbol{C}_1(1), \boldsymbol{S}_2(1)$
2	Monoclinic	2	$\boldsymbol{C}_{2h}$	$\boldsymbol{C}_{1h}(4), \boldsymbol{C}_2(3), \boldsymbol{C}_{2h}(6)$
3	Rombic	4	$\boldsymbol{D}_{2h}$	$\boldsymbol{C}_{2v}(22), \boldsymbol{D}_2(9), \boldsymbol{D}_{2h}(28)$
4	Tetragonal	2	$\boldsymbol{D}_{4h}$	$\boldsymbol{S}_4(2), \boldsymbol{D}_{2d}(12), \boldsymbol{C}_4(6), \boldsymbol{C}_{4h}(6), \boldsymbol{C}_{4v}(12), \boldsymbol{D}_4(10), \boldsymbol{D}_{4h}(20)$
5	Rombohedral	1	$\boldsymbol{D}_{3d}$	$\boldsymbol{C}_3(4), \boldsymbol{S}_6(2), \boldsymbol{C}_{3v}(6), \boldsymbol{D}_3(7), \boldsymbol{D}_{3d}(6)$
6	Hexagonal	1	$\boldsymbol{D}_{6h}$	$\boldsymbol{C}_{3h}(1), \boldsymbol{D}_{3h}(4), \boldsymbol{C}_6(6), \boldsymbol{C}_{6h}(2), \boldsymbol{C}_{6v}(4), \boldsymbol{D}_6(6), \boldsymbol{D}_{6h}(4)$
7	Cubic	3	$\boldsymbol{O}_h$	$\boldsymbol{T}(5), \boldsymbol{T}_h(7), \boldsymbol{T}_d(6), \boldsymbol{O}(8), \boldsymbol{O}_h(10)$

It became clear that translational and isogonal point groups, together with fractional translations, completely determine one of the space groups. Various choices of fractional translations differ space groups from the same crystal class. Two space groups are considered as equivalent if they are conjugated as the subgroups of the Euclid's group. Then there are 230 nonequivalent space groups, distributed over 32 crystal classes (table 2.1). Their main common characteristics is the invariant translational subgroup; the corresponding factor group, isomorphic to the isogonal point group, specifies the crystal class and the crystal system. If the isogonal group is also subgroup of the space group, *i.e.* if all fractional translations vanish, the structure of the space group is $S = T \wedge P_I$ (to see this it suffices to repeat the discussion on the analogous relation for the symmetry group of the lattice); there are 73 such groups, known as the *symorphic* space groups.

Since the set of translations is commutative invariant subgroup of any space group, the

irreducible representations can be found by the induction from this subgroup (§ A.2.8). The orbit of the representation $D^{(\boldsymbol{k})}(T)$ of the translational group is the set of the vectors of the Brillouin's zone, called the *star of* $\boldsymbol{k}$; these vectors are mapped one to another by the elements of the isogonal group. If vector $\boldsymbol{k}$ is in the interior of the Brillouin's zone, outside the plains and the axes of symmetries (this is called *general position*), the stabilizer is the translational subgroup, T, itself, and the order of the orbit is $|P_I|$. On the contrary, when $\boldsymbol{k} = 0$, the stabilizer is the whole space group, S, and the order of the orbit is 1. Between these extreme cases, there are vectors of *special positions*, called (*Lifshic's points*): their stabilizer are nontrivial subgroups of S and the orders of their orbits are less then $|P_I|$. When the representative vector is chosen for each star and its stabilizer is determined, the allowable irreducible representations are to be found; then, inducing these representations from the stabilizer to the total space group, the irreducible representations of S are obtained.

Construction of the allowable representations is the main difficulty in this algorithm, [23]. For the symorphic group $S = T \wedge P_I$, the stabilizer $S_{\boldsymbol{k}}$ is semidirect product of T and the subgroup $P_{\boldsymbol{k}}$ of the isogonal group. The allowable representation of $S_{\boldsymbol{k}}$ are found as direct products of $D^{(\boldsymbol{k})}(T)$ with the irreducible representations of $P_{\boldsymbol{k}}$ (the later are called *little representations*). Even for nonsymorphic groups, the stabilizer $S_{\boldsymbol{k}}$ is a space group, with same translational subgroup as S, and the isogonal group $P_{\boldsymbol{k}}$ being a subgroup of P_I. It turns out that the procedure is similar to the case of symorphic groups, but in the role of little representations appear projective representations of $P_{\boldsymbol{k}}$ (§ A.2.7, [11]), or, equivalently, irreducible representations of the covering group of $P_{\boldsymbol{k}}$. The dimensions of the irreducible representations of the space groups are 1, 2, 3, 4, 6 or 8.

The described construction causes that among the labels of the irreducible representations of the space groups is the vector $\boldsymbol{k}$ of Brillouin's zone, indicating the orbit (star) of induction. Therefore, the selection rules obtained when Clebsch-Gordan's coefficients are calculated, manifest the conservation of quasi-momenta. As for the quasi angular momenta and parities, they are related to the isogonal group; therefore, they are conserved only if the corresponding symmetries are also in the space group (*i.e.* if the associated fractional translation is zero), but, depending on representations, these conservation rules are satisfied in other cases.

2.4 Layers: diperiodic groups

The diperiodic groups can be treated along the same lines as the space groups. Also there are some structural similarities to the line groups, enabling easier construction of the irreducible representations. Systems with such symmetries were rarely analyzed in the solid state physics until, during this decade, high temperature superconductivity and planar dislocations in the crystals have been related to diperiodic symmetry.

Each diperiodic group is a subgroup of some of the space groups. Since one diperiodic group can be subgroup of different space groups, all those 3-dimensional holohedries differing only by the translations in the direction outside the plain of the diperiodic lattice, give the same two dimensional holohedry (same refers to the corresponding Bravais's lattices). The

isogonal groups satisfy crystallographic conditions for the order of the principle rotational axis derived for the crystals. Therefore they are subgroups of the crystallographic point groups which leave the lattice plain invariant. There are 10 such groups at all: $\boldsymbol{C}_n$ and $\boldsymbol{C}_{nv}$ for $n = 1, 2, 3, 4, 6$; other point groups either act in the lattice plane (xOy) as some of the encountered, or do not leave this plane invariant. The holohedry can be any group containing the inversion in the lattice plane, *i.e.* the rotation C_2. When, for the reasons discussed in § 2.3.2, the groups $\boldsymbol{C}_3, \boldsymbol{C}_4$ i $\boldsymbol{C}_6$ are left out, the remaining groups, $\boldsymbol{C}_2$, $\boldsymbol{C}_{2v}$, $\boldsymbol{C}_{4v}$ and $\boldsymbol{C}_{6v}$ are the holohedries. The reflection σ_h acts trivially on the lattice, and it is not considered as its symmetry; still, diperiodic physical system may not be two dimensional, and σ_h may be nontrivial symmetry. Therefore, in this context it is usual to enlarge the holohedries by σ_h, yielding $\boldsymbol{C}_{2h}$ (monoclinic system, 7 groups), $\boldsymbol{D}_{2h}$ (rombohedral, 41), $\boldsymbol{D}_{4h}$ (tetragonal, 16) and $\boldsymbol{D}_{6h}$ (hexagonal, 16).

Analogously to the line groups, each diperiodic group is weak direct product of the generalized 2-dimensional translational group $\boldsymbol{Z}$ and the point group $\boldsymbol{P}$: $D = \mathbf{ZP}$. The generalized translational group, $\boldsymbol{Z}$, is two dimensional, and describes the periodical arrangement of the elementary motifs along two independent directions in the xOy-plane. It can be formed of the generalized one-dimensional translational groups leaving the xy-plane invariant, and these are: the pure translational group $\boldsymbol{T}$ along an axis in the plane, the screw axis group $\mathbf{2}_1$ with the C_2 axis in the plane, the glide plane group $\boldsymbol{T}_h$ of the horizontal, xy, glide plane, and the glide plane group $\boldsymbol{T}_v$ of the vertical glide plane (containing z axis). The point factors are chosen among the enumerated 10 axial crystallographic point groups.

The list of all diperiodic groups (in the numerical, [27], and international notation), factorized in the described form **PZ**, is given in the Table 2.2.

2.5 Polymers: line groups

Polymers, nanotubes and subsystems of the structures periodical in two or three directions (*e.g.* spin subsystem of 3-dimensional crystal can be periodical in one direction only) are typical systems periodical along one direction. In this section any such system will be called *polymer*.

Clearly, polymer is infinite along the direction of the periodicity (z-axis, by convention); thus, it is infinite series of the finite identical units, called *monomers*. These are regularly arranged along z-axis: the n-th monomer is obtained from the previous one by the same transformation $z = (R|\boldsymbol{v})$ mapping the n-th monomer to the next one. If certain monomer is singled out as the initial one, then all others can be obtained from this by the successive action of z. Therefore, the group L of geometrical symmetries of polymer contains infinite cyclic (therefore Abel's) subgroup, Z, generated by the element z. On the other hand, monomer itself may have some symmetry group, P, being one of the point groups. Thus, the elements of L are combinations (products [25]) of the symmetries of the arrangement of monomers (group Z) and the internal symmetries of the monomer (group P).

The generator z certainly translates along z-axis, and its most general form is $z = (R|v)$

Table 2.2: **Factorization of diperiodic groups.** For each group $\boldsymbol{Dg}$, its holohedry $\boldsymbol{H}$, isogonal point group $\boldsymbol{I}$, factorization $\boldsymbol{PT}$ and international symbol [27] are given. The last column points to the table in Ref. [**?**], with irreducible representation of the group.

$\boldsymbol{Dg}$	**H**	**I**	**P T**	Int. simb.	Tabela	$\boldsymbol{Dg}$	**H**	**I**	**P T**	Int. simb.	Tabela
1	$\mathbf{C}_{2h}$	$\mathbf{C}_1$	$\boldsymbol{T}$	p1	2	41	$\mathbf{D}_{2h}$	$\mathbf{D}_{2h}$	$\mathbf{C}_{2v}\boldsymbol{T}_h$	$\mathrm{p}\frac{2}{a}\frac{2_1}{m}\frac{2}{m}$	11
2		$\mathbf{S}_2$	$\mathbf{S}_2\boldsymbol{T}$	p$\bar{1}$	3	42		$\mathbf{D}_{2h}$	$\mathbf{D}_{1d}\boldsymbol{T}'_h$	$\mathrm{p}\frac{2}{n}\frac{2}{m}\frac{2_1}{a}$	17
3		$\mathbf{C}_2$	$\mathbf{C}_2\boldsymbol{T}$	p211	3	43		$\mathbf{D}_{2h}$	$\mathbf{D}_1 2_1 T_h$	$\mathrm{p}\frac{2}{a}\frac{2}{b}\frac{2_1}{a}$	12
4		$\mathbf{C}_{1h}$	$\mathbf{C}_{1h}\boldsymbol{T}$	pm11	2	44		$\mathbf{D}_{2h}$	$\mathbf{C}_{2h}\boldsymbol{T}'_v$	$\mathrm{p}\frac{2}{m}\frac{2_1}{b}\frac{2_1}{a}$	15
5		$\mathbf{C}_{1h}$	$\boldsymbol{T}_h$	pb11	2	45		$\mathbf{D}_{2h}$	$\mathbf{C}_2 2_1 T_h$	$\mathrm{p}\frac{2}{a}\frac{2_1}{b}\frac{2_1}{m}$	10
6		$\mathbf{C}_{2h}$	$\mathbf{C}_{2h}\boldsymbol{T}$	$\mathrm{p}\frac{2}{m}11$	3	46		$\mathbf{D}_{2h}$	$\mathbf{C}_{2v}\boldsymbol{T}'_h$	$\mathrm{p}\frac{2}{n}\frac{2_1}{m}\frac{2_1}{m}$	17
7		$\mathbf{C}_{2h}$	$\mathbf{C}_2\boldsymbol{T}_h$	$\mathrm{p}\frac{2}{b}11$	4	47		$\mathbf{D}_{2h}$	$\mathbf{D}_{2h}\boldsymbol{T}'$	$\mathrm{c}\frac{2}{m}\frac{2}{m}\frac{2}{m}$	14
8	$\mathbf{D}_{2h}$	$\mathbf{D}_1$	$\mathbf{D}_1\boldsymbol{T}$	p112	5	48		$\mathbf{D}_{2h}$	$\mathbf{C}_{2v}\boldsymbol{T}'_h$	$\mathrm{c}\frac{2}{a}\frac{2}{m}\frac{2}{m}$	18
9		$\mathbf{D}_1$	$\mathbf{2}_1$	$\mathrm{p}112_1$	7	49	$\mathbf{D}_{4h}$	$\mathbf{C}_4$	$\mathbf{C}_4\boldsymbol{T}$	p4	19
10		$\mathbf{D}_1$	$\mathbf{D}_1\boldsymbol{T}'$	c112	13	50		$\mathbf{S}_4$	$\mathbf{S}_4\boldsymbol{T}$	p$\bar{4}$	19
11		$\mathbf{C}_{1v}$	$\mathbf{C}_{1v}\boldsymbol{T}$	p11m	5	51		$\mathbf{C}_{4h}$	$\mathbf{C}_{4h}\boldsymbol{T}$	p4/m	19
12		$\mathbf{C}_{1v}$	$\boldsymbol{T}_v$	p11a	7	52		$\mathbf{C}_{4h}$	$\mathbf{C}_4\boldsymbol{T}'_h$	p4/n	20
13		$\mathbf{C}_{1v}$	$\mathbf{C}_{1v}\boldsymbol{T}'$	c11m	13	53		$\mathbf{D}_4$	$\mathbf{D}_4\boldsymbol{T}$	p422	21
14		$\mathbf{D}_{1d}$	$\mathbf{D}_{1d}\boldsymbol{T}$	$\mathrm{p}11\frac{2}{m}$	6	54		$\mathbf{D}_4$	$\mathbf{C}_4\mathbf{2}'_1$	$\mathrm{p}42_12$	22
15		$\mathbf{D}_{1d}$	$\mathbf{S}_2\mathbf{2}_1$	$\mathrm{p}11\frac{2_1}{m}$	8	55		$\mathbf{C}_{4v}$	$\mathbf{C}_{4v}\boldsymbol{T}$	p4mm	21
16		$\mathbf{D}_{1d}$	$\mathbf{D}_{1d}\boldsymbol{T}'$	$\mathrm{c}11\frac{2}{m}$	14	56		$\mathbf{C}_{4v}$	$\mathbf{C}_4\boldsymbol{T}'_v$	p4bm	22
17		$\mathbf{D}_{1d}$	$\mathbf{S}_2\boldsymbol{T}_v$	$\mathrm{p}11\frac{2}{a}$	8	57		$\mathbf{D}_{2d}$	$\mathbf{D}_{2d}\boldsymbol{T}$	p$\bar{4}$2m	21
18		$\mathbf{D}_{1d}$	$\mathbf{S}_2\boldsymbol{T}'_v$	$\mathrm{p}11\frac{2_1}{a}$	15	58		$\mathbf{D}_{2d}$	$\mathbf{S}_4\mathbf{2}'_1$	$\mathrm{p}\bar{4}2_1\mathrm{m}$	22
19		$\mathbf{D}_2$	$\mathbf{D}_2\boldsymbol{T}$	p222	6	59		$\mathbf{D}_{2d}$	$\mathbf{D}_{2d}\boldsymbol{T}$	p$\bar{4}$m2	21
20		$\mathbf{D}_2$	$\mathbf{C}_2\mathbf{2}_1$	$\mathrm{p}222_1$	8	60		$\mathbf{D}_{2d}$	$\mathbf{S}_4\boldsymbol{T}'_v$	p$\bar{4}$b2	22
21		$\mathbf{D}_2$	$\mathbf{C}_2\mathbf{2}'_1$	$\mathrm{p}22_12_1$	15	61		$\mathbf{D}_{4h}$	$\mathbf{D}_{4h}\boldsymbol{T}$	$\mathrm{p}\frac{4}{m}\frac{2}{m}\frac{2}{m}$	21
22		$\mathbf{D}_2$	$\mathbf{D}_2\boldsymbol{T}'$	c222	14	62		$\mathbf{D}_{4h}$	$\mathbf{D}_{2d}\boldsymbol{T}'_h$	$\mathrm{p}\frac{4}{n}\frac{2}{b}\frac{2}{m}$	23
23		$\mathbf{C}_{2v}$	$\mathbf{C}_{2v}\boldsymbol{T}$	p2mm	6	63		$\mathbf{D}_{4h}$	$\mathbf{C}_{4h}\boldsymbol{T}'_v$	$\mathrm{p}\frac{4}{m}\frac{2_1}{b}\frac{2}{m}$	22
24		$\mathbf{D}_{1h}$	$\mathbf{D}_{1h}\boldsymbol{T}$	pmm2	5	64		$\mathbf{D}_{4h}$	$\mathbf{D}_{2d}\boldsymbol{T}'_h$	$\mathrm{p}\frac{4}{n}\frac{2_1}{m}\frac{2}{m}$	23
25		$\mathbf{D}_{1h}$	$\mathbf{C}_{1h}\mathbf{2}_1$	$\mathrm{pm}2_1\mathrm{a}$	7	65	$\mathbf{D}_{6h}$	$\mathbf{C}_3$	$\mathbf{C}_3\boldsymbol{T}$	p$\bar{3}$	24
26		$\mathbf{D}_{1h}$	$\mathbf{C}_{1v}\mathbf{2}_1$	$\mathrm{pbm}2_1$	7	66		$\mathbf{S}_6$	$\mathbf{S}_6\boldsymbol{T}$	p$\bar{3}$	27
27		$\mathbf{D}_{1h}$	$\mathbf{D}_1\boldsymbol{T}_v$	pbb2	7	67		$\mathbf{D}_3$	$\mathbf{D}_3\boldsymbol{T}$	p312	26
28		$\mathbf{C}_{2v}$	$\mathbf{C}_2\boldsymbol{T}_v$	p2ma	8	68		$\mathbf{D}_3$	$\mathbf{D}_3\boldsymbol{T}$	p321	25
29		$\mathbf{D}_{1h}$	$\mathbf{D}_1\boldsymbol{T}_h$	pam2	9	69		$\mathbf{C}_{3v}$	$\mathbf{C}_{3v}\boldsymbol{T}$	p3m1	26
30		$\mathbf{D}_{1h}$	$2_1 T_h$	$\mathrm{pab}2_1$	9	70		$\mathbf{C}_{3v}$	$\mathbf{C}_{3v}\boldsymbol{T}$	p31m	25
31		$\mathbf{D}_{1h}$	$\mathbf{D}_1\boldsymbol{T}'_h$	pnb2	13	71		$\mathbf{D}_{3d}$	$\mathbf{D}_{3d}\boldsymbol{T}$	$\mathrm{p}31\frac{2}{m}$	28
32		$\mathbf{D}_{1h}$	$\mathbf{C}_{1v}\boldsymbol{T}'_h$	$\mathrm{p\ nm}2_1$	13	72		$\mathbf{D}_{3d}$	$\mathbf{D}_{3d}\boldsymbol{T}$	$\mathrm{p}3\frac{2}{m}1$	28
33		$\mathbf{C}_{2v}$	$\mathbf{C}_2\boldsymbol{T}'_v$	p2ba	15	73		$\mathbf{C}_6$	$\mathbf{C}_6\boldsymbol{T}$	p6	27
34		$\mathbf{C}_{2v}$	$\mathbf{C}_{2v}\boldsymbol{T}'$	c2mm	14	74		$\mathbf{C}_{3h}$	$\mathbf{C}_{3h}\boldsymbol{T}$	p6	24
35		$\mathbf{D}_{1h}$	$\mathbf{D}_{1h}\boldsymbol{T}'$	cmm2	13	75		$\mathbf{C}_{6h}$	$\mathbf{C}_{6h}\boldsymbol{T}$	p6/m	27
36		$\mathbf{D}_{1h}$	$\mathbf{D}_1\boldsymbol{T}'_h$	cam2	16	76		$\mathbf{D}_6$	$\mathbf{D}_6\boldsymbol{T}$	p622	28
37		$\mathbf{D}_{2h}$	$\mathbf{D}_{2h}\boldsymbol{T}$	$\mathrm{p}\frac{2}{m}\frac{2}{m}\frac{2}{m}$	6	77		$\mathbf{C}_{6v}$	$\mathbf{C}_{6v}\boldsymbol{T}$	p6mm	28
38		$\mathbf{D}_{2h}$	$\mathbf{D}_2\boldsymbol{T}_h$	$\mathrm{p}\frac{2}{a}\frac{2}{m}\frac{2}{a}$	11	78		$\mathbf{D}_{3h}$	$\mathbf{D}_{3h}\boldsymbol{T}$	p$\bar{6}$m2	26
39		$\mathbf{D}_{2h}$	$\mathbf{D}_2\boldsymbol{T}'_h$	$\mathrm{p}\frac{2}{n}\frac{2}{b}\frac{2}{a}$	17	79		$\mathbf{D}_{3h}$	$\mathbf{D}_{3h}\boldsymbol{T}$	p62m	25
40		$\mathbf{D}_{2h}$	$\mathbf{C}_{2h}\boldsymbol{T}_v$	$\mathrm{p}\frac{2}{m}\frac{2_1}{m}\frac{2}{a}$	8	80		$\mathbf{D}_{6h}$	$\mathbf{D}_{6h}\boldsymbol{T}$	$\mathrm{p}\frac{6}{m}\frac{2}{m}\frac{2}{m}$	28

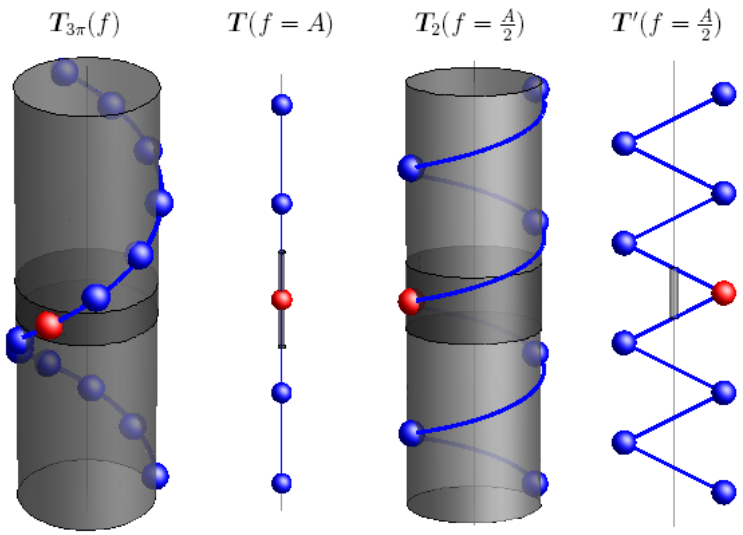

Figure 2.1: **Generalized translational groups:** *screw axis* $\boldsymbol{T}_Q(f)$, *pure translations* $\boldsymbol{T}(a)$, *achiral (zig-zag) screw axis* $\boldsymbol{T}_2(f)$, *and glide plane* $\boldsymbol{T}'$.

(*i.e.* $\boldsymbol{v} = v\boldsymbol{e}_z \neq 0$), with the orthogonal transformation R leaving the z-axis invariant. Such elements are $R(\phi)$, σ_v, σ_h and U. Irrespectively of v, the elements $(\sigma_h|v)$ and $(U|v)$ cannot generate infinite cyclic group (their square is the identity). Thus, the possible generators of the groups of the monomers arrangements are $(C_Q|f)$ and $(\sigma_v|f)$, where Q is real number not less than 1. Since $(\sigma_v|f)^2 = (I|2f)$ is pure translation, in the second case there is translation period $a = 2f$. In the first case, only if Q is rational number, there is a pure translation: if $Q = q/r$, with r being nonnegative integer, less than q and coprime with q, than $(C_q^r|f)^q = (I|qf)$; otherwise, systems are called *incommensurate* or *modulated*. To summarize, $(C_Q|f)$ and $(\sigma_v|f)$ generate the groups of the *generalized translations*, Z: *screw axes* $\boldsymbol{T}_Q$ (infinite family of the groups generated by $(C_Q|f)$) and *glide plane*, $\boldsymbol{T}'$ (generated by $(\sigma_v|\frac{1}{2})$); pure translational group, $\boldsymbol{T}$, is a special case of screw axis with $Q = 1$ (Fig. 2.1).

Note that some elements of the full symmetry group P' of monomer may not leave z-axis invariant. Nevertheless, such elements are discarded when L is constructed, *i.e.* P is the maximal axial subgroup of P': $P = P' \cap \boldsymbol{D}_{\infty h}$.

Since each symmetry of the polymer is composed of the elements of the subgroups Z and P, the whole group is the product $L = ZP$, implying the equality $ZP = PZ$ (weak direct product, § A.1.5). Test of this condition for each generalized translational group ($Z = \boldsymbol{T}_Q, \boldsymbol{T}'$) and each axial point group ($P = \boldsymbol{C}_n, \boldsymbol{S}_{2n}, \boldsymbol{C}_{nv}, \boldsymbol{C}_{nh}, \boldsymbol{D}_n, \boldsymbol{D}_{nd}, \boldsymbol{D}_{nh}$) gives all the line groups in the factorized form. Encountering that some of the obtained products are different factorizations of the same group, all of the 13 infinite families of the line groups are found (Table 2.3).

As well as for the space and diperiodic groups, when exists, translational subgroup is invariant in the line group, and corresponding factor group is isomorphic to the isogonal group, P_I, obtained when the translational parts of the line group transformations are neglected. The

Table 2.3: **Line groups.** *For each family of the line groups the international symbol, different factorizations, generators, the subgroup $\boldsymbol{L}^{(1)}$ and the isogonal point group $\boldsymbol{P}_I$, are given. Here, $\boldsymbol{T}_{cd}$ and U' are the glide plane and horizontal axis bisecting vertical mirror planes of $\boldsymbol{P}$. For the groups of the families 1 and 5, q is a multiple of n (instead of r the helicity in the international symbol is given by its modular inverse $p = n(r^{-1}|q/n|)$). For the first and fifth family, when Q is irrational, the isogonal groups are $\boldsymbol{C}_\infty$ and $\boldsymbol{D}_\infty$, respectively.*

	International symbol		Factorizations	Generators	$\boldsymbol{L}^{(1)}$	$\boldsymbol{P}_I$
	n even	n odd				
1	$\boldsymbol{L}q_p$		$\boldsymbol{T}_Q \otimes \boldsymbol{C}_n$	z_q^r, C_n	$\boldsymbol{T}_Q \otimes \boldsymbol{C}_n$	$\boldsymbol{C}_q$
2	$\boldsymbol{L}(\overline{2n})$	$\boldsymbol{L}\overline{n}$	$\boldsymbol{T} \wedge \boldsymbol{S}_{2n}$	$z_0, C_{2n}\sigma_h$	$\boldsymbol{T} \otimes \boldsymbol{C}_n$	$\boldsymbol{S}_{2n}$
3	$\boldsymbol{L}(\overline{2n})$	$\boldsymbol{L}n/m$	$\boldsymbol{T} \wedge \boldsymbol{C}_{nh}$	z_0, C_n, σ_h	$\boldsymbol{T} \otimes \boldsymbol{C}_n$	$\boldsymbol{C}_{nh}$
4	$\boldsymbol{L}(2n)_n/m$		$\boldsymbol{T}_{2n}\boldsymbol{C}_{nh} = \boldsymbol{T}_{2n}\boldsymbol{S}_{2n}$	z_{2n}^1, C_n, σ_h	$\boldsymbol{T}_{2n}\boldsymbol{C}_n$	$\boldsymbol{C}_{2nh}$
5	$\boldsymbol{L}q_p22$	$\boldsymbol{L}q_p2$	$\boldsymbol{T}_Q \wedge \boldsymbol{D}_n$	z_q^r, C_n, U	$\boldsymbol{T}_Q \otimes \boldsymbol{C}_n$	$\boldsymbol{D}_q$
6	$\boldsymbol{L}nmm$	$\boldsymbol{L}nm$	$\boldsymbol{T} \otimes \boldsymbol{C}_{nv} = \boldsymbol{C}_{nv} \wedge \boldsymbol{T}_{cd}$	z_0, C_n, σ_v	$\boldsymbol{T} \otimes \boldsymbol{C}_n$	$\boldsymbol{C}_{nv}$
7	$\boldsymbol{L}ncc$	$\boldsymbol{L}nc$	$\boldsymbol{C}_n \wedge \boldsymbol{T}_c$	z_v, C_n	$\boldsymbol{T} \otimes \boldsymbol{C}_n$	$\boldsymbol{C}_{nv}$
8	$\boldsymbol{L}(2n)_nmc$		$\boldsymbol{C}_{nv} \wedge \boldsymbol{T}_{2n} = \boldsymbol{C}_{nv} \wedge \boldsymbol{T}_{cd}$	z_{2n}^1, C_n, σ_v	$\boldsymbol{T}_{2n} \otimes \boldsymbol{C}_n$	$\boldsymbol{C}_{2nv}$
9	$\boldsymbol{L}(\overline{2n})2m$	$\boldsymbol{L}\overline{n}m$	$\boldsymbol{T} \wedge \boldsymbol{D}_{nd} = \boldsymbol{T}_c \wedge \boldsymbol{D}_{nd}$	z_0, C_n, U', σ_v	$\boldsymbol{T} \otimes \boldsymbol{C}_n$	$\boldsymbol{D}_{nd}$
10	$\boldsymbol{L}(\overline{2n})2c$	$\boldsymbol{L}\overline{n}c$	$\boldsymbol{T}_c\boldsymbol{S}_{2n} = \boldsymbol{T}_{cd}\boldsymbol{D}_n$	z_v, C_n, U'	$\boldsymbol{T} \otimes \boldsymbol{C}_n$	$\boldsymbol{D}_{nd}$
11	$\boldsymbol{L}n/mmm$	$\boldsymbol{L}(\overline{2n})2m$	$\boldsymbol{T} \wedge \boldsymbol{D}_{nh} = \boldsymbol{T}_c\boldsymbol{D}_{nh}$	z_0, C_n, U, σ_v	$\boldsymbol{T} \otimes \boldsymbol{C}_n$	$\boldsymbol{D}_{nh}$
12	$\boldsymbol{L}n/mcc$	$\boldsymbol{L}(\overline{2n})2c$	$\boldsymbol{T}_c\boldsymbol{C}_{nh} = \boldsymbol{T}_c\boldsymbol{D}_n$	z_v, C_n, U	$\boldsymbol{T} \otimes \boldsymbol{C}_n$	$\boldsymbol{D}_{nh}$
13	$\boldsymbol{L}(2n)_n/mcm$		$\boldsymbol{T}_{2n}\boldsymbol{D}_{nh}=\boldsymbol{T}_{2n}\boldsymbol{D}_{nd}$ $=\boldsymbol{T}_c\boldsymbol{D}_{nh}=\boldsymbol{T}_c\boldsymbol{D}_{nd}$	$z_{2n}^1, C_n, U, \sigma_v$	$\boldsymbol{T}_{2n} \otimes \boldsymbol{C}_n$	$\boldsymbol{D}_{2nh}$

families 2, 3, 6, 9, 11 are symorphic, as well as the families 1 and 5 for $Q = 1$.

Irreducible representations of the commensurate line groups can be obtained by the method described for the space groups. Nevertheless, the specific structure of the line groups allows significantly simpler procedure, applicable to the incommensurate ones, too. The groups of the first family are direct products of cyclic groups, and their (one dimensional) irreducible representations are easily calculated. The groups of the families 2-8 have halving subgroups from the family 1, while themselves are halving subgroups of the groups in the remaining families. Thus, the method of the induction from the halving subgroup can be completely performed to find the irreducible representations of the line groups.

These are characterized by the quantum number of helical quasi momentum $\tilde{k}$, related to the screw-axis subgroup; it takes values from the helical Brillouin's zone (one dimensional interval $(-\pi/f, \pi/f]$ in this case). When there is translational subgroup (Q rational and glide plane), usual quasi momentum k can be used, with values from the linear Brillouin's zone $(-\pi/a, \pi/a]$. Additional labels originate from the point group (z component of the angular momentum, different parities). Corresponding selection rules manifest conservation of quasi momenta and parities. From the described procedure it is clear that possible dimensions of the irreducible representations are 1, 2 and 4.

2.6 Magnetic symmetries

The frequent symmetry of the systems and the corresponding equations, the time reversal, due to its physical contents, slightly differs with respect to the previously studied symmetries, and requires different treatment within quantum mechanical formalism.

2.6.1 Time reversal

The Wigner's theorem (§ B.2) restricts the quantum mechanical operators associated to the symmetries onto the unitary and antiunitary, [5, 18]. The most important antiunitary represented operation is the *time reversal*, θ. Indeed, if θ is symmetry of the system, then the operator Θ, representing θ, commutes with H. On the other hand, for arbitrary state $|\, x,t\rangle$ obviously holds $\Theta \mid x,t\rangle = U(-t)\Theta \mid x,0\rangle$, implying the relation $\Theta U(t) = U(-t)\Theta$, *i.e.* $\Theta \mathrm{e}^{\frac{\mathrm{i}}{\hbar}Ht} = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht}\Theta$. This is compatible with assumed $[\Theta, H] = 0$ only if Θ is antiunitary[5]. It is obvious that θ leaves the coordinates invariant, $\Theta \boldsymbol{q} \Theta^\dagger = \boldsymbol{q}$, and commutes with the geometrical transformations, $\Theta D(R|\boldsymbol{a})\Theta^\dagger = D(R|\boldsymbol{a})$. Only the antiunitarity of Θ makes this property compatible to the obvious change of sign of the momentum and the angular momentum (generating the translations and the rotations): $\Theta \boldsymbol{p} \Theta^{-1} = -\boldsymbol{p}$ i $\Theta \boldsymbol{l} \Theta^{-1} = -\boldsymbol{l}$.

Another important property of the time reversal is that it is involutive transformation, $\theta^2 = e$; thus, Θ^2 does not change the physical state of the system, *i.e.* each ray in the state space must be invariant for it, and this is accomplished only by $\Theta^2 = cI$, with $c = \pm 1$, for antiunitary Θ (in fact, $|c| = 1$ since Θ^2 is unitary, and $\Theta^2\Theta^\dagger = \Theta = \Theta^\dagger\Theta^2$, gives $c = c^*$, since $U^\dagger$ is antiunitary and nonsingular). If $\Theta^2 = I$, there is basis in $\mathcal{S}$ with real vectors, meaning that they satisfy conditions $\Theta\,|i\rangle = |i\rangle$ (for any vector $|x\rangle$, the vector $|x\rangle + \Theta\,|x\rangle$ is real). The operator Θ acts as the complex conjugation of the columns representing the vectors in this basis, while the real matrices represent in this basis the linear operators commuting with Θ. In the second case, $\Theta^2 = -1$, no such basis exists, but each vector $|\, x\rangle$ is orthogonal to the conjugated vector $\Theta \,|\, x\rangle$[6]; therefore in each invariant subspace of Θ, there is basis consisted of the pairs of the orthogonal conjugated vectors. Obviously, the dimension of such subspace is even; in the basis $\{|\, x_1\rangle, \ldots, |\, x_n\rangle, \Theta \mid x_1\rangle, \ldots, \Theta \mid x_n\rangle\}$, the linear operator commuting with Θ are represented by the matrix of the form $\begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}$ (a and b are n-dimensional submatrices). Consequently, the operator Θ can be factorized as $\Theta = TK$, where T is unitary operator, and K is the antiunitary operator of the complex conjugation of the columns in some basis; from $\Theta^2 = \pm I$ and $K^2 = I$ it follows that, in the basis in which K is the complex conjugation, the matrix representing T satisfies $TT^* = \pm I$.

If G is group of the geometrical transformation (or some other transformations commuting with θ), and $D(G)$ its linear irreducible representation in $\mathcal{S}$, the properties of $D(G)$ partly

[5] The attempt to treat Θ as unitary operator, implies that this operator anticommute with the hamiltonian; consequently, the eigen energies would appear in the pairs of the opposite signs, contradicting both to the existence of the lower bound to the energy and to the independence of the energy on the signs of the velocities.

[6] Antiunitary operators satisfy $(\Theta x, \Theta y) = (x,y)^*$ for all x and y. Thus: $(x, \Theta x) = (\Theta x, \Theta^2 x)^* = (\Theta x, -x)^* = -(x, \Theta x) = 0$.

determine the representation of θ, [12], since the representative operators also commute, $D(g) = \Theta D(g)\Theta^\dagger = TD^*(g)T^\dagger$. Schur's lemas (§ A.2.2) immediately give $T = 0$ for the representations of the III type (§ A.3). If $D(G)$ is a representation of the I kind, there is a basis such that $D(G)$ is real, i.e. $D(g) = \Theta D(g)\Theta^\dagger = TD(g)T^\dagger$, yielding $T = \mathrm{e}^{\mathrm{i}\phi} I$ and $TT^* = I$. Also, if $TT^* = I$, the representation $R(g) = (T + \mathrm{e}^{\mathrm{i}\alpha} I)^{-1} D(g)(T + \mathrm{e}^{\mathrm{i}\alpha} I)$ (for any α such that $T + \mathrm{e}^{\mathrm{i}\alpha} I$ is nonsingular) is equivalent to $D(g)$ and real (since $R^*(g) = (T + \mathrm{e}^{\mathrm{i}\alpha} I)^{-1*}(T^* D(g) T)(T + \mathrm{e}^{\mathrm{i}\alpha} I)^*$. Therefore, it becomes clear that the case $TT^* = -I$ corresponds to the representations of the II kind, when $\Theta^2 = TT^*$ (but not T) commutes with $D(G)$ and satisfies the Schur's lema. It follows that the irreducible subspaces of the representations of the second kind of any group are even dimensional, with the time reversal operator characterized by $\Theta^2 = -I$.

Let $D(G)$ be reducible real representation, and $\mathcal{S}'$ its subspace carrying real irreducible representation $D'(G)$. For $D'(G)$ of the I kind, this subspace is irreducible, while for the representations of the II and III it can be decomposed onto the pair of the irreducible subspaces, $\mathcal{S}^{(\mu)}$ and $\mathcal{S}^{(\mu)*}$ (of the same dimensions). In the latter case, there is basis in $\mathcal{S}'$, such that the representative matrices of $D'(G)$ are block-diagonal: $D'(g) = \begin{pmatrix} D^{(\mu)}(g) & 0 \\ 0 & D^{(\mu)*}(g) \end{pmatrix}$. With $T' = \begin{pmatrix} 0 & \mathrm{e}^{\mathrm{i}\varphi} I_\mu \\ \mathrm{e}^{\mathrm{i}\varphi} I_\mu & 0 \end{pmatrix}$, the operator $\Theta' = T' K_0$ commutes with $D'(G)$, while its square is $\Theta^2 = I'$. It is shown above that these conditions are fulfilled also for the representations of the I kind, and consequently the direct sum $\oplus\Theta'$ is also the involutive operator commuting with $D(G)$: if $D(G)$ is real representation, time reversal can be represented by the antiunitary involution. The condition that $D(G)$ and H commute, provides the reduction of H into the irreducible subspaces. Therefore, for the representations of the I kind, the reduced operator H' in $\mathcal{S}'$ can be represented by real matrix, with real eigen vectors; for the representations of the II and III kind, in the basis in which $D'(G)$ is decomposed (to the pair of the conjugated irreducible representations), the reduced operator takes the form $H' = \begin{pmatrix} H_\mu & 0 \\ 0 & H_\mu^* \end{pmatrix}$ (since H and $D(G)$ commute the matrix is block diagonal, and the blocks are conjugated because H and commutes with Θ).

The representation of rotational group in the orbital space is decomposed to the integer irreducible components, being of the I kind (real); furthermore, although the components (except the identical one) of the representation of the translational group are of the III kind, they appear in the complex conjugated pairs. Therefore, in the orbital space time reversal is represented by the involutive operator, and in the appropriate basis it can be identified with the operator of the complex conjugation of columns. On the contrary, in the spin space of the halfinteger spin, the corresponding representation of the group SU(2) is half integer, and of the II kind. In the eigenbasis of the third component of spin, S_z, the condition $\Theta \boldsymbol{S} \Theta^\dagger = \boldsymbol{S}$ implies $\Theta = \mathrm{e}^{\mathrm{i}\pi S_y} K$ (for the integer spin, $(\mathrm{e}^{\mathrm{i}\pi S_y} K)^2 = 1$ and the same definition is retained). Therefore, for the system invariant under the time reversal, with the halfinteger spin, the invariant subspaces for Θ, including the eigenspaces of the hamiltonian, are even dimensional. This property is known as the *Kramers's degeneracy*, [28]. It should be noted

that the condition $\Theta^2 = -I$ coincides to the fact that within halfinteger representations to the rotation for 2π (this is identical transformation, as well as θ^2 is) two operators are associated, I and sa $-I$; in fact, the underlying requirement of the compatibility with the universal covering group (with doubly covered rotations) makes this type of the representing of the time reversal necessary.

2.6.2 Magnetic groups

Magnetic groups are the groups containing the elements which combine the geometrical transformations and the time reversal, [21, 12]. Since θ is involution commuting with the geometrical symmetries, each magnetic group, M, contains the halving subgroup G of the pure spatial symmetries. Two cases are possible: if θ is symmetry of the system (*e.g.* there is no magnetic field in the hamiltonian, and the potential is time independent), then $M = G \otimes \{e, \theta\} = G + \theta G$; on the contrary, when θ is not symmetry itself, but there is spatial transformation s, such that system is invariant under θs, then $M = G + \theta s G$ (of course, $s \notin G$ since then θ is symmetry of the system). The first type is called the *magnetic gray group*, and the other one is the *magnetic black and white group*. The black and white group is isomorphic to the group $G + sG$, of the spatial transformations. Hence, for each geometrical group, G, the family of the magnetic group is formed, containing one gray group, $G1' = G \otimes \{e, \theta\}$, and one black and white group, $G(H) = H + \theta s H$ for each halving subgroup, H, in G (all the groups $G(H)$ are isomorphic to G).

Due to the special properties of the time reversal, the magnetic groups are represented by the corepresentations, (§ A.3): the coset containing θs ($s = e$ for the gray groups) is represented by the antiunitary operator. Irreducible corepresentations define symmetry based properties of the vectors and the operators, and their dimension determines the degeneracy of the eigen subspaces of the hamiltonian. The method used for the unitary representations to obtain the standard tensors, and possible properties of the physical systems of the given symmetry, can be applied analogously to the magnetic groups and their corepresentations. Especially when the spin systems are considered, the time reversal becomes nontrivial operation, which is used in the classification of the possible ferro- or antiferromagnetic orders. In the construction of the irreducible corepresentations by the $*$-induction method, the irreducible representations of the spatial part of the magnetic group are used; those of the II and III kind give the corepresentations of the doubled dimension (this enables the uniqueness of the representing of the elements). Restricting to the spatial symmetries, the additional degeneracy of the eigen energies seems to be accidental.

The magnetic groups and their corepresentations are derived for most of the geometrical groups. There are 24 infinite families of the axial point groups (7 of them are families of the gray groups) and 11 (5) magnetic groups related to the spatial groups $\boldsymbol{T}$, $\boldsymbol{T}_d$, $\boldsymbol{T}_h$, $\boldsymbol{O}$ and $\boldsymbol{O}_h$, [21]. Among them there are 90 (32) magnetic crystallographic point groups, enumerating the magnetic crystallographic classes for 1421 (230 gray) magnetic space groups, [23]. Similarly, there are 68 (13) infinite families of the magnetic line groups, [25].

2.7 Spin groups

After classification of the magnetic groups it became clear that there were magnetic systems with spin arrangements which did not match any of the magnetic groups, i.e. that these groups are insufficient to describe the complete variety of the magnetic orderings in the real compounds. This refers to the conical helimagnets (observed in the fifties of the 20th century), and in particular to incommensurate spin order (which does not match the periodicity of the lattice). Therefore need for an extension of the magnetic groups was obvious, and this inspired several attempts, which finally resulted by the spin groups. During the past decade many of the nanosystems, having quasi one-dimensional spin subsystems [**?**] have the described peculiar properties, which reinforced interest for these groups.

At first, note that here spin (magnetic moment) of an atom is a vector $\boldsymbol{s}$ (of the expected values of the spin observables S_i, $i = x, y, z$) in the spin space which is the three dimensional real space (in the theory of magnetism this is usually called classical approximation). Consequently, geometrical transformations of symmetry in this space are represented by real (thus orthogonal) matrices. More precisely, if atomic system consists of the atoms positioned at $\boldsymbol{x}_i$, then the corresponding spin arrangement is given by a spin field over atoms, i.e. by the pairs $(\boldsymbol{x}_i, \boldsymbol{s}_i)$ for each atom (this includes also magnetically inactive atoms, for which $\boldsymbol{s}_i = 0$). Then, if the symmetry transformation g maps an atom from $\boldsymbol{x}$ to $g\boldsymbol{x}$, the corresponding spins are $\boldsymbol{s}(\boldsymbol{x})$ and $\boldsymbol{s}(g\boldsymbol{x})$. Thus, for consistent symmetry based description of the spin field transformations, it is necessary that transformations of the spins correspond to the geometrical transformations, i.e. that $\boldsymbol{s}(g\boldsymbol{x}) = D^{\mathrm{sp}}(g)\boldsymbol{s}(\boldsymbol{x})$, where D^{sp} is the mentioned three dimensional orthogonal representation of the symmetry group, called *spin representation*, i.e. homomorphism of G into O(3).

As a result, explicating the fact that spin space is independent on the atomic space, the spin arrangement is described by the pairs $(\boldsymbol{x}_i, \boldsymbol{s}_i)$, and the action of the symmetry group on the pairs is defined by

$$(g, D^{\mathrm{sp}}(g))(\boldsymbol{x}, \boldsymbol{s}) \stackrel{\mathrm{def}}{=} (g\boldsymbol{x}, D^{\mathrm{sp}}(g)\boldsymbol{s}). \tag{2.6}$$

The set of pairs $G_{D^{\mathrm{sp}}} = \{(g, D^{\mathrm{sp}}(g)) \,|\, g \in G\}$ is a group with respect to the multiplication $(g, D^{\mathrm{sp}}(g))(g', D^{\mathrm{sp}}(g')) = (gg', D^{\mathrm{sp}}(g)D^{\mathrm{sp}}(g'))$. Since D^{sp} is representation of the symmetry group G, the group $G_{D^{\mathrm{sp}}}$, called *spin group* is obviously isomorphic to G.

Note that each spin representation generates one spin group. Thus the problem of classification of the spin groups reduces to the classification of the nonequivalent spin representations. This problem can be solved using the irreducible representations of G. In fact, one should find all possible combinations of the irreducible representations of G, which as a direct sum give a three-dimensional real representation of G. Recall that there are three types of the irreducible representations $d(G)$: real ones, those which are equivalent to the conjugated but without equivalent real representation, and complex representations. In the last two cases, instead of $d(G)$, real form is achieved with the representation $d(G) + d^*(G)$ of the doubled dimension. Thus, one concludes that irreducible components of D^{sp} may be of the dimension 1, 2 or 3 for real type, and only 1 for the other two types. Having this in mind, all

possible combinations can be systematically find, and all nonequivalent spin groups derived. Of course, for one spin representation, their equivalent forms $RD^{\rm sp}R^T$ for $R \in$SO(3) may be realized. The spin groups are found for point, space [**?**] and and line groups.

In general, magnetic system consists of several orbits. Then, the symmetry group independently acts on each of the orbits, and the definition (2.6) should be generalized. In fact, let the coordinates of the symcell be $\boldsymbol{X}_0 = (\boldsymbol{x}_{10}, \dots, \boldsymbol{x}_{n0})$, where $\boldsymbol{x}_{i0}$ is position of the i-th orbit representative. Accordingly, $\boldsymbol{S}_0 = (\boldsymbol{s}_{10}, \dots, \boldsymbol{s}_{n0})$ is spin of the symcell, being vector in the space $\mathbb{R}^{3n}$. Than the group action on the spins is independently described for each orbit by its spin representation $D^{\rm sp}_i$, giving:

$$(g, D^{\rm sp}(g))(\boldsymbol{X}_0, \boldsymbol{S}_0) \stackrel{\rm def}{=} (g\boldsymbol{x}_{10}, \dots, g\boldsymbol{x}_{n0}; D^{\rm sp}_1\boldsymbol{s}_{10}, \dots, D^{\rm sp}_N\boldsymbol{s}_{n0}). \tag{2.7}$$

It becomes clear that the total spin representation is direct sum of the orbital ones:

$$D^{\rm sp} = D^{\rm sp}_1 \oplus \dots \oplus D^{\rm sp}_n. \tag{2.8}$$

Spin groups are successfully used in the description of the spin arrangements. Namely, to this end it is necessary to give spins in the symcell atoms, and then the spin group distribute them over the whole system. This can be utilized also in the prediction of the possible spin arrangements. For this purpose classification of the orbits of the group is needed together with stabilizers of orbit representatives, as well as all single orbital spin representations. Then, for each orbit, independently all allowed spin representations should be applied to all allowed spins of the orbit representative. Precisely, for each element g of the stabilizer $G_{\boldsymbol{x}}$ of the orbit representative at $\boldsymbol{x}$, the fixed point condition

$$D^{\rm sp}(g)\boldsymbol{s}(\boldsymbol{x}) = \boldsymbol{s}(\boldsymbol{x}) \tag{2.9}$$

provides uniqueness of the spin vector. If such *allowed* vector $\boldsymbol{s}(\boldsymbol{x})$ exists, the spin representation is *allowed* itself. In particular, ferromagnetic order appears when allowed vector is fixed point (i.e. obeys (2.9)) for each element of the group G; for antiferromagnetic order one has $D^{\rm sp}(g)\boldsymbol{s}(\boldsymbol{x}) = \pm\boldsymbol{s}(\boldsymbol{x})$ for all symmetries of the system.

Finally, note that ordinary magnetic group correspond to the spin group with axial vector representation as $D^{\rm sp}$, while to obtain black-and-white magnetic group the elements of the subgroup H are represented by $D^{\rm sp}(h) = D^{\rm av}(h)$, and those from the coset sH by $D^{\rm sp}(sh) = -D^{\rm av}(sh)$. Obviously, the matrix $-I_3$ takes the role of the time reversal Θ; in fact, the time reversal was introduced because there is no geometrical transformation reversing all axial vectors.

2.8 Double groups

The well known physical arguments justify that the systems with the half-integer spin are related to half-integer representations of the group SU(2). Therefore, when such systems are studied, SU(2) is unavoidably used instead of the rotational group. This must be taken

into account when the spin systems with discrete spatial symmetries are considered, and two-valued representations (due to rotational symmetries) of the symmetry group naturally appear. They can be found by the procedure neatly following the one used to find such representation of the rotational group (§ 2.1.2). In fact, the double (covering) group is found firstly, and then its (ordinary) representations. Some of them are two-valued and the others ordinary representations of the initial symmetry group [3, 8].

If $P_+ < \mathrm{SO}(3,\mathbb{R})$ is a point group containing rotations only ($\boldsymbol{C}_n$, $\boldsymbol{D}_n$, $\boldsymbol{T}$, $\boldsymbol{O}$ or $\boldsymbol{Y}$; including n infinite), then $\tilde{P}_+ \stackrel{\text{def}}{=} h^{-1}(P_+)$ of SU(2) corresponds to P_+ by the homomorphism (2.4). However, besides identity I_2, $h^{-1}(e)$ contains $\tilde{e} = -I_2$, commuting with all other elements of $\tilde{P}_+$, and each rotation $C = R(\alpha, \boldsymbol{a})$ in P_+ corresponds to spin-rotations $\tilde{C} = U(\alpha, \boldsymbol{a})$ and $\tilde{e}\tilde{C} = -U(\alpha, \boldsymbol{a})$ in $\tilde{P}_+$. The easiest way to find the group structure of the rotational double point groups is to find spin rotations (2.3b) for the generators by the same Euler angles as for ordinary rotations. For example, $\boldsymbol{C}_n$ structure is determined by the generator $C_n = R(2\pi/n, \boldsymbol{e}_z)$ satisfying condition $C_n^n = R(2\pi, \boldsymbol{e}_z) = e$; the corresponding spin rotation $\tilde{C}_n = U(2\pi/n, \boldsymbol{e}_z)$ of $\tilde{\boldsymbol{C}}_n$ is of order $2n$, as $\tilde{\boldsymbol{C}}_n^n = U(2\pi, \boldsymbol{e}_z) = \tilde{e}$, and only squared gives $\tilde{\boldsymbol{C}}_n^{2n} = (4\pi, \boldsymbol{e}_z) = e$, making $\tilde{\boldsymbol{C}}_n$ algebraically isomorphic to $\boldsymbol{C}_{2n}$. Similarly, for $\boldsymbol{D}_n$, the generators C_n and $U = R(\pi, \boldsymbol{e}_x)$ satisfy $C_n^n = U^2 = (C_n U)^2 = e$ ($C^n U = R(\pi, \boldsymbol{b})$, with $\boldsymbol{b} = R(\pi/n, \boldsymbol{e})\boldsymbol{a}$); automatically, $\tilde{C}_n^n = \tilde{U}^2 = \tilde{e}$, thus $\tilde{U}$ is of order four, and the intersection of the two cyclic subgroups generated by $\tilde{C}_n$ and by $\tilde{U}$ is $\{e, \tilde{e}\}$. Consequently, double group is $\tilde{\boldsymbol{D}}_n = \tilde{C}_n + \tilde{U}\tilde{C}_n$, with $(\tilde{C}_n\tilde{U})^2 = \tilde{e}$ (as the direct check gives; this enables standard construction of the irreducible representations), but not a semidirect product as $\boldsymbol{D}_n$.

For other point groups, P_-, the double groups are constructed from the double groups of the rotational subgroup, which is halving subgroup in P_-. Precisely, each such group has rotational subgroup P_+ of index two, and the coset consisted of the rotations multiplied by spatial inversion P. There are only two structural possibilities: either $P_- = P_+ + PRP_+$ (for some rotation R out of P_+) or $P_- = P_+ + PP_+ = P_+ \otimes \{e, P\}$. In the first case $P' = P_+ + RP_+ \cong P_-$ is subgroup in $\mathrm{SO}(3,\mathbb{R})$, and $\tilde{P}_-$ is isomorphic to $\tilde{P}' = \tilde{P}_+ + \tilde{R}\tilde{P}_+$ with the same irreducible representations (as a reminder to geometric source, it is convenient to retain symbol $P\tilde{R}$ in the algebraic structure $\tilde{P}_- = \tilde{P}_+ + P\tilde{R}\tilde{P}_+$). In the second case $\tilde{P}_-$ is isomorphic to the direct product of $\tilde{P}_+ \otimes \{e, P\}$. Thus, in all the cases the relation between the group and its rotational (sub)group, is completely preserved at the level of double groups. After construction of the double groups, their irreducible (ordinary) representations are constructed by the standard methods.

The two valued representations and the double groups of the other geometrical symmetries can be found using the structure of the relevant groups: the isogonal point groups are substituted by their double groups (recall that the necessity for double group construction stems from the nontrivial topology of the rotational group; translations and spatial inversion, when involved, obviously do not contribute to complexity of the total topology), and then to $(R\,|\,\boldsymbol{x})$ the elements $(\tilde{R}\,|\,\boldsymbol{x})$ and $(\tilde{e}R\,|\,\boldsymbol{x})$ are associated. Finally, when the time reversal is involved for the systems with half integral spin, the double magnetic and spin groups must be considered.

At the moment in the literature are available double crystallographic point groups, double spatial groups and magnetic groups of these two. For all of them irreducible representations (corepresentations) are also found.

2.9 Identical particles: permutations

Due to the intuitively obvious fact that the permutation of the identical particles can cause no observable effect, the symmetrical group S_N must be included in the symmetry analysis of the system with N identical particles. Straightforward and simple application of group theory in this case gives one of the most beautiful illustrations of the essential importance of the symmetry in physics.

The order of the group S_N is $N!$, and each of its elements — permutations — is the composition of a number of the transpositions, the most simple permutation of two particles. Therefore, there is the index-two subgroup A_N of all even permutations (composed of even number of the transpositions), and the corresponding coset decomposition is $S_N = A_N + \tau A_N$ (τ is any transposition, or another odd permutation). Consequently, for each N there is one-dimensional (thus irreducible) *alternative* representation of S_N: $A^-(\pi) \stackrel{\text{def}}{=} (-1)^\pi$ (as it is usual, the same symbol, π, is used for the permutation and its parity). Additionally, there is the important fact in the theory of the symmetric groups, that the identical, $A^+(S_N)$ (given by $A^+(\pi) \stackrel{\text{def}}{=} 1$), and the alternative, $A^-(S_N)$, representations are the only one-dimensional representations of S_N.

If $\mathcal{S}$ is the state space of one particle, and $\{|\,1\rangle, \ldots, |\,n\rangle\}$, is its basis, then the principles of quantum mechanics a priory prescribe that the state space of the system of N particles is $\mathcal{S}^N = \underbrace{\mathcal{S} \otimes \cdot \otimes \mathcal{S}}_{N}$. In the basis

$$|\,i_1, \ldots, i_N\rangle \stackrel{\text{def}}{=} |\,i_1\rangle_1 \otimes \cdots \otimes |\,i_N\rangle_N,\ i_1, \ldots, i_n = 1, \ldots, n, \tag{2.10}$$

the permutation π of the particles is manifested as the permutation of their states, defining the representative operator $D(\pi)\ |i_1, \ldots, i_N\rangle = |i_{\pi 1}, \ldots, i_{\pi N}\rangle$. This representation of S_N is not irreducible, since there are at least two invariant subspaces: the symmetrical, $\mathcal{S}^N_+$, and antisymmetrical, $\mathcal{S}^N_-$, subspaces are multiple irreducible subspaces of the representations $A^\pm(S_N)$, determined by the corresponding group projectors, called *symmetrizer* and *antisymmetrizer*, $P^\pm = \frac{1}{N!}\sum_\pi (\pm)^\pi D(\pi)$. Requirement that the action of the permutation is not observable, means that the physically relevant states are transformed according to the one-dimensional representations of S_N, *i.e.* that these states are from the subspaces $\mathcal{S}^N_\pm$. Moreover, if $|\,+\rangle$ is from $\mathcal{S}^N_+$, while $|\,-\rangle$ is from $\mathcal{S}^N_-$, the transposition τ maps $|\,x\rangle = \alpha\ |\,+\rangle + \beta\ |\,-\rangle$ to vector which is not proportional to $|\,x\rangle$, which points out the observable difference of the two vectors. Consequently, the superposition of the states of the different parity is forbidden, and the physically relevant part of the space $\mathcal{S}^N$ is either $\mathcal{S}^N_+$ or $\mathcal{S}^N_-$, only. Bosons are particles described within symmetric subspace, and fermions are related to the antisymmetric

one. Within the relativistic quantum theory, the locality condition (§ 2) determines that the spin of the bosons is integral, while the spin of the fermions must be half-integral, [29]. Note that the permutational symmetry is, in contrast to the previously studied space-time symmetries, given as the group of symmetry of state, and this caused the restriction of the a priory state space $\mathcal{S}^N$, by the so called *superselection* of a subspace. Consequently, the physically meaningful operators, *i.e.* those representing physical quantities, must reduce in the relevant subspace, which immediately shows that these operators are invariants of the group S_N, that is they must commute with the operators representing permutations.

A number of important results can be derived using the (anti)symmetrizers. Each vector $|\ x\rangle = |\ i_1, \ldots, i_N\rangle$ of the basis (2.10) defines n-tuple of the *occupation numbers* $\boldsymbol{p}(x) = (p_1(x), \ldots, p_n(x))$: $p_k(x)$ is the number of appearance of the state $|\ k\rangle$ among the single-particle states $|\,i_1\rangle, \ldots, |\,i_N\rangle$ forming $|\,x\rangle$; obviously, $p_k(x) \geq 0$ and $\sum_{k=0}^{n} p_k(x) = N$.

Definition of $D(\pi)$ shows that this operator maps $|\,x\rangle$ into a state with the same occupation numbers. Consequently, the matrix element $D_{xx'}(\pi)$ vanishes if $\boldsymbol{p}(x) \neq \boldsymbol{p}(x')$, and the same holds for the matrix elements of (anti)symmetrizer. But this matrix element is the scalar product of the states obtained by the (anti)symmetrization of the non-correlated basis vectors $|\,x\rangle$ and $|\,x'\rangle$: $\langle x\,|\,P^{\pm}P^{\pm}\,|\,x'\rangle = \langle x\,|\,P^{\pm}\,|\,x'\rangle$. Therefore, the (anti)symmetrized vectors with different occupation numbers are mutually orthogonal.

On the other hand, if $\boldsymbol{p}(x) = \boldsymbol{p}(x')$, there is a permutation ρ such that $D(\rho)\,|\,x\rangle = |\,x'\rangle$. Thus, the projections satisfy

$$P^{\pm}\,|\,x'\rangle = \frac{1}{N!}\sum_{\pi}(\pm)^{\pi}D(\pi\rho)\,|\,x\rangle = (\pm)^{\rho}P^{\pm}\,|\,x\rangle, \tag{2.11}$$

i.e. the (anti)symmetrization of any vector of the basis (2.10) with given occupation numbers gives the same vector (up to the sign for the fermions). The previous result, concerning the orthogonality of such states, shows that the spaces $\mathcal{S}^N_{\pm}$ can be obtained as follows: for each possible choice of the occupation numbers, $\boldsymbol{p}$, choose from the basis (2.10) arbitrary vector $|\,x\rangle$ with $\boldsymbol{p}(x) = \boldsymbol{p}$, and (anti)symmetrize it to get the vector $|\,\boldsymbol{p}\rangle_{\pm}$; for all different $\boldsymbol{p}$, the vectors $|\boldsymbol{p}\rangle_{\pm}$ are mutually orthogonal and span $\mathcal{S}^N_{\pm}$.

To find the dimension of the bosonic and fermionic space, the number of the independent vectors $|\ \boldsymbol{p}\rangle$ must be calculated. Due to their orthogonality, it remains to find which of them are nonvanishing. Since the matrix elements $D(\pi)$ is either 1 or 0, the scalar product $\langle x\,|\,P^{+}\,|\,x\rangle = \frac{1}{N!}\sum_{\pi}\langle x\,|\,D(\pi)\,|\,x\rangle$ is always nonvanishing (no cancellation is possible, and $\langle x\,|\,D(e)\,|\,x\rangle = 1$). Hence, for each choice of $\boldsymbol{p}$ there is exactly one nonzero vector $|\,\boldsymbol{p}\rangle_{+}$ in $\mathcal{S}^N_{+}$, and $\dim \mathcal{S}^N_{+} = \binom{N+n-1}{N}$. In the case of fermions, it can be seen that if for some k the corresponding $p_k(x)$ is greater than 1 (*e.g.* $i_1 = i_2 = k$), there is at least one transposition permuting only the particles in the same state (the first and the second particle in the same example), and this transposition does not change the corresponding vector $|x\rangle$. Then, for the antisymmetrized vector $P^{-}\,|x\rangle$ the equation (2.11) gives $\langle x|\ P^{-}\,|x\rangle = \langle x|\ P^{-}D(\rho)\,|x\rangle = -\langle x|\ P^{-}\,|x\rangle = 0$. Eventually, the nonvanishing vectors $|\boldsymbol{p}\rangle_{-}$ are those with the occupation numbers 0 or 1, all together $\dim \mathcal{S}^N_{-} = \binom{n}{N}$ of them. In fact, this is *Pauli's principle*, transparently

derived from symmetry only. In both the cases (bosons and fermions), the normalization of the obtained nonvanishing vectors $|\boldsymbol{p}\rangle_{\pm}$ gives the *basis of the occupation numbers*.

Chapter 3

NORMAL MODES

Harmonic oscillations are among basic types of dynamic of systems. Possibility of their exact description both in classical and in quantum mechanics, caused attempts to reduce even more complex situations to this one within different approximations. Just this method of the harmonic approximation[1] underlies indispensable (quasi)-particle model in quantum mechanics. In this sense study of harmonic oscillations (irrespectively of the contents they have in a particular situation) is fundamental part of all physical theories, and fruitful incorporation of the symmetry in this problem has far reaching importance.

3.1 Harmonic potential

A complex physical system, composed of n atoms (here "atom" is used in almost original antic meaning: elementary, at the accepted level of study, constituent of the system, *i.e.* ion, molecule, electron, etc., depending on the context), is described by the $6n$-dimensional phase space, within the classical mechanics, [1], and by the orbital Hilbert's space with $3n$ coordinates and momenta in the quantum mechanics. To each atom 3 Descartes's orthonormal vectors are attached both in the configuration and momentum spaces, and the basis of the whole space is:

$$\{\mid \boldsymbol{q}, \alpha i \rangle, \mid \boldsymbol{p}, \alpha i \rangle \mid \alpha = 1, ..., n; i = 1, 2, 3\}. \tag{3.1}$$

In this way vector $\sum_{\alpha i}(q_{\alpha i}\mid \boldsymbol{q}, \alpha i \rangle + p_{\alpha i}\mid \boldsymbol{p}, \alpha i \rangle)$ of the phase space becomes a column of coordinates $\begin{pmatrix} q \\ p \end{pmatrix} = (q_{11}, \dots p_{n3})^T$. The basis (3.1) is chosen to satisfy *canonical commutation relations*[2]

$$[q_{\alpha i}, q_{\beta j}] = [p_{\alpha i}, p_{\beta j}] = 0, \quad [q_{\alpha i}, p_{\beta j}] = c\delta^{\alpha}_{\beta}\delta^{i}_{j}.$$

Under canonical transformations the vectors of the configuration space change contragrediently with respect to the vectors of the momentum space.

[1] $\chi\alpha\rho\rho\mu\sigma\nu\eta$ or $\chi\alpha\rho\alpha$ means joy, happiness.

[2] In order to treat simultaneously both classical and quantum framework, less standard notation is used in this chapter. Constant c and braces $[\,,\,]$, stand for 1 and Poisson's bracket in classical mechanics, while for $\mathrm{i}\hbar$ and operator commutator in quantum mechanics; $\hbar$ is Planck's constant.

Configuration of stable equilibrium, i.e. the point of the minimum of potential, will be chosen as the origin of the coordinates. Therefore, the coordinate $q_{\alpha i}$ is the displacement of the atom α from the equilibrium position along i-th direction. The *harmonic approximation* is obtained when the potential is expanded into the power series over the displacements, and all the terms of the order higher than two are rejected. Since the constant term $V(0)$ can be always removed from the hamiltonian, and the first derivatives in the linear terms vanish in the equilibrium, the hamiltonian becomes:

$$H = \frac{1}{2}\sum_{\alpha i}\frac{1}{m_\alpha}p_{\alpha i}^2 + \frac{1}{2}\sum_{\alpha\beta ij}V_{\beta j}^{\alpha i}q_{\alpha i}q_{\beta j} = \frac{1}{2}\begin{pmatrix} q, & p\end{pmatrix}\boldsymbol{H}\begin{pmatrix} q \\ p\end{pmatrix}, \quad \boldsymbol{H} = \begin{pmatrix} V & 0 \\ 0 & M^{-1}\end{pmatrix}, \tag{3.2}$$

where the matrix $V = (V_{\beta j}^{\alpha i}) = (\frac{\partial^2 V(0)}{\partial q_{\alpha i}\partial q_{\beta j}})$ is symmetric and nonnegative (due to the stability of the equilibrium point), while $M = (M_{\beta j}^{\alpha i}) = (m_\alpha \delta_\beta^\alpha \delta_j^i)$ is positive diagonal matrix. In this sense, the hamiltonian is given by the matrix $\boldsymbol{H}$.

If the matrix V is diagonal, the whole system can be considered as the set of the non interacting linear harmonic oscillators, with the well known properties both in the classical and in the quantum theory. Since V is symmetric, it can be diagonalized, with use of its eigenbasis. However, in order to perform the canonical transformation in the phase space, this transition to the eigenbasis of V in the configurational space, must be accompanied by the contragredient transformation in the momentum space, which may cause the appearance of the non diagonal terms in M. To overcome this problem, the scalar product is changed firstly: the new one is in the momentum space defined by the metric M^{-1}. As M is diagonal, the basis vectors $\mid \boldsymbol{p}, \alpha i \rangle$ remain orthogonal, but they must be normalized by the factor $\sqrt{m_\alpha}$. To achieve canonical transformation, this is accompanied by the multiplication of $\mid \boldsymbol{q}, \alpha i \rangle$ by $\frac{1}{\sqrt{m_\alpha}}$, corresponding to the change of metric of the configuration space to M. Thus, the kinetic energy determines the metric of the phase space, and the orthonormal basis is:

$$\{\mid \boldsymbol{Q}, \alpha i \rangle = \frac{1}{\sqrt{m_\alpha}}\mid \boldsymbol{q}, \alpha i \rangle, \quad \mid \boldsymbol{P}, \alpha i \rangle = \sqrt{m_\alpha}\mid \boldsymbol{p}, \alpha i \rangle \mid \alpha = 1, ..., n; i = 1, 2, 3\}. \tag{3.3}$$

The point with coordinates $\begin{pmatrix} q \\ p\end{pmatrix}$ in the basis (3.1) is in the basis (3.3) represented by the column $\begin{pmatrix} Q \\ P\end{pmatrix}$, with the coordinates $Q_{\alpha i} = \sqrt{m_\alpha}q_{\alpha i}$, $P_{\alpha i} = \frac{1}{\sqrt{m_\alpha}}p_{\alpha i}$. Using the *dynamical matrix*

$$W = M^{-\frac{1}{2}}VM^{-\frac{1}{2}} = \sum_{\alpha\beta}E^{\alpha\beta}\otimes W_\beta^\alpha, \quad W_{\beta j}^{\alpha i} = \frac{1}{\sqrt{m_\alpha m_\beta}}V_{\beta j}^{\alpha i}$$

($E^{\alpha\beta}$ is the standard basis in the space of n-dimensional matrices: $E_{\eta\rho}^{\alpha\beta} = \delta_\eta^\alpha\delta_\rho^\beta$), which is obviously symmetric and nonnegative, (3.2) reads:

$$H = \frac{1}{2}\begin{pmatrix} Q, & P\end{pmatrix}\boldsymbol{H}_M\begin{pmatrix} Q \\ P\end{pmatrix}, \quad \boldsymbol{H}_M = \begin{pmatrix} W & 0 \\ 0 & I\end{pmatrix}. \tag{3.4}$$

The identity matrix standing for the kinetic part of the hamiltonian (momentum space) is invariant under arbitrary change of basis. Thus, the transition to the eigenbasis of the

potential energy, W, can be deliberately performed and accompanied by the contragredient transformation in the momentum space, giving the final basis in the whole space:

$$\{|\ \boldsymbol{Q},\omega_k l\ \rangle, |\ \boldsymbol{P},\omega_k l\ \rangle\ |\ l=1,...,n_k, \sum_k n_k = 3n\}, \quad W|\ \boldsymbol{Q},\omega_k l\ \rangle = \omega_k^2|\ \boldsymbol{Q},\omega_k l\ \rangle.$$

In the coordinates Q_{ki}, P_{ki} of this basis, the hamiltonian obtains the characteristic form (as for the quantum theory, the star denotes adjoined operator):

$$H = \frac{1}{2}\sum_{ki}(P_{ki}^2 + \omega_k^2 Q_{ki}^2) = \frac{1}{2}\sum_{ki}\hbar\omega_k(b_{ki}^* b_{ki} + b_{ki} b_{ki}^*). \tag{3.5}$$

The second expression is in the coordinates of the basis

$$\{|\ \boldsymbol{b},ki\ \rangle = \sqrt{\hbar}\frac{|\ \boldsymbol{Q},\omega_k i\ \rangle - \mathrm{i}\omega_k|\ \boldsymbol{P},\omega_k i\ \rangle}{\sqrt{2\omega_k}}, \quad |\ \boldsymbol{b}^*,ki\ \rangle = \sqrt{\hbar}\frac{|\ \boldsymbol{Q},\omega_k i\ \rangle + \mathrm{i}\omega_k|\ \boldsymbol{P},\omega_k i\ \rangle}{\sqrt{2\omega_k}}\}. \tag{3.6}$$

These coordinates satisfy the *bosonic commutation relations*

$$[b_{ki}, b_{lj}^*] = b\delta_l^k\delta_j^i, \quad [b_{ki}, b_{lj}] = [b_{ki}^*, b_{lj}^*] = 0$$

($b = -\mathrm{i}$ and $b = 1$ in the classical and quantum mechanics). The vectors of the eigenbasis, being linear combinations of the displacements of the different atoms, describe the independent vibrations of the whole system. Therefore they are known as the *normal modes*. When the system is in the equilibrium position, all the normal coordinates vanish, meaning that non vanishing of any of them reflects excitation of the system. The dynamics in the vicinity of the equilibrium is reduced to the independent exciting of certain normal excitations. Therefore, these normal excitations in the various theories are *elementary particles* or *quasi particles*, and the equilibrium state, when the excitations are absent, is called *vacuum*. After the quantization, the bosonic coordinates become the operators, $b_{ki}^\dagger$ and b_{ki}, while the hamiltonian gets the familiar form $H = \sum_{ki}\hbar\omega_k(b_{ki}^\dagger b_{ki} + \frac{1}{2})$. The eigen energies of each single term in the hamiltonian are equidistant ($\hbar\omega_k(n_{ki}+\frac{1}{2})$, $n_{ki} = 0, 1, ...$), which justify the particle picture: by creation of the boson of energy $\hbar\omega_k$ from the vacuum, the operator $b_{ki}^\dagger$ performs the transition from the state $|\ldots, n_{ki}, \ldots\rangle$, to the state $|\ldots, n_{ki}+1, \ldots\rangle$.

3.2 Application of symmetry

It has turned out that the determination of the normal modes has been reduced to the solution of the eigenvalue problem of the dynamical matrix W, since the basis in the momentum space is easily obtained as the canonically conjugated to the eigenbasis of W in the configurational space. Therefore, the application of symmetry, performed along the lines described in the chapter § 1, can simplify, and in some cases completely solve this problem.

For application of the group theoretical methods, [6], the starting point is to note that the configurational space, $\mathcal{H}_q = \mathbb{R}^{3n}$, can be understood as the space $\mathbb{R}^n$, with the vectors

of the absolute basis corresponding to different particles; therefore, each particle contributes by its own configurational space $\mathbb{R}^3$, with the coordinates being its displacements from the equilibrium. Thus the total configurational space is reconstructed in the form $\mathcal{H}_q = \mathbb{R}^n \otimes \mathbb{R}^3$ (this type of mathematical objects is called fibber bundle, to reflect that the total space is "bundle" of the "fibbers" $\mathbb{R}^3$, attached to the particles). The sets $\{|\ \boldsymbol{q}, \alpha i\ \rangle = |\ \alpha\rangle\ |\ i\rangle\}$ and $\{|\ \boldsymbol{Q}, \alpha i\ \rangle = \frac{1}{\sqrt{m_\alpha}}\ |\alpha\rangle\ |i\rangle\}$ are uncorrelated bases of the product space. All this refers also to the momentum space, $\mathcal{H}_p$, and the phase space $\mathcal{H} = \mathcal{H}_q \oplus \mathcal{H}_p = \mathbb{R}^n \otimes (\mathbb{R}^3 \oplus \mathbb{R}^3)$. The introduced picture allows to factorize the geometrical transformation leaving the system invariant: the first factor permutes the atoms (and as for the symmetries only the atoms of the same type are mutually permuted), while the second acts the in $\mathbb{R}^3$, describing the transformation of the coordinates (and the momenta) of the single particle. The last factor is in fact the polar vector representation, both for the coordinates and for the momenta. Thus, to each element g of the symmetry group G, there corresponds the orthogonal matrix $D^d(g) \stackrel{\text{def}}{=} D^P(g) \otimes D^v(g)$ acting in $\mathcal{H}_q$ (or in $\mathcal{H}_p$) as $D^d(g)|\ \boldsymbol{Q}, \alpha i\ \rangle = \sum_{\beta j} D^{P\,\beta}_{\ \alpha}(g) D^{v\,j}_{\ i}(g)|\ \boldsymbol{Q}, \beta j\ \rangle$, *i.e.* with the matrix elements $D^{d\,\beta j}_{\alpha i}(g) = D^{P\,\beta}_{\ \alpha}(g) D^{v\,j}_{\ i}(g)$. Here, $D^P(G)$ is the *permutational representation* of G, giving the action of the group on the atoms of the system; $D^v(G)$ is the polar-vector representation of G, which is essentially defined by the geometrical contents of the symmetry transformation, and does not depend on the system considered.

The *dynamical representation* of G, constructed above, commutes with M and V, and, therefore with W. This means that the standard formulation of the problem is achieved, $(\mathcal{S} = \mathcal{S}_q, H = W, D(G) = D^d(G))$, and the usual procedure should be applied to find the standard stationary basis. For each irreducible representation appearing in the decomposition of $D^d(G)$, the group projector $P_1^{(\mu)}$ and its range $\mathcal{H}_{q1}^{(\mu)}$ should be determined. The dynamical matrix, W, is reduced in this subspace. and the eigen problem of the matrix $W(\mu 1) = P_1^{(\mu)} W$ is to be solved, giving the standard stationary basis in $\mathcal{S}_q$:

$$\{|\ \boldsymbol{Q}, \mu t_\mu m\ \rangle\ |\ \mu = 1, ..., s; t_\mu = 1, ..., a_\mu; m = 1, ..., n_\mu\} \quad W|\ \boldsymbol{Q}, \mu t_\mu m\ \rangle = \omega^2(\mu t_\mu)|\ \boldsymbol{Q}, \mu t_\mu m\ \rangle.$$

As usually, this basis determines the canonically conjugated basis i $|\ \boldsymbol{P}, \mu t_\mu m\ \rangle$ in $\mathcal{S}_p$.

Note that the presented procedure is based on the complex representations of the group G. This has implicitly introduced the complex configurational space $\mathbb{C}^{3n}$ (instead of the real one, $\mathbb{R}^{3n}$), with $3n$ additional degrees of freedom (the complexified space can be also considered as the real decomplexified space with doubled dimension). Also, the vectors $|\ \boldsymbol{P}, \mu t_\mu m\ \rangle$, are transformed according to the contragredient, *i.e.* conjugated representation $D^{(\mu)^*}(G)$, in the momentum space. Since the new coordinates and momenta, $Q_{\mu t_\mu m}$ and $P_{\mu t_\mu m}$, may not be real anymore, the scalar product (3.4) becomes:

$$H = \frac{1}{2} \sum_{\mu, t_\mu, m} (P^*_{\mu t_\mu m} P_{\mu t_\mu m} + \omega^2(\mu t_\mu) Q^*_{\mu t_\mu m} Q_{\mu t_\mu m}),$$

where $Q^*_{\mu t_\mu m}$, $Q_{\mu t_\mu m}$, $P^*_{\mu t_\mu m}$ and $P_{\mu t_\mu m}$ are independent variables. On the other hand, the formulation of the problem itself warranties that there are real coordinates. This apparent

controversy, introduced by the application of symmetry, is also resolved by the group theory when the reality, (§ 2.6.1), of the dynamical representation $D^d(G)$ is encountered:

(i) if $D^{(\mu)}(G)$ is real representation (type I), then $W(\mu 1)$ is symmetrical matrix, with real eigenvectors, and the displacements are described by the real coordinates;

(ii) if $D^{(\mu)}(G)$ is pseudoreal representation (type II), then its frequency number in $D^d(G)$, a_μ, is even, as well as the degeneracy of the eigenvalues of the hermitean operator $W(\mu 1)$, and the real basis can be chosen in the same way and with the same consequences as in the case

(iii) if $D^{(\mu)}(G)$ is complex representation (type III), when $a_\mu = a_{\mu^*}$, and $W(\mu 1) = W^*(\mu^* 1)$ (μ^* is label of the representation conjugated to $D^{(\mu)}$). Since $W(\mu 1)$ and $W(\mu^* 1)$ are hermitean, with real eigenvalues, the last relation implies that their eigenvalues are equal, while the columns representing the corresponding eigenvectors in the basis (3.3), are mutually conjugated: $\langle \boldsymbol{Q}, \alpha i \mid \mu t_\mu m \rangle = \langle \boldsymbol{Q}, \alpha i \mid \mu^* t_{\mu^*} m \rangle^*$ for $t_\mu = t_{\mu^*}$.

In other words, since the dynamical representation is real, and the initial hamiltonian is invariant upon the time reversal, the irreducible corepresentations of the magnetic group $G \otimes \{e, \theta\}$ are essentially involved. Therefore, for the representations of the types II and III, the real, but still not standard, eigenbasis in $\mathcal{S}_q^{(\mu t_\mu)} \oplus \mathcal{S}_q^{(\mu^* t_\mu)}$ for W can be found (and supplemented by the canonically conjugated basis in $\mathcal{S}_p^{(\mu t_\mu)} \oplus \mathcal{S}_p^{(\mu^* t_\mu)}$:

$$
\begin{aligned}
\mid \boldsymbol{Q}, \mu t_\mu m, r \rangle &= \frac{\mid \boldsymbol{Q}, \mu t_\mu m \rangle + \mid \boldsymbol{Q}, \mu^* t_\mu m \rangle}{\sqrt{2}} \quad , \quad \mid \boldsymbol{Q}, \mu t_\mu m, i \rangle = \frac{\mid \boldsymbol{Q}, \mu t_\mu m \rangle - \mid \boldsymbol{Q}, \mu^* t_\mu m \rangle}{-\sqrt{2}\mathrm{i}}, \\
\mid \boldsymbol{P}, \mu t_\mu m, r \rangle &= \frac{\mid \boldsymbol{P}, \mu t_\mu m \rangle + \mid \boldsymbol{P}, \mu^* t_\mu m \rangle}{\sqrt{2}} \quad , \quad \mid \boldsymbol{P}, \mu t_\mu m, i \rangle = \frac{\mid \boldsymbol{P}, \mu t_\mu m \rangle - \mid \boldsymbol{P}, \mu^* t_\mu m \rangle}{\sqrt{2}\mathrm{i}}.
\end{aligned}
\tag{3.7}
$$

In this basis the displacements are real, while the hamiltonian is:

$$
H = \frac{1}{2} \sum_I \sum_{t_\mu m} (P^2_{\mu t_\mu m} + \omega^2(\mu t_\mu) Q^2_{\mu t_\mu m}) + \frac{1}{2} \sum_{II,III}{}' \sum_{t_\mu m} \sum_{l=r,i} (P^2_{\mu t_\mu m l} + \omega^2(\mu t_\mu) Q^2_{\mu t_\mu m l}) =
$$

$$
= \frac{\hbar}{2} \sum_I \sum_{t_\mu m} \omega(\mu t_\mu)(b^*_{\mu t_\mu m} b_{\mu t_\mu m} + b_{\mu t_\mu m} b^*_{\mu t_\mu m}) + \frac{\hbar}{2} \sum_{II,III}{}' \sum_{t_\mu m l} \omega(\mu t_\mu)(b^*_{\mu t_\mu m l} b_{\mu t_\mu m l} + b_{\mu t_\mu m l} b^*_{\mu t_\mu m l})
$$

(the primed sum, $\sum'$, is over the half of the set of the complex representations – types II and III). The later expression is in the basis $\{\mid \boldsymbol{b}, \mu t_\mu m \rangle, \mid \boldsymbol{b}^*, \mu t_\mu m \rangle\}$ for the real, and $\{\mid \boldsymbol{b}, \mu t_\mu m, r \rangle, \mid \boldsymbol{b}^*, \mu t_\mu m, r \rangle, \mid \boldsymbol{b}, \mu t_\mu m, i \rangle, \mid \boldsymbol{b}^*, \mu t_\mu m, i \rangle\}$ for the complex representations. Note that in the case of the complex representations, the vectors labeled by r (or i) do not span an irreducible subspace, and the basis is not a standard one. Nevertheless, the coordinates $b_{\mu t_\mu m, r}, b^*_{\mu t_\mu m, r}$ (analogously for i) satisfy the bosonic commutation relations.

Since the canonical transformation are manifested as the mutually contragredient change of bases in the coordinate and in the momentum space, the coordinates in the basis of the

type (3.6), formed directly with the vectors of the standard basis, would not have neither the expected symmetry properties, nor they would satisfy the bosonic relations. Therefore, another basis is introduced for the complex representations in the space $\mathcal{S}_q^{(\mu t_\mu)} \oplus \mathcal{S}_q^{(\mu^* t_\mu)} \oplus \mathcal{S}_p^{(\mu t_\mu)} \oplus \mathcal{S}_p^{(\mu^* t_\mu)}$:

$$\begin{aligned}
\{ \mid \boldsymbol{b}, \mu t_\mu m \rangle &= \sqrt{\frac{\hbar}{2\omega(\mu t_\mu)}} \mid \boldsymbol{Q}, \mu t_\mu m \rangle - \mathrm{i}\sqrt{\frac{\hbar\omega(\mu t_\mu)}{2}} \mid \boldsymbol{P}, \mu^* t_\mu m \rangle, \\
\mid \boldsymbol{b}^*, \mu t_\mu m \rangle &= \sqrt{\frac{\hbar}{2\omega(\mu t_\mu)}} \mid \boldsymbol{Q}, \mu^* t_\mu m \rangle + \mathrm{i}\sqrt{\frac{\hbar\omega(\mu t_\mu)}{2}} \mid \boldsymbol{P}, \mu t_\mu m \rangle, \\
\mid \boldsymbol{b}, \mu^* t_\mu m \rangle &= \sqrt{\frac{\hbar}{2\omega(\mu t_\mu)}} \mid \boldsymbol{Q}, \mu^* t_\mu m \rangle - \mathrm{i}\sqrt{\frac{\hbar\omega(\mu t_\mu)}{2}} \mid \boldsymbol{P}, \mu t_\mu m \rangle, \\
\mid \boldsymbol{b}^*, \mu^* t_\mu m \rangle &= \sqrt{\frac{\hbar}{2\omega(\mu t_\mu)}} \mid \boldsymbol{Q}, \mu t_\mu m \rangle + \mathrm{i}\sqrt{\frac{\hbar\omega(\mu t_\mu)}{2}} \mid \boldsymbol{P}, \mu^* t_\mu m \rangle \; \}.
\end{aligned} \tag{3.8}$$

At very last, in the coordinates of this basis, the hamiltonian obtains form (3.5) (with slightly changed meaning of the symbols!):

$$H = \frac{1}{2} \sum_{\mu t_\mu m} \hbar\omega(\mu t_\mu)(b^*_{\mu t_\mu m} b_{\mu t_\mu m} + b_{\mu t_\mu m} b^*_{\mu t_\mu m}).$$

Since $Q_{\mu t_\mu m} = \sqrt{\frac{\hbar}{2\omega(\mu t_\mu)}}(b_{\mu t_\mu m} + b^*_{\mu^* t_\mu m})$ i $P_{\mu t_\mu m} = \mathrm{i}\sqrt{\frac{\hbar\omega(\mu t_\mu)}{2}}(b^*_{\mu t_\mu m} - b_{\mu^* t_\mu m})$, the bosonic commutation relations are easily verified. Note that the subspaces of the conjugated irreducible representations cannot be separately considered, because the corresponding conjugated coordinates, which are simultaneously used, are transformed according to them. Finally, while the creation operators in the previous hamiltonian connect different irreducible representations, in the last one they induce complex displacements. The standard usage of the coordinates in the so called canonical quantization, originated the incompatibility of this procedure with the symmetrical coordinates, [33].

Using the properties of the dynamical representation, its explicit construction and the reduction, being the most important steps in the calculation of the standard stationary basis, are performed surprisingly simply. Since each element of the symmetry group connects the atoms of the same sort, only the matrix elements of $D^d(g)$ connecting such pairs of atoms are non vanishing; in addition, the diagonal element is zero unless the corresponding atom remains invariant under the transformation g. More precisely, $D^P_{\alpha\beta}(g) = \delta_{\beta,g\alpha}$, and, since the character of $D^d(g)$ is the product of the characters of the permutational and the polar vector representations, the frequencies a_μ in the decomposition $D^d(G) = \sum_\mu a_\mu D^{(\mu)}(G)$ are:

$$a_\mu = \frac{1}{\mid G \mid} \sum_g \chi^{(\mu)*}(g)\chi^d(g), \quad \chi^d(g) = n(g)\chi^v(g).$$

This is the instance where the most powerful simplifications occur. Firstly, $n(g) = \chi^P(g)$ is exactly the number of the atoms remaining fixed under the transformation g, and it is found by simple inspection in each concrete problem. Secondly, the character of the polar-vectors representation, $\chi^v(g)$, is independent of the problem. It is easily calculated, and well known for any geometrical transformation: the translations do not change the vectors (because they move both of its ends), and $\chi^v(\ I\ |\boldsymbol{z}\ ) = 3$; the character of the rotation for the angle φ is $\chi^v(R(\varphi)) = 1 + 2\cos(\varphi)$; the product of the spatial inversion with the rotation has character $\chi^v(PR(\varphi)) = -1-2\cos(\varphi)$. If the transformation g has no fixed points in $\mathbb{R}^3$, it a priori moves all the atoms, and $\chi^d(g) = n(g) = 0$; besides the pure translations, some other geometrical transformations share this property. For example, if $R\boldsymbol{t} = \boldsymbol{t}$, the action of $(R|\boldsymbol{t})$ involves a translational part, and $\chi^d(R|\boldsymbol{t}) = 0$, independently of the regarded system (warning: in general, the non vanishing of the translational part $\boldsymbol{t}$ does not prevent the existence of the fixed points of $(R|\boldsymbol{t})$; *e.g.*, for $\boldsymbol{t} = t\boldsymbol{e}_z$ and $R = \sigma_h$, giving $R\boldsymbol{t} = -\boldsymbol{t}$, the element $(\sigma_h|t\boldsymbol{e}_z)$ is the reflection in the horizontal plane, $z = \frac{t}{2}$, and each point of the plain is fixed).

Another important property of the dynamical representation, inherited from the permutational factor $D^P(G)$, comes from the fact that the orbits of the group action on the system are disjoint. The configurational (or phase) space of the single orbit is invariant subspace in the configurational (phase) space of total system. Therefore, the dynamical representation is reduced in the orbital subspaces, appearing as the sum of the dynamical representations of the orbits. This inspired the attempts to classify all the possible orbits of the geometrical groups in $\mathbb{R}^3$, in order to analyze the vibrations of arbitrary system of the given symmetry.

The dynamical representation involves all the displacements of the systems from the equilibrium configuration: vibrations, translations and rotations. The translations and the rotations are global motions of the system, which do not change the relative positions of the atoms, and they should be separated in order to study only essentially vibrational degrees of freedom. These global displacements are transformed according to the polar vector (translations) and axial vector (rotations) representations, and the resulting normal modes correspond to the irreducible components of these representations. Therefore, these components should be subtracted from the dynamical representation, to achieve the *vibrational* representation, related to pure vibrations. For the finite system, there are 3 translational and 3 rotational modes if it is nonlinear, while for linear system any rotation around its axis is identical mapping (thus not movement), and 2 axial vectors orthogonal to the system axis are rotational modes. For the infinite systems the rotational modes do not exist (since far from the rotational axis the displacements induced by the rotation are large), except when the system is quasi one-dimensional, when the rotation around the system axis is the degree of freedom (this does not refer to the exactly one dimensional systems: again, the mentioned rotation is not real motion and the degree of freedom). In the spectrum of the harmonic hamiltonian, the translational and the allowed rotational modes are characterized by the vanishing frequencies, reflecting the fact that the since for translational and rotational hamiltonians are degenerated cases of the harmonic one for the zero frequency (the constant in the quadratic term).

To illustrate these concepts, the isolated system, with the usual two-particle central in-

teraction, *i.e.* depending only on the distance $r_{\alpha\beta} = ||\boldsymbol{r}_\alpha - \boldsymbol{r}_\beta||$ of the atoms) is considered. Quite generally, its potential, $V = \frac{1}{2}\sum_{\alpha,\beta} V_{\alpha\beta}(r_{\alpha\beta})$, is invariant under the rotations and the translations of the whole system. The harmonic term in the equilibrium configuration $\boldsymbol{R}_\alpha$ is, [30]: $\frac{1}{2}\sum_{\alpha,\beta}\frac{d^2V_{\alpha\beta}(R_{\alpha\beta})}{dr^2_{\alpha\beta}}(\frac{\boldsymbol{R}_{\alpha\beta}}{R_{\alpha\beta}}(\boldsymbol{q}_\alpha - \boldsymbol{q}_\beta))^2$. Therefore the coefficients in the expansion (3.2) are:

$$V^{\alpha i}_{\beta j} = \begin{cases} -V_{\alpha\beta}\frac{R^i_{\alpha\beta}R^j_{\alpha\beta}}{R^2_{\alpha\beta}}, & \text{for } \alpha \neq \beta, \\ \sum_\gamma V_{\alpha\gamma}\frac{R^i_{\alpha\gamma}R^j_{\alpha\gamma}}{R^2_{\alpha\gamma}}, & \text{for } \alpha = \beta. \end{cases}$$

The direct inspection shows that the translational and the rotational displacements are the eigenvectors of the dynamical matrix for the eigenvalue equal to zero. Indeed, a translational mode is described by the equal displacements, vector $\boldsymbol{a}$, of each atom, *i.e.* by the vector $\sum_{\alpha i} a_i |\, \boldsymbol{q}, \alpha i \,\rangle$ in the configurational space; the requirement that this vector is the eigenvector of V for the vanishing eigenvalue (for any $\boldsymbol{a}$), gives the equality $\sum_\alpha V^{\beta j}_{\alpha i} = 0$, for all i, j and β. In fact, these turn out to be the identities, when the derived values for the coefficients $V^{\alpha i}_{\beta j}$ are encountered. Analogously, the form of rotational modes is determined by the form of the rotation, $R(\varphi) = \mathrm{e}^{A\varphi}$ (A is a skew symmetric matrix): $\varphi\sum_{\alpha ij} A^i_j R_{\alpha j}|\, \boldsymbol{q}, \alpha i \,\rangle$. Such vector is the eigenvector of V for the vanishing eigenvalue if $\sum_\alpha (R_{\alpha j}V^{\beta k}_{\alpha i} - R_{\alpha i}V^{\beta k}_{\alpha j}) = 0$, for all β, i, j and k, and the last condition is fulfilled in the considered case.

3.3 Normal modes of crystals

It has been explained, § 2.3.1, that translational periodicity is the main characteristic of the crystal structure, since the translational group, T, is always included in the symmetry group of the crystal. Therefore, when the results referring to all crystals are looked for, methods of the solid state physics [31] apply this symmetry only; the full space group treatment is postponed for precise studies of the concrete compounds, [32, 33]. The consequences of the translational symmetry only will be the subject of this section.

The irreducible representations of T are parameterized by the vectors of the Brillouin's zone. All of them are complex, except for $\boldsymbol{k} = 0$ (the identical representation), and several representations for $\boldsymbol{k}$ at the boundary of the zone (these are alternative representations), and satisfy $D^{(\mathbf{k})*}(T) = D^{(-\mathbf{k})}(T)$. Therefore, the expressions bellow are simplified to involve only the complex representations (consequently, the summations are performed over the half of the Brillouin's zone — $\frac{BZ}{2}$).

The notation of the previous section can be slightly adapted to the crystal structure. Thus, instead by the single index α, it is convenient to enumerate the atoms of the system by double label, $\boldsymbol{z}\alpha$: the first part, $\boldsymbol{z}$, being the vector with integral coordinates, $z_i = 0, \ldots, N_i - 1$, specifies the elementary cell, and $\alpha = 1, ..., r$ distinguishes between the atoms in the cell. The total number of the atoms[3] is $n = Nr$, where $N = N_1N_2N_3$. The basis (3.3) becomes

[3] In fact, the finite order of the translational group, $|T| = N$, is temporary introduced only to avoid the question of normalization of the vectors; this technical assumption, with no relationship to the symmetry, cannot disturb the results, since they are independent on N.

$|\ \boldsymbol{Q}, \boldsymbol{z}\alpha i\ \rangle$, and the dynamical representation is defined by:

$$D^d(\ I\ |\boldsymbol{l}\ )|\ \boldsymbol{Q}, \boldsymbol{z}\alpha i\ \rangle = |\ \boldsymbol{Q}, (\boldsymbol{l}+\boldsymbol{z})\alpha i\ \rangle.$$

Its matrices and characters

$$D^{d\,\boldsymbol{z}\alpha i}_{\boldsymbol{z}'\alpha' i'}(\ I\ |\boldsymbol{l}\ ) = \delta^{\boldsymbol{z}}_{\boldsymbol{z}'+\boldsymbol{l}}\delta^{\alpha}_{\alpha'}\delta^{i}_{i'} \quad \chi^d(\ I\ |\boldsymbol{l}\ ) = 3Nr\delta_{\boldsymbol{l},0}, \tag{3.9}$$

give, applying (A.1), the decomposition onto the irreducible components:

$$D^d(T) = \sum_{\boldsymbol{k}} 3rD^{(\boldsymbol{k})}(T).$$

Therefore, the dimension of each subspace $\mathcal{H}^{(\boldsymbol{k})}_q$ is $3r$ (the index m is omitted since the representations are one-dimensional). It is easily verified that the vectors

$$\{|\ \boldsymbol{Q}, \boldsymbol{k}\alpha i\ \rangle = \sqrt{N}P^{(\boldsymbol{k})}|\ \boldsymbol{Q}, 0\alpha i\ \rangle = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{z}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{z}}|\ \boldsymbol{Q}, \boldsymbol{z}\alpha i\ \rangle\ |\ \alpha = 1,\dots,r; i = 1,2,3\}$$

are orthonormal, forming the basis of $\mathcal{H}^{(\boldsymbol{k})}_q$. Due to the translational symmetry of the system, $D^d(T)$ commutes with V and W. Using (3.9), this gives relation $W^{\boldsymbol{z}\alpha i}_{\boldsymbol{z}'\alpha' i'} = W^{\boldsymbol{z}-\boldsymbol{z}'\alpha i}_{0\alpha' i'}$ among matrix elements of W. In the last basis W is in the reduced form: since $\langle\ \boldsymbol{Q}, \mathbf{k}\alpha i\ |W|\ \boldsymbol{Q}, \mathbf{k}'\alpha' i'\ \rangle = \sum_{\mathbf{z}} \mathrm{e}^{-\mathrm{i}\mathbf{k}\mathbf{z}}W^{\mathbf{z}\alpha i}_{0\alpha' i'}\delta^{\mathbf{k}}_{\mathbf{k}'}$, $\mathcal{S}^{(\boldsymbol{k})}_q$ is invariant subspace for W, and in this subspace the W acts as the matrix $W^{\alpha i}_{\alpha' i'}(\boldsymbol{k}) = \sum_{\mathbf{z}} \mathrm{e}^{-\mathrm{i}\mathbf{k}\mathbf{z}}W^{\mathbf{z}\alpha i}_{0\alpha' i'}$.

Solving the eigenproblem in each $\mathcal{S}^{(\boldsymbol{k})}_q$, the eigenvalues $\omega^2_t(\mathbf{k})$ and the eigenbasis $\{|\ \boldsymbol{Q}, \mathbf{k}t\ \rangle\ |\ \mathbf{k} \in BZ, t = 1, ...3r\}$ (there is no need for the usual subscript of t, since T takes on the same $3r$ values independently of $\boldsymbol{k}$) are found. Note that $\omega_t(\boldsymbol{k}) = \omega_t(-\boldsymbol{k})$, since $W(\boldsymbol{k}) = W^*(\boldsymbol{k})$. In the coordinates of this basis, the hamiltonian is:

$$H = \frac{1}{2}\sum_{kt}(P^*_{\mathbf{k}t}P_{\mathbf{k}t} + \omega^2_t(\mathbf{k})Q^*_{\mathbf{k}t}Q_{\mathbf{k}t}).$$

To obtain the form of the system of the harmonic oscillators, the described methods for the representations of the type III would be applied: either in the real basis (3.7) the hamiltonian takes the form

$$H = \frac{1}{2}\sum_{\mathbf{k}\in\frac{\mathrm{BZ}}{2}}\sum_{t}\sum_{l=r,i}(P^2_{\mathbf{k}tl} + \omega^2_t(\mathbf{k})Q^2_{\mathbf{k}tl}) = \frac{1}{2}\sum_{\mathbf{k}\in\frac{\mathrm{BZ}}{2}}\sum_{t}\sum_{l=r,i}\omega_t(\mathbf{k})(b^*_{\mathbf{k}tl}b_{\mathbf{k}tl} + b_{\mathbf{k}tl}b^*_{\mathbf{k}tl}),$$

or, more frequently, substituting $Q_{\boldsymbol{k}t} = \frac{1}{\sqrt{2\omega_t(\boldsymbol{k})}}(b_{\boldsymbol{k}t} + b^*_{-\boldsymbol{k}t})$, $P_{\boldsymbol{k}t} = \mathrm{i}\sqrt{\frac{\omega_t(\boldsymbol{k})}{2}}(b^*_{\boldsymbol{k}t} - b_{-\boldsymbol{k}t})$, the basis (3.8) is used, to rewrite hamiltonian as

$$H = \frac{1}{2}\sum_{\mathbf{k}t}\omega_t(\mathbf{k})(b^*_{\mathbf{k}t}b_{\mathbf{k}t} + b_{\mathbf{k}t}b^*_{\mathbf{k}t}).$$

In the solid state physic, after the quantization, the last expression describes the energy of the thermal excitations of the lattice, *i.e.* the quasi particles, *phonons*, created by the operators $b^{\dagger}_{\boldsymbol{k}t}$.

The usual physical reasons imply that the eigen frequencies, $\omega_t(\boldsymbol{k})$, are continuous functions on $\boldsymbol{k}$. This means that for fixed t, these frequencies form the hyper surfaces over the Brillouin's zone, known as the *vibrational bands*. This is a special case of the energy bands, (§ 2.3.1, § 5.4), manifesting the translational symmetry. It has been mentioned that there are 3 translational modes , transforming according to the identical representations, $\boldsymbol{k} = 0$ (only translational group is considered!), giving raise to the 3-fold degeneracy of the frequency $\omega = 0$. These three bands $\omega_t(\boldsymbol{k})(t = 1, 2, 3)$ vanishing in the center of the Brillouin's zone ($\omega_t(0) = 0$) are called *acoustic*, to distinguish from the remaining *optical* bands ($t = 4, \dots 3r$). In fact, for $\boldsymbol{k} = 0$ the displacements of the atoms are same in any cell, but the acoustic mode induces the same displacements of all the atoms within cell, displacing the cell in its eternity, like the acoustic wave; in other modes the relative distances between the atoms within single cell are oscillating, also. Clearly, the full space group treatment will relate the band index t to the irreducible representations of the symmetry group of the elementary cell (which is realized through the induced representations of the space group).

3.4 Analysis of the results

The obtained classification of the normal vibrations is directly observed in the spectroscopy of the atoms and molecules. When the typical masses and force constants (characterizing the interactions) are substituted in the harmonic potential, it turns out that the obtained frequencies correspond to the infra red domain of the electromagnetic waves; being much less then the energies of the electronic transitions, the corresponding spectral lines are easily recognized. In the standard theoretical prescription, the transitions are described through the interaction with the electromagnetic waves. In the first, *dipole* approximation, [2], relevant for the most probable one-phonon transitions, the unperturbed hamiltonian is (3.2), and the perturbation (being proportional to the dipole moment of the system) is transformed according to the polar vector representation, $D^v(G)$. To derive the selection rules, all the Clebsch-Gordan's coefficients for the irreducible components of $D^v(G)$ should be calculated. Assuming that the ground state of the system is symmetrical, *i.e.* corresponds to the identical representation, Wigner-Eckart's theorem gives that, within the dipole approximation, the excited states allow normal modes transforming according to the irreducible components of $D^v(G)$. Therefore, these are called *active* modes.

The described method is easily generalized to other physical problems. Usually, only the *"interior" space* is changed: depending on the physical situation, instead of $\mathbb{R}^3$ (for the mechanical motion), some other space, $\mathcal{S}_{in}$, is attached to every atom. This implies the change of the relevant representation of the symmetry group; analogously to the polar vector representation, the another representation, $D^{in}(G)$ is defined in $\mathcal{S}_{in}$.

For example, when the spin ordering is studied, the spin corresponding to the site (atom)

α ($\alpha = 1, \ldots, n$) is described in the spin space $\mathcal{S}$, forming total state space $\mathcal{S}^{\otimes n}$, and the general hamiltonian with pairwise interaction only is:

$$H = -\sum_{\alpha\beta} \boldsymbol{S}_\alpha J^\alpha_\beta \boldsymbol{S}_\beta = -\sum_{\alpha\beta}\sum_{ij} J^{\alpha i}_{\beta j} S_{\alpha i} \odot S_{\beta j}. \tag{3.10}$$

Here, $\odot$ is matrix multiplication if $\alpha = \beta$ and tensor product otherwise, $\boldsymbol{S}_\alpha$ is triple of the spin operators associated to the site α, and J^α_β is three-dimensional tensor of interaction of the spins in the sites α and β; clearly, terms are tacitly directly multiplied by identity operators in all but α and β site-spaces. Depending on J^α_β various models are obtained: most frequently it is assumed that this tensor is diagonal and depends only on the distance between sites (*e.g.* nonzero only for the first neighbors) one gets generalizations of the Heisenberg's hamiltonian, which is isotropic since uses only scalar matrices (*i.e.* J^α_β become coupling constants).

Being intrinsically many-body problem, model (3.10) is not solvable in geneal, and a typical approach is the variational one. *Classical* approximation takes uncorrelated spin states $|\,\psi_1, \psi_2, \ldots\rangle$ ($|\,\psi_\alpha\rangle$ is the state of the spin of the site α) for the trial set. The derived average energy is $E(\boldsymbol{s}) = -\sum_{\alpha\beta} \boldsymbol{s}_\alpha J^\alpha_\beta \boldsymbol{s}_\beta$, where $\boldsymbol{s}_\alpha$ is the three-dimensional axial vector (with components $\boldsymbol{s}_{\alpha i} = \langle\psi_\alpha|\, S_{\alpha i}\, |\psi_\alpha\rangle$), interpreted as the spin (correctly: spin operators averages) of the site α. Thus, within this approximation ground state minimizes energy over spin arrangements $\boldsymbol{s} = \{\boldsymbol{s}_1, \boldsymbol{s}_2, \ldots\}$. Obviously, it can be obtained as the minimal eigenvalue of the "classical" hamiltonian $H_{cl} = -\sum_{\alpha\beta} E^{\alpha\beta} \otimes J^\alpha_\beta$. This problem is quite analogous to that of normal modes: the permutational representation is the same, only spin vectors are axial (to differ from the polar displacements). Note that, as it is usual in the variational approach, eigenstates corresponding to higher eigenvalues are not expected to give good description of excitations, and perturbative methods are employed to get *spin waves*, also called *magnons*. In this case the time reversal can be less trivially involved, as it reverses spins, which points to the importance of the of the magnetic groups and their corepresentations. On the other hand, as the lengths of the spin vectors are same along the orbits of the group (this is not the case with vibrational amplitudes), spin groups give the most efficient way to find classical ground state. Finally, let it be mentioned that the original quantum problem, being solved only for some very special configurations and hamiltonians (*e.g.* for one-dimensional periodic chain solution is known as *Bethe anztz*), still is one of the greatest challenges of the condensed matter theory; it can be expected that further substantial breakthroughs can be performed only with systematic (though complicated) application of symmetry.

Further example of the analogous construction will be connected to electronic states of the molecules and crystals, (§ 5.3): each atom gives a subspace of its electronic states, and these chosen states are altogether used to construct the one electron states of the whole molecule (or crystal).

The invariance of the potential in the Heisenberg's method under the rotations (of the spin operators) in each site of the lattice, introduces additional interior symmetry. The treatment of such symmetries leads to the *gauge theories*; the formulation of such problems is based on the differential geometry, making them beyond the scope of the text (still, some of the notions will be implicitly introduced within the adiabatic method, § 5.1).

Chapter 4

SYMMETRY BREAKING

Symmetry breaking is common name for the processes in which the symmetry of the final state is subgroup of the symmetry of the initial state. Many diverse and important physical phenomena (phase transitions, Jahn-Teller effect, Peierls transitions, symmetry breaking in particle physics) fall into this class, and their unique explanation is perhaps the most impressive success of the concept of symmetry.

4.1 Invariant functionals

Let $\mathcal{S}$ be real space carrying the representation $D(G) = \sum_\mu a_\mu D^{(\mu)}(G)$ of the group G. *Functional* (real) on $\mathcal{S}$, *i.e.* the map $F : \mathcal{S} \to \mathbb{R}$, is *invariant* if $F(D(g)\,|x\rangle) = F(|x\rangle)$ for all $|x\rangle \in \mathcal{S}$ and $g \in G$. Functional is *differentiable* in $|x\rangle \in \mathcal{S}$, if for any unit vector $|y\rangle \in \mathcal{S}$ the real function of the real variable ε, $F(|x\rangle + \varepsilon\,|y\rangle)$, is differentiable in $\varepsilon = 0$.

Note that the linearity of the functional is not requested. Also, the differentiability of the certain order is not necessary, although it customary to use the sufficiently smooth functionals; in fact, for the simplicity, it is usually assumed that the physical functionals are infinitely differentiable.

Frequently appearing functional in the spaces with scalar product is the square of the norm of the vectors:

$$F(|x\rangle) = \langle\, x\,|x\rangle = \sum_i \xi_i^2 = F(\xi_1, \ldots, \xi_n); \tag{4.1}$$

here, ξ_i are the coordinates of the vector $|\, x\rangle$ in some orthonormal basis. This example clearly illustrates how the choice of the basis transforms the functional in $\mathcal{S}$ to the function of the coordinates: the function $F(\xi_1, \ldots, \xi_n)$ from $\mathbb{R}^n$ to $\mathbb{R}$, is differentiable if the functional $F(|\, x\rangle)$ is differentiable. The potentials of different physical systems can be understood as the invariant functionals (over the configurational space in classical, or over the space spanned by the observables of the coordinates in quantum mechanics); then the group of the geometrical (or other) symmetries is easily incorporated. Especially, the harmonic potential (§ 3) is quadratic functional. Another, quite general example is the functional obtained from the hamiltonian of the system: $V(|\, x\rangle) = \langle x \mid H \mid x\rangle$; its extremal points in $\mathcal{S}$ are the

eigenvectors of H.

In the coordinates of some chosen basis, the group action, $D(g)\,|x\rangle = |x'\rangle$, takes the matrix form $\xi'_i = \sum_j D_{ij}(g)\xi_j$, and the invariance of the functional reads

$$F(\xi_1,\dots,\xi_n) = F(\xi'_1,\dots,\xi'_n) = F(\sum_j D_{1j}(g)\xi_j,\dots,\sum_j D_{nj}(g)\xi_j).$$

In the complex spaces the real coordinates can be introduced by the decomplexification procedure (consequently, the coordinates ξ_i and ξ_i^* are independent). Also in this case, the square of the norm is frequent example of the functional. Especially, the harmonic potential (§ 3)

The differentiability of the functional enables to expand it in the vicinity of arbitrary point $|x_1\rangle$

$$F(|x_1\rangle + \varepsilon\,|x\rangle) = F(|x_1\rangle) + \varepsilon\sum_i C^{[1]}_i\xi_i + \varepsilon^2\sum_{ij} C^{[2]}_{ij}\xi_i\xi_j + \dots. \tag{4.2}$$

Here $C^{[1]}_i \overset{\text{def}}{=} \frac{\partial F(|x_1\rangle)}{\partial\xi_i}$, $C^{[2]}_{ij} \overset{\text{def}}{=} \frac{1}{2}\frac{\partial^2 F(|x_1\rangle)}{\partial\xi_i\partial\xi_j}$ and generally $C^{[r]}_{i_1,\dots,i_r} \overset{\text{def}}{=} \frac{1}{n!}\frac{\partial^r F(|x_1\rangle)}{\partial\xi_{i_1}\cdots\partial\xi_{i_r}}$; all these tensors are symmetric with respect to the permutations of indices.

In the context of the symmetry breaking, the properties of the functional in the vicinity of the *fixed points* of the group action are of especially important. Therefore, $|\,x_1\rangle$ will be assumed to be such point, *i.e.* it will be from the subspace $\mathcal{S}^{(1)}$ of the identity representation: $D(g)\,|x_1\rangle = |x_1\rangle$. The value of the functional in the point $D(g)(|x_1\rangle + \varepsilon\,|x\rangle) = |x_1\rangle + \varepsilon D(g)\,|x\rangle$ (being also in the ε-vicinity of $|x_1\rangle$ due to the unitarity of $D(G)$) is given by (4.2) again, with the coordinates ξ_i of the vector $|x\rangle$ substituted by the new ones, ξ'_i of $|x'\rangle = D(g)\,|x\rangle$:

$$F(D(g)(|x_1\rangle + \varepsilon\,|x\rangle)) = F(|x_1\rangle) + \varepsilon\sum_i C^{[1]}_i\xi'_i + \varepsilon^2\sum_{ij} C^{[2]}_{ij}\xi'_i\xi'_j + \dots.$$

Therefore, the r-th term reads

$$\varepsilon^r\sum_{i_1\cdots i_r} C^{[r]}_{i_1\cdots i_r}\xi'_{i_1}\cdots\xi'_{i_r} = \varepsilon^r\sum_{i_1\cdots i_r} C^{[r]}_{i_1\cdots i_r}D_{i_1j_1}(g)\cdots D_{i_rj_r}(g)\xi_{j_1}\cdots\xi_{j_r}. \tag{4.3}$$

Obviously, the coordinates in r-th term of the expansion form homogeneous polynomial of r-the degree, transforming according to the r-th tensor power of the representation $D(G)$. Nevertheless, after the action on the (mutually commuting!) coordinates, only the symmetric part of this tensor product remains (other parts mutually cancels). Thus, each term in the expansion transforms according to the corresponding symmetric power (§ A.2.5) of the representation $D(G)$ (this can be equivalently explained by the contraction of the tensor formed by the coordinates with the symmetric tensor $C^{[r]}$ of the coefficients).

The invariance of the functional induces additional properties of the expansion in the vicinity of the fixed point. To provide the invariance of the whole functional, each order of expansion must be invariant (due to the different exponent of ε). In other words, the r-th term (4.3) is homogeneous *invariant polynomial* (of order r) in coordinates. Thus, the differentiable invariant functional is expanded as a sum of the invariant homogeneous polynomials of the group G. Since the homogeneous polynomial transforms according to the corresponding

symmetric power of the representation $D(G)$, invariant polynomial of the r-th degree, *i.e.* polynomial transforming according to the identity representation of G, can be constructed only if the identical representation appears in the decomposition of the symmetric r-th power $[D^r(G)]$; if this is not the case, the r-th degree term of any invariant functional is absent.

In the previous example, the functional (4.1) is obviously invariant for the group $\mathrm{O}(n,\mathbb{R})$ ($\mathrm{U}(n)$), and the coordinates form quadratic invariant polynomial for this group. Also, (4.1) can be understood as the second order expansion of some functional invariant for $\mathrm{O}(n,\mathbb{R})$ ($\mathrm{U}(n)$), in the vicinity of the coordinate origin (being the only fixed point in the considered example). In fact, the quadratic functional obtained this way, is usully called the harmonic approximation, as discussed in § 3.

The algorithm for the construction of the differentiable invariant functionals is easily found using their derived properties in the vicinity of the fixed points (note that the set of the fixed points is defined by the group action only, independently on the characteristics of the functional under consideration). In the vector space S_r (of the dimension $\binom{n+r-1}{r}$), spanned by the monomials of the order r over the coordinates, the action of the group G is defined by the representation $[D^r(G)]$; the range $S_r^{(1)}$ of the group projector of the identical representation in S_r is the set of all invariant polynomials of the degree r. If the polynomials $\{p_i^{[r]} \mid i = 1, ..., a_1^{[r]}\}$ are the basis in $S_r^{(1)}$, $\quad r = 1, 2, ...$, the most general form of the invariant differentiable functional is:

$$F(|\,x_1\rangle + \varepsilon\,|x\rangle) = F(|\,x_1\rangle) + \sum_r \varepsilon^r \sum_{i=1}^{a_1^{[r]}} A_i^{[r]} p_i^{[r]}. \tag{4.4}$$

Each choice of the coefficients $A_i^{[r]}$ completely defines one invariant functional.

This reveals the importance of the invariant polynomials in the description of the system with nontrivial symmetry[1]. Their calculation is relatively complicated task, and the suitable mathematics is developed during last century, to achieve important result at its end [35, 36]: for any representation of the compact group, there is the finite set, $\{p_i(\xi_1, \ldots, \xi_n) | i = 1, \ldots, q\}$, of the invariant polynomials over the coordinates of the representation, called the *integral basis*, such that each invariant polynomial is a polynomial over this set: $P(\xi_1, \ldots, \xi_n) = P(p_1, \ldots, p_q)$. This means that the classification of the invariant functionals can be performed using the integral basis. Unfortunately, the proof is not constructive, and the algorithm to find this basis is a problem itself, with complexity depending on the group structure and on the dimension of the irreducible representation.

As usually, the implementation of symmetry in the physical problems, starts by the reduction of the relevant representation on the irreducible components and usage of the standard basis. At first, note that the invariant polynomials of the first order can be made only by the coordinates of the vectors from the subspace $\mathcal{S}^{(1)}$ (the other coordinates are changed

[1] In fact, as it has been mentioned, the potential of the system is invariant functional, and in any physically relevant approximative method the potential is reduced to several invariant polynomials. Thus, their importance in the prediction of the dynamics of the system is obvious even at this instance, independently of the symmetry breaking processes considered in the rest of the chapter.

by the action of the group). The second order term of the invariant functional gives the most convenient standard basis: the matrix $C^{[2]}$ of the coefficients in this polynomial can be diagonalized, and its standard eigenbasis $\{|\ \mu t_\mu m\ \rangle\}$ in $\mathcal{S}$ is usually used to define the coordinates $\xi_{\mu t_\mu m}$. The group projector technique gives such basis as it has been explained in the context of normal vibrations (§ 3), and only the main results will be summarized here: *(i)* since $C^{[2]}$ is symmetric, the real standard basis can be used (even when the representation $D^{[2]}(G)$ contains the irreducible components of the types II and III, the conjugated pairs of the irreducible components are joined into one reducible, called *physically* or *real* irreducible representation of the group G); *(ii)* since the only quadratic invariant polinomial of the physicaly irreducible representation is the sum of the squares of the coordinates $p^{[2\mu]} = \sum_m \xi^2_{\mu t_\mu m}$, the quadratic term obtains the diagonal form $\sum_{\mu t_\mu} A^{[2]}_{\mu t_\mu} p^{[2\mu]}$. Thus, in the standard eigenbasis, for $|\,x\rangle = \sum_{\mu t_\mu m} \xi_{\mu t_\mu m} |\ \mu t_\mu m\ \rangle$, the equality (4.4) becomes

$$F(|\,x_1\rangle + \varepsilon\,|\,x\rangle) = F(|\,x_1\rangle) + \varepsilon \sum_{t_1}^{a_1} A^{[1]}_{1t_1}\xi_{1t_1} + \varepsilon^2 \sum_{\mu t_\mu} A^{[2]}_{\mu t_\mu} \sum_m \xi^2_{\mu t_\mu m} + \sum_{r>2} \varepsilon^r \sum_{i=1}^{a_1^{[r]}} A^{[r]}_i p^{[r]}_i. \quad (4.5)$$

Naturally, the coefficients $A^{[2]}_{\mu t_\mu}$ are the eigenvalues of the matrix $C^{[2]}$; they correspond to the eigen frequencies of the previous chapter, but their positivity is not necessary, unless some additional requirement has been imposed (like the condition of the stable equilibrium in § 3).

4.2 Extremes of the invariant functional

Vanishing of the first order terms (over ε) is sufficient condition for the functional (4.5) to be stationary at the fixed point $|x_1\rangle$. This point is a local minimum if all the coefficients $A^{[2]}_{\mu t_\mu}$ are positive (or equal zero, but then suitable conditions on the higher order terms are fulfilled).

Most relevant for the physical problems are the extreme properties of the functional in the directions of the vectors of the defined symmetry [34], *i.e.* in the case when $|\,x\rangle = |\,x, \mu t_\mu\rangle = \sum_m \xi_{\mu t_\mu m} |\ \mu t_\mu m\ \rangle$ is in the standard subspace $\mathcal{S}^{(\mu t_\mu)}$. Moreover, the motions toward some other fixed point are not to be considered, meaning that $\mu \neq 1$; consequently, the stabilizer $G_{|x\rangle} = G_{|x_1\rangle + \varepsilon|x\rangle}$ of the vector $|\ x\rangle$ (and $|\ x_1\rangle + \varepsilon\ |\ x\rangle$) is proper subgroup of $G = G_{|x_1\rangle}$. Under these conditions, the invariant polynomials are formed by the coordinates $\xi_{\mu t_\mu m}$, only. The first order term vanishes immediately (as it has been explained), and this shows that in the considered directions each fixed point of the group action is stationary for any invariant functional. Therefore, for the normalized vector $|\,x, \mu t_\mu\rangle$ (the norm is not essential in what follows), (4.5) reads:

$$F(|\,x_1\rangle + \varepsilon\,|\,x, \mu t_\mu\rangle) = F(|\,x_1\rangle) + \varepsilon^2 A^{[2]}_{\mu t_\mu} + \sum_{r>2} \varepsilon^r \sum_{i=1}^{a_1^{[r\mu]}} A^{[r]}_i p^{[r\mu]}_i,$$

where the polynomials $\{p^{[r\mu]}_i \mid i = 1, \ldots, a^{[r\mu]}_1\}$ span the subspace of the identical representation in the space spanned by the r-th order monomials over the coordinates $\xi_{\mu t_\mu m}$.

When the identical representation is not among the irreducible components of $[D^{(\mu)^r}]$, then $a_1^{[r\mu]} = 0$, and there is no r-th degree invariant polynomial. Thus, the term of order r in the expansion (4.5) disappears (in the vicinity of the fixed point) along the direction of $|x, \mu t_\mu\rangle$. There are invariant polynomials of even orders for any irreducible representation: the square of the norm of the vector, $p^{[2\mu]} = \sum_m \xi^2_{\mu t_\mu m}$, is the unique quadratic invariant of any irreducible representation, and its powers are even order invariants. Therefore, some odd-degree terms for some irreducible representations disappear *a priory* ($a_1^{[r\mu]} = 0$ is sufficient condition, related to the group only; other terms may vanish also, due to some specific properties of the considered functional). The example of this type has been already used: $a_1^{[r\mu]} = 0$ holds for $r = 1$ and any $\mu \neq 1$. If $A^{[2]}_{\mu t_\mu}$ is positive (negative), $|x_1\rangle$ is minimum (maximum) for the chosen direction; if $A^{[2]}_{\mu t_\mu} = 0$ the higher orders must be examined to determine the type of the stationary point. For example, if $A^{[2]}_{\mu t_\mu} = 0$ and there are third order terms, then $|x_1\rangle$ is a point of inflection, and if the third order terms vanish too, the sign of the fourth order term must be discussed. It is also possible that the functional is constant along some direction, which is manifested as the reduction of the expansion to the constant: $F(|x_1\rangle + \varepsilon\,|x\rangle) = F(|x_1\rangle)$; this has been the case for the translational and rotational modes of the harmonic potential. In such examples $|x_1\rangle$ is not isolated extreme point[2].

4.3 Spontaneous symmetry breaking

The physical theories are based on some invariant functional on the state space (*e.g.* potential energy in the classical mechanics is the functional over the phase space), which governs the dynamics of the system, in the sense that its minimal points are the equilibrium (stationary) states of the system (the states taken by the isolated system). It has been shown that the fixed points are stationary along the directions of the irreducible representations (except the identical one). If the coefficient $A^{[2]}_{\mu t_\mu}$ is negative, such point is maximal, and the system is instable for the displacements along the vectors $|x, \mu t_\mu\rangle$ from $\mathcal{S}^{(\mu t_\mu)}$: it spontaneously departs the state $|x_1\rangle$, and evolves in the direction of $|x, \mu t_\mu\rangle$, being stabilized if some local minimum lays along this line, or turns in some other direction at non minimal stationary points. The symmetry of all the points along the line $|\,x_1\rangle + \alpha\,|\,x, \mu t_\mu\rangle$ is the same, $G_{|x,\mu t_\mu\rangle}$, meaning that at the very beginning of the motion from $|\,x_1\rangle$ in the direction of the vector $|\,x, \mu t_\mu\rangle$, the symmetry of the system is instantaneously (*i.e.* discontinuously) diminished from G to $G_{|x,\mu t_\mu\rangle}$. This process is called the *spontaneous symmetry breaking*, since it occurs without any external change of symmetry (note that there are systems with spontaneously broken symmetry: the symmetry of their ground state — the stable state minimizing the mean value of the hamiltonian — is a proper subgroup of the hamiltonian symmetry group, [3, 39]). Some common characteristics of such processes will be studied in this section.

[2] In fact, the fixed points for the linear action of the group (given by $D(G)$) form the subspace $\mathcal{S}^{(1)}$, and they cannot be isolated. Their isolation can appear in the physical sense: the one-dimensional subspace in the state space of the system describes the same physical state, while among the operators $c\rho$ collinear with the statistical operator ρ, there is no other mixed state.

The symmetry of the vector in $\mathcal{S}$ is defined as the group of the state (§ 1), *i.e.* the stabilizer of that vector when G acts by the representation $D(G)$. Thus, the symmetry of the point $|x\rangle \in \mathcal{S}$ is the group $G_{|x\rangle} \stackrel{\text{def}}{=} \{g \in G \mid D(g)\,|x\rangle = |x\rangle\}$. If $G_{|x\rangle}$ is a proper subgroup of G, the representation $D(G)$ is not reduced to the identical representation in the subspace spanned by $|x\rangle$, but the subduced representation, $D(G) \downarrow G_{|x\rangle}$ is reduced, and it acts as the identical representation in this subspace as well as in the subspace spanned by the vector $|x_1\rangle + \varepsilon\,|x\rangle$.

Let $|x\rangle = |x, \mu t_\mu\rangle \in \mathcal{S}^{(\mu t_\mu)}$, where $|x, \mu t_\mu\rangle$ is the vector of the standard basis found in the previous section. In the space $\mathcal{S}^{(\mu t_\mu)}$ the operators $D(G)$ are reduced, and act as the representation $D^{(\mu)}(G)$. Therefore, in the lineal over $|x, \mu t_\mu\rangle$ the subduced representation $D^{(\mu)}(G) \downarrow G_{|x,\mu t_\mu\rangle}$ is reduced to identical representation, meaning that the coefficient a_1^μ in the compatibility relations $D^{(\mu)}(G) \downarrow G_{|x,\mu t_\mu\rangle} = \sum_\nu a_\nu^\mu D^{(\nu)}(G_{|x,\mu t_\mu\rangle})$, is positive.

Useful generalization of the notion of the stabilizer is the *epikernel*, [37], of the representation $D^{(\mu)}(G)$ for the subspace $\mathcal{S}^{(\mu)'}$ (being subspace in $\mathcal{S}^{(\mu)}$). This is the maximal subgroup $\mathrm{Ek}(G, \mathcal{S}^{(\mu)'})$ of G, such that all the vectors of subspace $\mathcal{S}^{(\mu)'}$ are fixed points for the subduced irreducible representation $D^{(\mu)}(G)$ onto this epikernel. Obviously the kernel of the representation is the epikernel for the complete carrying space of the representation: $\ker(D^{(\mu)}(G)) = \mathrm{Ek}(G, \mathcal{S}^{(\mu)})$ (this is the source of the name epikernel). Since the stabilizer is also an epikernel, $G_{|x,\mu t_\mu\rangle} = \mathrm{Ek}(G, \mathrm{span}(|x, \mu t_\mu\rangle))$, but in general case it is not required that the subspace $\mathcal{S}^{(\mu)'}$ is one-dimensional, the epikernel appears as a generalization of the stabilizer. It is important in slightly more general theory, because it includes the cases when $G_{|x\rangle}$ acts as identity onto some vectors outside the lineal over $|x\rangle$, and thus appears as the epikernel of the many dimensional subspace. The epikernels of the different irreducible representations of the group G are the symmetries of the states after the symmetry breaking. Thus, list of the epikernels for all the irreducible representations of the group G gives the possible symmetry groups of the system in the different states.

Let $|y\rangle = |x_1\rangle + \alpha\,|x, \mu t_\mu\rangle$ be the local minimum on the trajectory in the direction $|x, \mu t_\mu\rangle$ of the functional. Due to its invariance, the same extreme properties of the functional are found at the points of the whole orbit of the vector $|y\rangle$, *i.e.* at the points $G\,|y\rangle = \{D(g)\,|y\rangle \mid g \in G\}$. This set is obtained by the action of the transversal (set of the cosets representatives) of the stabilizer $G_{|y\rangle} = G_{|x,\mu t_\mu\rangle}$ on $|y\rangle$. Thus, all these points are minimal for the functional, and all of them are of the form $|x_1\rangle + \alpha D^{(\mu)}(g)\,|x, \mu t_\mu\rangle$. Accordingly, at $|x_1\rangle$ the functional equally allows motions toward all these points of the orbit, and the system, being isolated, *randomly* departs toward one of them. Since the orbit consists of the equivalent minima, if these points are connected (making a continuous set), the functional enables deliberate transitions between them; the tunnel effect in the quantum mechanics gives the non vanishing probabilities for the transitions between the minima even if they form a discrete set. Therefore, if there is a continuous set formed by the transversal of the stabilizer, *i.e.* if the *coset space* $G/G_{|y\rangle}$ is a manifold of the non zero dimension, the functional allows free motion along these continuous parts of the orbits (these degrees of freedom are called *Goldstone modes*). An example appears when the stabilizer is invariant subgroup, and the corresponding factor group is Lie group G' (and this is the case whenever $G = G_{|y\rangle} \otimes G'$).

In the vicinity of the minimal point $|\,y\rangle$, the same analysis can be performed again, but with the stabilizer $G_{|y\rangle}$ in the role of the group G (since $G_{|y\rangle} < G$, the functional is still invariant). Now, the whole space is decomposed onto the irreducible subspaces $\mathcal{S}^{(\nu t_\nu)}$ of the stabilizer, and for the motions along the vectors from $\mathcal{S}^{(\nu t_\nu)}$ the series $F(|\,y\rangle + \varepsilon\,|\,x, \nu t_\nu\rangle) = F(|\,y\rangle) + \varepsilon^2 A_{\nu t_\nu} \sum_n \xi^2_{\nu t_\nu n} + ...$ is found.

Since the subspaces of the different irreducible components of $D(G)$ are mutually orthogonal, the vectors from the subspaces of the non identical irreducible representations are orthogonal to all the fixed points, and especially to $|\,x_1\rangle$. Nevertheless, after the beginning of motion along $|\,x, \mu t_\mu\rangle$, some of the vectors from the standard basis in $\mathcal{S}^{(\mu t_\mu)}$ are no more orthogonal to the instant state, and the corresponding scalar products are proportional to the distance from the fixed point: $\langle \mu t_\mu m|\,(|\,x_1\rangle + \varepsilon\,|\,x, \mu t_\mu\rangle) = \varepsilon\langle\ \mu t_\mu m\,|\,x, \mu t_\mu\rangle$.

4.4 Phase transitions

Phase transitions are among main objectives of solid state physics. Although there are many different types of them, inspiring many elaborated theories, some phenomenological characteristics are quite general. *(i)* When the parameters of the system are varied (*e.g.* the temperature is decreased), and some critical values attained and passed through, the crystal with the space group G changes the structure; its new space group is G' (the magnetic or the double groups can be also taken into account, depending on their relevance for the transition). *(ii)* It has been observed that the mean value of some physical quantity, Q, called the *order parameter*, is changed during the transition from 0 (before the transition) to some other value (after the transition). *Landau's theory* [4, 38] describes such *continuous phase transitions* as spontaneous symmetry breakings. It is based on the following common properties.

The state space $\mathcal{S}$ is the set of all the states of the system, meaning the real space of all the observables, since this is the minimal linear space containing all the statistical operators. Scalar product is standard: $(A, B) = \mathrm{Tr}AB$ (observables are hermitean operators). The functional relevant for the considered dynamics is *free energy*, being invariant with respect to the space group G, and the equilibrium states are minimal points of free energy. The set of all relevant thermodynamic parameters of the system (temperature, pressure, external fields etc.) is denoted by T, and their possible values are points of the *parameter space*, being the manifold defined by the ranges of the parameters. Continuous motion of the system defines a curve in the parameter space, and the phase transition occurs when the *critical point*, $T = T_c$, lies on this curve.

Before coming to T_c (the domain denoted by T_-), the state of the system is the fixed point $\rho_1(T_-)$, being the minimal point of the free energy. In the critical point the state of the system $\rho_1 = \rho_1(T_c)$ is still stable. Nevertheless, after passing through T_c (domain T_+), the state ρ_1 is not stable any more, and the transition occurs to the state with the symmetry G'. The thermodynamic parameters are incorporated in the coefficients $A^{[r]}_{i_r}$, which are therefore the functions $A^{[r]}_{i_r}(T)$. Continuity of these functions is assumed within the model. In the simplest case (the generalization is straightforward), the order parameter is the element, Q,

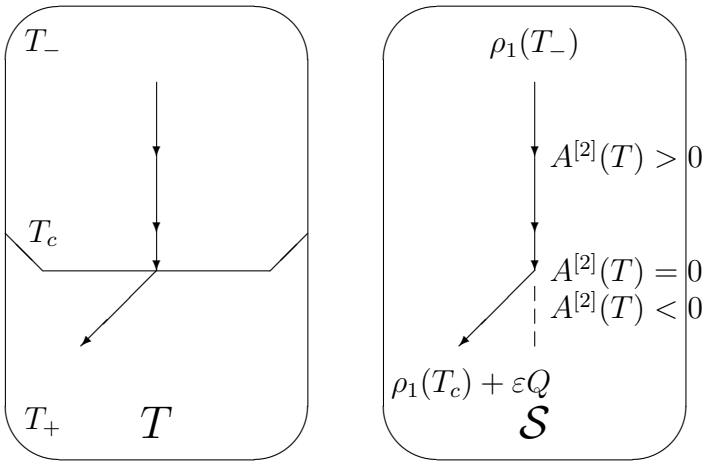

Figure 4.1: The evolution of the system in the parameter space, T, and in the state space, $\mathcal{S}$, during the phase transition. The curve T_c, confining the phases, solves the equation $A^{[2]}_{\mu t_\mu}(T_c) = 0$.

of the standard basis in the space of the observables; this implies that the other observables of the standard basis with vanishing mean values before the transition retain this property immediately after the transition. Thus, the change of the mean value of Q, from $\mathrm{Tr}Q\rho_1 = 0$ (before the transition) to non vanishing one after the transition, indicates that the system evolves along the direction of $\rho_1 + \varepsilon Q$ (in accordance with the last conclusion in § 4.3). Consequently, if $Q \in \mathcal{S}^{(\mu t_\mu)}$, then $A^{[2]}_{\mu t_\mu}(T_-) > 0$ before the transition, and $A^{[2]}_{\mu t_\mu}(T_+) < 0$ afterwards. Due to the continuity assumption, the parameters of the critical point fulfill the equation $A^{[2]}_{\mu t_\mu}(T_c) = 0$. This equation determines the hyper surface confining different phases. Stability of the state ρ_1 implies that in T_c the third term of the expansion vanishes also (since the quadratic term is 0). To differ from the previous one, this condition cannot be treated as the requirement on the coefficient $A^{[3]}_{\mu t_\mu}(T_c)$ yielding the equation over the parameters: the dimension of the surface confining the phases in the parameter space would be less for two then the dimension of the parameter space (two simultaneous equations for $A^{[2]}_{\mu t_\mu}(T_c)$ and $A^{[3]}_{\mu t_\mu}(T_c)$), and it could be bypassed — the transition and the symmetry breaking would be avoided. Therefore, the third order term must be *a priori* annihilated by the symmetry based condition: there is no third order invariant polynomial, *i.e.* $[D^{(\mu)^3}]$ does not contain the identical representation. Finally, the stability of ρ_1 at T_c is realized by the condition of the positivity of the fourth order term.

Since the space groups are discrete, the orbit of the final equivalent stable configurations is discrete, too. As it has been explained, the crystal randomly comes to one of them. In the large enough realistic crystals, the parts of it are not correlated, and the transition occurs independently in the different *domains*, showing the different choices of the orbit points. In fact, the averaging over all the points of an orbit restore the initial symmetry, while the

symmetry of each single point is its stabilizer, *i.e.* one of the epikernels of the group G.

Two tasks are usually considered within this theory. The *Landau's problem* is to predict the symmetry of the new phase, if the order parameter and the initial symmetry group are known (*e.g.* it is known that in the ferromagnetic transition the order parameter is the corresponding component of the axial vector of the magnetic field). The solution of this problem consists of the encountering of the epikernels of the irreducible representation of the order parameter, giving the list of the possible new symmetry groups. The *inverse Landau's problem* is to find the order parameter for the transition, when the symmetry groups of both the phases are known. To solve it, all of the epikernels of all the irreducible representations should be found; then the representations having the new symmetry group as one of the epikernels are selected, and among them only those without identity component in the decomposition of the third symmetrical power are retained. The candidates for the order parameters are the physical quantities transforming according to one of these representations.

Incorporating some additional physical requirements, Landau's theory can be used for other predictions. *Lifshic's condition* is frequent and useful example. It is assumed that the new phase is spatially homogeneous, *i.e.* that the order parameter does not depend on the coordinates, or equivalently that the gradient of the order parameter vanishes. Obviously, in the free energy functional the components of the gradient must be incorporated, and the analogous expansion straightforwardly gives the group theoretical equivalent of the requirement: there is no common irreducible component in the skew symmetrical square of the representation of the order parameter, and the polar vector representation. Incommensurate phase transitions, crystal defects and some other phenomena are considered along the same lines. Also, the critical exponents are introduced through the choice of the invariant polynomials within different models of the free energy functional, [38].

4.5 Theories of the fourth order

In the different fields of physics the important role is given to the *standard model*, or φ^4 *theories*, [39, 40]. This significant example of the spontaneous symmetry breaking is given by the functional of the simplest nontrivial, but quite fruitful form:

$$F(|\,x\rangle) = A^{[2]}x^2 + A^{[4]}x^4, \tag{4.6}$$

(x is the norm of the vector $|\,x\rangle$). Applicability of the results greatly increases if (4.6) is interpreted as the fourth order expansion in the vicinity of $|x_1\rangle = 0$ of some more complicated functional, invariant under the group $\mathrm{SO}(n,\mathbb{R})$ (or $\mathrm{U}(n)$ in the complex case): $|x_1\rangle$ is obviously the fixed point of this group, and zero order term is ignored since it does not influence the physical results. Note that this is the fourth order invariant polynomial for the identifying representation of the group (for the classical matrix groups, the group itself is one of its irreducible representations — identifying representation, § A.2.1).

If $\{|i\rangle | i = 1,\dots,n\}$ is an orthonormal basis, and $|x\rangle = \xi_n\,|n\rangle$, the potential takes the form $F(\xi_n) = A^{[2]}\xi_n^2 + A^{[4]}\xi_n^4$. The first and the second derivatives are $F'(\xi_n) = (2A^{[2]} + 4A^{[4]}\xi_n^2)\xi_n$

and $F''(\xi_n) = 2A^{[2]} + 12A^{[4]}\xi_n^2$. The point $|\,x_1\rangle = 0$ is stationary (the first derivative vanishes for $\xi_n = 0$), and to provide the maximality (which is the source of the spontaneous symmetry breaking), it is sufficient that $A^{[2]}$ is negative (fig. 4.2). Then the next extreme in the direction of the vector $|\,x\rangle)$ is at $\xi_n^0 = \sqrt{-\frac{1}{2}\frac{A^{[2]}}{A^{[4]}}}$. This point is minimum, since the value of the second derivative at ξ_n^0 is $-4A^{[2]} > 0$.

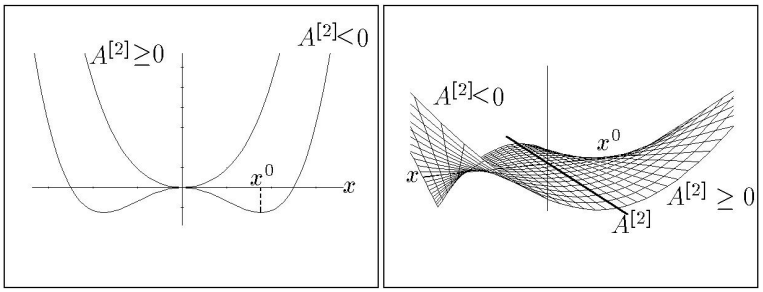

Figure 4.2: The potential $F(|\,x\rangle) = A^{[2]}x^2 + A^{[4]}x^4$ as the function of x and $A^{[2]}$ (right), and as a function of x with two fixed values of $A^{[2]}$ (left): for $A^{[2]} \geq 0$, the point $x = 0$ is minimum, and for $A^{[2]} < 0$ the same point is maximum, causing instability of the system and the transition to the minimal position $x^0 = \sqrt{-\frac{1}{2}\frac{A^{[2]}}{A^{[4]}}}$.

The form of the functional around this point is easily found substituting $\xi_n = \xi_n^0 + \eta$ in (4.6):

$$\begin{aligned} F(\eta) &= -\frac{{A^{[2]}}^2}{4A^{[4]}} - 2A^{[2]}\eta^2 \\ &+ \sqrt{-8A^{[2]}A^{[4]}}(\sum_{i=1}^{n-1}\xi_i^2)\eta + \sqrt{-8A^{[2]}A^{[4]}}\eta^3 + A^{[4]}(\sum_{i=1}^{n-1}\xi_i^2)^2 + 2A^{[4]}(\sum_{i=1}^{n-1}\xi_i^2)\eta^2 + A^{[4]}\eta^4. \end{aligned} \tag{4.7}$$

The coefficient of the quadratic term is in field theory interpreted as the half of the square of the mass of the (quasi)-particle described by the field x; the quadratic terms correspond to the free fields (without interaction interaction), while the interaction is represented by the higher order terms. Thus, the expression (4.6) describes the *multiplet* of n particles, with equal masses $m_\xi = \sqrt{2A^{[2]}}$, transforming among themselves under the action of the group $\mathrm{SO}(n,\mathbb{R})$ (or $\mathrm{U}(n)$). Negative square of the mass indicates instability of the system, resulting in the transition to the new state. The dynamics is now governed by the functional (4.7), and it describes one particle field, η, of the mass $m_\eta = 2\sqrt{-A^{[2]}}$, interacting with the massless fields $\xi_1, ..., \xi_{n-1}$, called *Goldstone's bosons*.

To understand this result, note that the direction of the n-th vector is chosen arbitrarily, and any other vector from the subspace of the initial particles (in the initial subspace, $\mathbb{R}^n$ or $\mathbb{C}^n$, the orthogonal or the unitary group acts) could be used with the same result. Therefore, it is clear that the found minimum must be continuously degenerate: the orbit of the point $\xi_n^0 \neq 0$ is the sphere S^{n-1}. The stabilizer of the same point is the group $\mathrm{SO}(n-1,\mathbb{R})$, describing the rotations in the subspace orthogonal to ξ_n^0. Therefore, the number of the generators of

the symmetry group of the state has decreased from $\frac{n(n-1)}{2}$ initially, to $\frac{(n-1)(n-2)}{2}$ finally. The remaining $n-1$ generators determine the coset space of the stabilizer, being manifold of the dimension $n-1$; these cosets generate the orbit — the sphere S^{n-1} (quite analogous results can be obtained for unitary groups). Therefore, the motions restricted to this sphere are free, and the excitations describing such motions are without quadratic term in the potential; within the standard language of the theory, the corresponding (quasi)-particles are massless, and these are the Goldstone's bosons.

4.6 Adiabaticity and Jahn-Teller effect

When complex physical systems are studied, the technical difficulty to solve the obtained equations, is usually surpassed by different approximation. In contrast to ones related to specific problems, the *adiabatic approximation* belongs to the common methods of physics.

Many systems can be approximately decomposed onto two subsystems, such that one of them ("light") follows evolution of the other one ("heavy"). Then the problem of the "light" subsystem is considered at first, incorporating explicitly in the potential its dependence on the state of the "heavy" subsystem. For the state $|x\rangle$ of the "heavy" subsystem, the potential $V_{|x\rangle}$ of the "light" one is obtained. Its minimal points are the stable states of the "light" subsystem when the "heavy" is in $|x\rangle$; thus, such stable state is function of the state of the "heavy" subsystem. The adiabatic approximation consists in the change of the potential (*i.e.* of the evolution), such that during the motion of the "heavy" subsystem the stability of the "light" one is not disturbed: all the terms causing transition of the "light" subsystem (during the motion of the "heavy" subsystem in the vicinity of $|x\rangle$) from the minimal point of $V_{|x\rangle}$ to some non minimal point of the potential $V_{|x'\rangle}$ are neglected. In other words, the "light" system is instantaneously stabilized during the motion of the "heavy" system. Quantum mechanical formulation of this procedure is postponed for the next chapter, and only the properties related to symmetry breaking of such modeled systems are discussed here.

The total state space is $\mathcal{S} = \mathcal{S}_L \otimes \mathcal{S}_H$. The evolution is determined by the total potential (invariant functional on the total space):

$$V(|x\rangle, |y\rangle) = V_L(|y\rangle) + V_H(|x\rangle) + V_{LH}(|x\rangle, |y\rangle),$$

where $V_{LH}(|x\rangle, |y\rangle)$ is the potential of the interaction, while $V_H(|x\rangle)$ and $V_L(|y\rangle)$ are the potentials of the isolated subsystems.

Let the "heavy" system be in the state $|x_1\rangle$. It is fixed point for its stabilizer group $G = G_{|x_1\rangle}$, being represented in $\mathcal{S}_H$ and $\mathcal{S}_L$ by $D_H(G)$ and $D_L(G)$, respectively. Due to the assumed adiabatic property, the dynamics of the "light" system is determined by the potential $V_{|x_1\rangle}(|y\rangle) = V(|x_1\rangle, |y\rangle)$. This is a functional on $\mathcal{S}_L$, and must be invariant with respect to G. Further, the state of the "light" system is stable, *i.e.* it is one of the minima of $V_{|x_1\rangle}$. If $|y, \nu t_\nu\rangle \in \mathcal{S}_L^{(\nu t_\nu)}$ is such a state[3], then the whole orbit contains equivalent minimal points, and

[3]The considered functionals are related to some hamiltonians, and their minimal points are hamiltonian

due to irreducibility of $D^{(\nu)}(G)$, these vectors span $\mathcal{S}_L^{(\nu t_\nu)}$ (§ A.2.2). Clearly, in the adiabatic approximation the dynamics that tosses the "light" subsystem from $\mathcal{S}_L^{(\nu t_\nu)}$ during the change of state of the "heavy" subsystem is neglected, and only displacements from $|\, y, \nu t_\nu\rangle$ within $\mathcal{S}_L^{(\nu t_\nu)}$ is considered. Therefore, the motion $|\, x_1\rangle + \varepsilon\, |\, x, \mu t_\mu\rangle$ of the "heavy" subsystem yields new stable state of the "light" subsystem in the form $|\, y, \nu t_\nu\rangle + \eta \sum_n \eta_{\nu t_\nu n}\, |\, \nu t_\nu n\rangle$. To provide stability of the "light" subsystem during the motion (the adiabatic approximation) no term linear over $\eta_{\nu t_\nu n}$ may appear in the expansion of the potential:

$$V(|\, x_1\rangle + \varepsilon\, |\, x, \mu t_\mu\rangle, |\, y, \nu t_\nu\rangle + \eta \sum_n \eta_{\nu t_\nu n}\, |\, \nu t_\nu n\rangle) =$$

$$V(|\, x_1\rangle, |\, y, \nu t_\nu\rangle) + \eta^2 \sum_{nn'} C_{nn'}(\varepsilon) \eta_{\nu t_\nu n} \eta_{\nu t_\nu n'} + \dots$$

The stability of the "heavy" subsystem depends on the leading term $\eta^2 \varepsilon \sum_{nn'm} C_{nn'm} \eta_{\nu t_\nu n} \eta_{\nu t_\nu n'} \xi_{\mu t_\mu m}$ in the additional expansion over ε. This polynomial is transformed according to the representation $[D^{(\nu)^2}(G)] \otimes D^{(\mu)}(G)$. Consequently, the system is instable for the displacements of the "heavy" subsystem along the vectors of $\mathcal{S}_H^{(\mu)}$, if there is invariant polynomial linear over $\xi_{\mu t_\mu m}$ and quadratic over $\eta_{\nu t_\nu n}$, *i.e.* if the above product of the representations contains the identical component. Equivalently, if $D^{(\mu)}(G)$ (the representations are real, otherwise this refers to the complex conjugated representation) is contained in $[D^{(\nu)^2}(G)]$, the "heavy" system is instable, and goes to the state of the lower symmetry. If $D^{(\nu)}$ is one dimensional (the state of the "light" system is not degenerated), the symmetrical square is the identical representation, and the displacements are allowed only in the directions of other fixed points, *i.e.* without symmetry breaking.

In the previous expression μ denotes any of the irreducible components of $D_H(G)$, and ν one of the components of $D_L(G)$. The system is *adiabatically instable* if in the symmetrical square of each of the irreducible representations of its group of symmetry there is at least one irreducible component, differing from the identical one, of $D_H(G)$. If the "heavy" subsystem is adiabatically instable, independently of the concrete "light" subsystem, the symmetry G of the "heavy" subsystem is breaking whenever the "light" one is in the degenerate state. Nevertheless, in the new state the whole procedure can be repeated, only instead of the group G, the symmetry group $G_{|x,\mu t_\mu\rangle}$, *i.e.* the corresponding epikernel of $D^{(\mu)}$ and its representations would be considered. If the condition of the adiabatic instability is fulfilled also for the epikernels, their epikernels, etc., the symmetry is breaking unless the "light" system attains the state of one-dimensional representation of the actual group of symmetry of the "heavy" system, *i.e.* unless the state of the state of the "light" subsystem becomes non degenerate.

Note that taking of the potential of the "light" system in the slices, $V(|\, x_1\rangle, |\, y\rangle)$, is not approximation, but only preparation of formalism for the forthcoming approximation. On the contrary, the prohibition of deverbs of the irreducible subspaces of $\mathcal{S}_L$ is the approximation. Its validity depends on the problem (it appears that the rate of the masses of the subsystems

eigenvectors. Therefore, the choice of the minimal point from an (multiple) irreducible subspace is naturally determined as eigenvector.

is important to justify the approximation, which has caused the use of the "attributes"). Note also, that although $|x_1\rangle$ is fixed point of G (by definition), it is not the extremal point, because the "heavy" system is not isolated: the first order term over $\xi_{\mu t_\mu m}$ is enabled by the "light" degrees of freedom of the "light" system (third order invariant polynomial over all the coordinates).

Following the conjecture of the Lav Landau, [3], Jahn and Teller showed, [41], that the nonlinear molecules are vibrationally instable if the electronic states are degenerate (Kramers degeneracy, referring to the antilinear time reversal operator, § 2.6.1, does not count). In fact, they showed that the symmetrical square of any physically irreducible many dimensional representation of any point group of the finite order, has an irreducible component in common with the vibrational representation of the molecule with such symmetry. Here, the ions are in the role of the "heavy" system, while the electrons are the "light" one, and $D_H(G)$ is the dynamical representation of the ionic system. The translational and the rotational modes should not be considered, since the whole system is isolated, and the invariant functional is constant along such displacements (the corresponding terms are absent in the first and the higher orders of the expansion, and cannot be responsible for the instability). This means that for the molecules there always exists vibrational (not translational or rotational) non symmetrical (*i.e.* corresponding to non identical representation) normal mode, which in the total potential appears in the first order terms (over ionic displacements), causing the instability of the ions. This is manifested as the change of their relative positions, with instantaneous symmetry breaking. Since the epikernel of the point group is again a point group, the described symmetry breaking occurs unless the electronic level is split to the non degenerate ones: only such states are stable for the whole molecule.

The same property is shared by the line groups, [26], *i.e.* by the polymers. As for the crystals, there is no systematic study of this type; some partial, mostly experimental, results in accordance with those for the molecules and polymers, [42], have established common belief in the universal validity of the Jahn-Teller's theorem. Nevertheless, although systematic research of diperiodic systems is not complete, it has been shown that the diperiodic groups break down the theorem: there are groups allowing degenerate electronic states with no electron-phonon interaction of the first order. For example, the high temperature superconducting compounds may not be periodical along the z-axis (perpendicular to the conducting plane), and their symmetry is diperiodic, determined by the geometry of the CuO_2 layers; it may be important that exactly this layer (containing two orbits of the group DG37) breaks the Jahn-Teller's theorem, allowing the degenerated electronic states.

Although this is an approximate conclusion, due to the rate of the masses of the electrons and ions, it is practically exact result, and frequently experimentally verified.

Chapter 5

ELECTRONIC LEVELS IN MOLECULES AND CRYSTALS

The dynamical problem of many particle systems cannot be solved exactly. This causes a series of approximations, and the first of them, the adiabatic or the Born-Oppenheimer's approximation, is separation of the electronic and the ionic subsystems. Also, some additional approximations are necessary, and all of of them incorporate the exact symmetry analysis, to provide at least qualitatively good results. This enable to use the results obtained in the rough approximation as a starting point for further more accurate calculations (*e.g.*, the states obtained in the Hückel's method are trial states in some variational methods).

5.1 Adiabatic model in quantum mechanics

General concept of the adiabatic behavior of the composite systems, [7, 3], considered briefly in the previous chapter, gives numerous important results within quantum mechanical applications. Therefore, precise quantum mechanical formalism is developed to introduce relevant notions, [43]. Since the system is composed of two subsystems, "light" and "heavy", the total state space is $\mathcal{S} = \mathcal{S}_L \otimes \mathcal{S}_H$. The evolution is determined by the hamiltonian:

$$H = T_L \otimes I_H + I_L \otimes T_H + V,$$

T denotes the kinetic, and $V = V_L \otimes I_H + I_L \otimes V_H + V_{LH}$ the potential energy (I_L and I_H are the identical operators in $\mathcal{S}_L$ and $\mathcal{S}_H$, respectively). Let $\hat{Q}$ be the operator of coordinate of the "heavy" subsystem (in fact, the set of the commuting operators of all the coordinates is understood); this is a complete observable in $\mathcal{S}_H$ (its eigenvalues, Q, uniquely correspond to the states of the "heavy" subsystem). The operator $\hat{Q}$ commutes with all the potentials and with T_L: $V_H = \int_Q V_H(Q) \mid Q\rangle\langle Q \mid \mathrm{d}Q$ (spectral form), $V_{LH} = \int_Q V_{LH}(Q) \mid Q\rangle\langle Q \mid \mathrm{d}Q$ (here $V_{LH}(Q)$ is operator in $\mathcal{S}_L$).

The total space $\mathcal{S}$ can be understand as orthogonal sum of the subspaces $\mathcal{S}_L(Q) \stackrel{\mathrm{def}}{=} \mathcal{S}_L \otimes |Q\rangle$ (precisely, $\mathcal{S}_L(Q)$ is the direct product of $\mathcal{S}_L$ with the one dimensional lineal over $\mid Q\rangle$): $\mathcal{S} = \oplus_Q \mathcal{S}_L(Q)$. Thus, the total space is sum of the *vertical subspaces* or *fibres* $\mathcal{S}_L(Q)$, each fibre

being isomorphic to $\mathcal{S}_L$. Since $\mathcal{S}_L(Q)$ is invariant subspace of the operator $H_L = T_L \otimes I_H + V$, in each fiber H_L is reduced to $H_L(Q)\,|Q\rangle\langle Q|$, where $H_L(Q) \stackrel{\text{def}}{=} T_L + V_L + V_{LH}(Q) + V_H(Q) I_L$ is operator in $\mathcal{S}_L$.

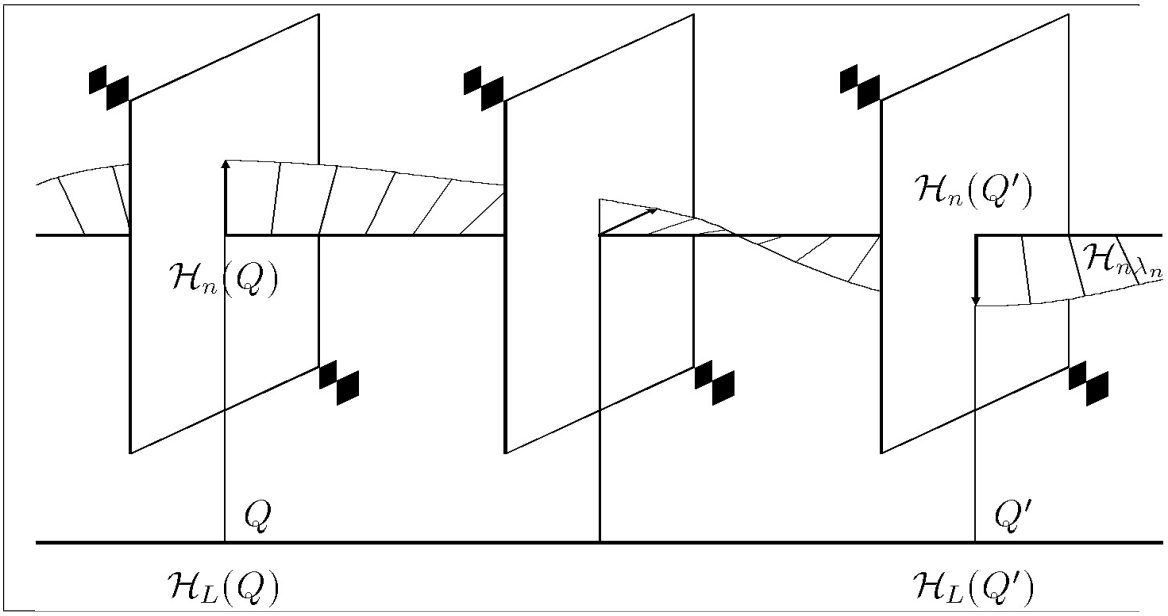

Figure 5.1: *The decomposition of the total space $\mathcal{S}$ onto the vertical subspaces $\mathcal{S}_L(Q)$. The vectors $|n\lambda_n, Q\rangle\,|Q\rangle$ in the different points Q span the horizontal subspace $\mathcal{S}_{n\lambda_n}$.*

Solving the eigenvalue problem of $H_L(Q)$, its spectral form $H_L(Q) = \sum_n \epsilon_n(Q) P_n(Q)$, orthonormal eigen basis $\{|n\lambda_n, Q\rangle\}$, and eigensubspaces $\mathcal{S}_{Ln}(Q)$, are found. In what follows, the spectrum of $H_L(Q)$ will be discrete. Obviously, the n-th eigenvalue is function of Q. To sumarize, Q becomes the parameter distingushing different operators of the family $H_L(Q)$ (fig. 5.1). This family generates the family of the eigen bases $\{|\, n\lambda_n, Q\rangle\}$: for each Q one eigenbasis in $\mathcal{S}_L$ is determined.

In this way in the total space the common eigenbasis $\{|n\lambda_n, Q\rangle\,|Q\rangle\}$ of H_L and $\hat{Q}$ is singled out (note that $[\hat{Q}, H_L] = 0$); the corresponding eigenvalues are $\epsilon_n(Q)$ and Q, respectively. It is important that this basis, called the *adiabatic basis*, is not the product of the bases of $\mathcal{S}_L$ and $\mathcal{S}_H$, although its vectors are not correlated[1]. Due to always assumed continuity of $H_L(Q)$ over Q, the eigen energies $\epsilon_n(Q)$ are continuous function of Q. Therefore, if the point Q' is in the vicinity of Q, the discretness of the eigenvalues of $H_L(Q)$ and $H_L(Q')$ provide the corespondence of the eigenergies: for each $\epsilon_n(Q)$ the nearest eigen energy of $H_L(Q')$ is singled out, and it will be labeled by the same index n: $\epsilon_n(Q')$. This also gives the correspondence of the eigen subspaces $\mathcal{S}_{Ln}(Q)$, enabling to chose their bases $\{|\, n\lambda_n, Q\rangle | \forall\lambda\}$

[1]If $\{|\, i\rangle\}$ and $\{|\, q\rangle\}$ are bases in the spaces $\mathcal{S}_L$ and $\mathcal{S}_H$ respectively, their product $\{|\, i\rangle\otimes|\, q\rangle | \forall i, q\}$ is a basis in $\mathcal{S}_L \otimes \mathcal{S}_H$, which is called *product* or *fixed* basis. Its vectors, being the products of the vectors from the factor spaces are not correlated. In the adiabatic basis, each vector $|\, Q\rangle$ from the second basis, is multiplied by diffrent basis of the first space.

continuously depending on Q. The *horizontal subspace* $\mathcal{S}_{n\lambda_n}$ in $\mathcal{S}$, spanned by the vectors $\{\mid n\lambda_n, Q\rangle \mid Q\rangle \mid \forall Q\}$ is now well defined; it is isomorphic to $\mathcal{S}_H$ (natural isomorphism is $\mid Q\rangle \mapsto \mid n\lambda_n, Q\rangle \mid Q\rangle$). Orthogonal summation of these horizontal subspaces yields the *horizontal slices*, the subspaces $\mathcal{S}_n = \oplus_{\lambda_n} \mathcal{S}_{n\lambda_n}$.

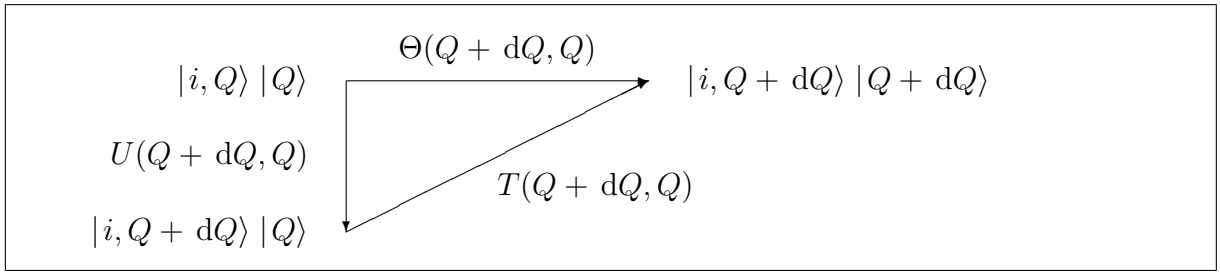

Figure 5.2: **Hamiltonian conection:** *the motion* $\Theta(Q + dQ, Q) = e^{\frac{-i}{\hbar} dQ P_H^0}$ *from* Q *for* dQ *of the total system is decomposed to the motion* $U(Q + dQ, Q) = e^{\frac{i}{\hbar} A(Q)\, dQ}$ *of the "light", and* $T(Q + dQ, Q) = e^{\frac{-i}{\hbar} dQ P_H}$ *of the "heavy" subsystem. The derivative* $-i\hbar\frac{\partial}{\partial Q}$ *in the fixed basis represents the operator* P_H*, while in the adiabatic basis it represents the operator* P_H^0*.*

In comparison to the choice of the fixed basis in $\mathcal{S}$ (see the footnote **??**), the adiabatic basis yields noticeable differences with respect to the representations of the relevant operators. The eigen basis of $\mathcal{S}_L$, corresponding to the operator $H_L(Q)$, is connected to the eigenbasis of $H_L(Q')$ by the unitary operator U: $\mid i, Q'\rangle = U(Q', Q) \mid i, Q\rangle$. Therefore, the infinitesimal displacement for $\mathrm{d}Q$, generated by the operator of the total space, is the transition $\mid i, Q\rangle \mid Q\rangle \mapsto \mid i, Q + \mathrm{d}Q\rangle \mid Q + \mathrm{d}Q\rangle$. It is not related exclusively to the "heavy" system, as it is the transition $\mid i\rangle \mid Q\rangle \mapsto \mid i\rangle \mid Q + \mathrm{d}Q\rangle$ generated by the operator $\frac{\partial}{\partial Q}$ in the fixed basis[2]. Indeed, the infinitesimal displacement of the "heavy" system solely, generated by its momentum P_H, is now, due to the interaction with the "light" system, only a part of the total change (fig. 5.2.). Thus, the relation

$$|i, Q + \mathrm{d}Q\rangle\,|Q + \mathrm{d}Q\rangle = \Theta(Q + \mathrm{d}Q, Q)\,|i, Q\rangle)\,|Q\rangle = T(Q + \mathrm{d}Q, Q)U(Q + \mathrm{d}Q, Q)\,|i, Q\rangle\,|Q + \mathrm{d}Q\rangle$$

is obtained. The first order terms of the expansion give $P_H^0 = P_H - A$. Thus in the adiabatic basis the momentum of the "heavy" system has the form

$$P_H = P_H^0 + A(Q) = -\mathrm{i}\hbar\frac{\partial}{\partial Q} + A(Q) \tag{5.1}$$

where $A(Q)$, coming through the derivation of U, is hermitean operator in $\mathcal{S}_L$. Only for $A = 0$ (this is the case of the "fixed" basis, when $U(q + \mathrm{d}Q, q) = I_L$), the operator $P_H^0 = -\mathrm{i}\hbar\frac{\partial}{\partial Q}$ is ordinary momentum of the "heavy" system. Otherwise, its physical contents is the generalized

[2]Note that when the basis of representation is changed, two different operators may have same matrix form. Here, this is the case with $\frac{\partial}{\partial Q}$, being the derivative over Q of the total wave function at in the adiabatic and in the fixed basis. It is defined in two different representations, and represents diferent operators, although the same symbol is used.

momentum for the displacements along Q; the term $A(Q)$ compensates the motion of the "light" system from $|\, i, Q\rangle$ to the corresponding state $|\, i, Q + \mathrm{d}Q\rangle$, restoring the momentum of the "heavy" system. The operator P_H^0 is reduced in the horizontal slices, since in the adiabatic basis it does not change the components from the "light" subspace (the index i remains fixed). The compensating operator A depend on the basis of representation, being itself determined by the hamiltonian, more precisely by the interaction terms (the "fixed" basis, i. e. $A = 0$, is obtained if $H_L(Q)$ is constant, meaning that there is no interaction depending on Q). Therefore, the operator field A is called *hamiltonian connection*, since it generates operator $U(Q + \mathrm{d}Q, Q)$ connecting the eigen bases of the family of the operators $H_L(Q)$ in the neighborhood of Q.

It appears that displacements of the "heavy" system in the adiabatic representation obtain "vertical" components (whenever A does not vanish), and may cause transition from one horizontal slice to another. This is immediately reflected in the dynamics of the total system. The kinetic energy of the heavy system, T_H, is the only term of the total hamiltonian not included in H_L, and thus not incorporated in the construction of the adiabatic basis. Therefore, involving P_H, and not P_H^0, it violates the invariance of the horizontal slices under H, meaning that the evolution causes the transition from one to another slice.

More precisely, using (5.1), T_H can be written in the form $T_H = T_H^0 + \Lambda$, where $T_H^0 = \frac{{P_H^0}^2}{2M}$ is reduced in the horizontal slices, since it, analogously to P_H^0, relates the dynamics of the "heavy" and "light" subsystems in the suitable way. The remainder, Λ, allows the vertical motions (exact expression for Λ in terms of A and $\frac{\partial}{\partial Q}$ can be easily found); in the adiabatic representation, Λ is the only term in the hamiltonian connecting different horizontal slices. In fact, this the only term in which the connection A appears, preventing complete separation of the "light" and "heavy" variables.

The adiabatic *approximation* forbids the transitions among the horizontal slices[3]. Accordingly, all the matrix elements of Λ connecting different slices are neglected: Λ is substituted by the operator $\Lambda^0 = \sum_n \int_Q P_n(Q)\Lambda(Q)P_n(Q) \mid Q\rangle\langle Q \mid \ \mathrm{d}Q$. This is usually performed in two steps: at first Λ (and therefore A) is completely neglected, and afterwards, it is included perturbatively. The first order corrections encounter only the restriction of the perturbation in the eigenspaces of the unperturbed hamiltonian, *i.e.* in the horizontal slices of these eigenvalues; therefore the adiabatic approximation is automatically provided (of course this is even slightly severe approximation than the original adiabatic condition requires). The unperturbed hamiltonian $H^o = T_H^0 + H_L$ reduces in the subspaces $\mathcal{S}_{n\lambda_n}$, acting in them as $H_n^o = T_H^0 + \epsilon_n$, with $\epsilon_n = \int_Q \epsilon_n(Q)P_n(Q) \mid Q\rangle\langle Q \mid \ \mathrm{d}Q$. Usually $H_L(Q)$ is considered as the hamiltonian of the "light" system in the field of the "heavy" one (being in the position Q), and in such context the eigenvectors $|n\lambda_n, Q\rangle$ are stationary states of the "light" system. Within this interpretation, the unperturbed hamiltonian (which reduces in the horizontal slices due to the approximation), describes the dynamics of the "heavy" system in the *adiabatic potential* $\epsilon_n(Q)$.

[3] $\alpha\delta\iota\alpha\beta\alpha\tau o\varsigma$ means impassable, not crossable.

Thus, the algorithm for the application of the adiabatic approximation is obtained. At first, the eigen problem of the "light" system in the field of the "heavy" subsystem is solved; this gives the eigen energies $\epsilon_n(Q)$ and eigenvectors $|n\lambda_n, Q\rangle$, as the functions of the position of the "heavy" system. Then the "heavy" system in the field $\epsilon_n(Q)$, for each n is studied, and stationary basis and the energies of the unperturbed hamiltonian are looked for. Finally, if more precise solution is required, perturbation $P_n(Q)\Lambda P_n(Q)$ is applied for each Q and n. Note that the above results are also called Born-Oppenheimer's approximation.

In different fields of physics factorizations of the same type are used. The obtained picture, naturally introduces techniques of differential geometry, being mathematical background of gauge theories and phenomena of the *geometrical* or *Berry's phase*, [44].

Frequently, the more severe, *Born's approximation* is introduced. If the ground state of the "heavy" system is known, *i.e.* its equilibrium state, the whole procedure can be applied, but with the potentials $V_H(Q)$ and $V_{LH}(Q)$ taken only in the vicinity of the equilibrium position. If only the equilibrium point is relevant, only the consideration of the "light" system remains.

5.2 Application of symmetry

The operator of the kinetic energy of any particle commutes with geometrical transformations, *i.e.* it is transformed according to the identity representation of the Euclid's group. Therefore, geometrical symmetry is always determined by the potentials. Adiabatic hypothesis, assuming that the "light" system neatly follows evolution of the "heavy" one, implies that the potential of the "heavy" system determines the total group of symmetry. This is manifested as the always fulfilled condition that the potentials depend on the relative positions of the particles composing the "light" system (meaning that geometrical symmetry of V_L is full Euclid's group) and configuration of the "heavy" system (V_{LH} i V_H). Therefore, symmetry of the total system, with the "heavy" subsystem in the position Q, is determined by geometry of the configuration Q. This group is denoted by G_Q.

All the potentials in the considered model are contained in $H_L(Q)$, and this operator must commute with the operators $D_L(G_Q)$, representing the group action. Clearly, the eigen subspaces $\mathcal{S}_{Ln}(Q)$ are invariant for $D_L(G_Q)$, and the corresponding standard stationary basis can be found: $|\mu t_\mu m, Q\rangle$ with the eigenvalue $\epsilon_{\mu t_\mu}(Q)$. The picture of the energy level as the function of Q appears, and the crossing of such levels will be studied immediately, while some other important applications of the described approach are postponed for the next section.

General considerations of the previous section show that the configurations of the "heavy" system in which the energy levels of the "light" system are crossed, are in a sense the singularities of the adiabatic potential. The degeneracy of the energy levels is increased in these points, and the horizontal slices can be rigorously defined only over the rest of the configurational manifold of the "heavy" system. In fact, this increased degeneracy reveals the very origin of the singularity: the symmetry in these points is greater than in their vicinity. Indeed, the more symmetric is the configuration Q, the greater is the degeneracy induced by symmetry. This is realized as junction of the energy levels $\epsilon_{\nu t_\nu}(Q')$, corresponding to the (lower

dimensional) irreducible representations of the lower symmetry groups of the surrounding configurations Q'. The symmetry group G_Q is stabilizer of the configuration Q, and characterizes the stratus (§ A.1.4) of the point Q: this is the set S_Q of all the configurations of the "heavy" system with stabilizers conjugated to G_Q. It is important result of the group theory that there is open and dense stratus, called the *generic stratus*, characterized by the minimal stabilizer[4]. The points of the higher symmetry occupy the lower dimensional submanifolds of the configurational space of the "heavy" system, the most symmetrical of them being isolated points. Therefore, these critical points of the adiabatic potential, being the more symmetrical than the surrounding ones enable the symmetry breaking.

Landau showed that the adiabatic potentials of the same symmetry, *i.e.* the slices corresponding to the same irreducible representation of the surrounding points symmetry group, cannot cross, [3]. Let $G_{Q'} < G_Q$ be the group of the low symmetry configuration Q' in the vicinity of Q. The level $\epsilon_{\mu t_\mu}(Q)$ may split in the course of the displacement from Q to Q', if the subduced representation $D^{(\mu)}(G_Q) \downarrow G_{Q'}$ becomes reducible (§ A.2.6): $D^{(\mu)}(G_Q) \downarrow G_{Q'} = \oplus a^\mu_\nu D^{(\nu)}(G_{Q'})$. Let $D^{(\nu)}(G_{Q'})$ and $D^{(\nu')}(G_{Q'})$ be two irreducible subrepresentations of the subduced representation, with the standard subbases $\{|\,\nu t_\nu n\rangle\}$ and $\{|\,\nu' t_{\nu'} n'\rangle\}$, respectively. In this basis the matrix of the perturbation $\Lambda(Q)$ is $\begin{pmatrix} \Lambda_{\nu\nu}(Q) & \Lambda_{\nu\nu'}(Q) \\ \Lambda_{\nu'\nu}(Q) & \Lambda_{\nu'\nu'}(Q) \end{pmatrix}$. Since Λ is determined by the parameters of the system only, its symmetry is at least G, *i.e.* it transforms according to the identity representation of G. The Wigner-Eckart's theorem implies that $\Lambda_{\nu\nu}(Q)$ and $\Lambda_{\nu'\nu'}(Q)$ are identity matrices, multiplied by the same scalar (due to the levels junction at Q). The off diagonal submatrices vanish, unless $\nu = \nu'$, when they are scalar matrices also. This means that if the levels of the unperturbed hamiltonian are crossed, the perturbation will remove this degeneracy for the levels of the same symmetry, and no crossing occurs.

5.3 Molecular orbitals

The adiabatic and the Born's approximations are successfully applied in molecular physics, due to the large difference in the masses of the electrons and ions (which appears as a criterion of the applicability of the adiabatic approximation). For example, the structure of molecules can be explained (if the ground adiabatic potential $\epsilon(Q)$ attains minimum at some finite point Q, this is the equilibrium configuration of the atoms in the molecule), the Jahn-Teller's effect has been observed, etc.

Theory of *molecular bond* and electronic spectra is among the greatest successes of quantum mechanics in molecular physics, [45, 46]. Within this theory it is assumed that the ionic configuration is known and fixed, and only the electronic subsystem is studied. Standard quantum mechanical approach, excellently confirmed by atomic electronic spectra, offers a scheme of one-electron states, which are one after another filled by the available electrons.

[4]The stabilizers on the same stratus are the same in the abstract sense, since they are conjugated (therefore isomorphic) subgroups of the Euclid's group. In the same abstract sense, this group for the generic stratus is a subgroup of the groups of other stratuses.

Only the electrons of the outer atomic shells are assumed to be relevant for molecular chemical bond: interacting weakly with their original ions, these are most intensively influenced by other ions. These states span the relevant electronic space, and the ground adiabatic potential with this "light" space $\mathcal{S}_e$, gets minimum in the stable molecular configuration, realizing molecular bonds.

To find these one electron states, called *molecular orbitals*, it is necessary to solve the eigen problem of $H_e = H_e(Q)$, for the equilibrium ionic configuration Q. Naturally, even this (already approximate) task is difficult enough, and further simplifications are introduced. Frequently, the initial step is Rayleigh-Ritz's variational method (§ 1.7): molecular orbitals are looked for in the subspace $\mathcal{S}^{AO} < \mathcal{S}_e(Q)$ over those atomic orbitals giving the electrons for the bond (the coefficients in the linear combinations of theses orbitals are varied). Therefore the method is known as the MOLCAO (molecular orbitals as linear combinations of atomic orbitals). Obviously, very important at this instant is additional assumption of the partial localization of the bonds. This is the approximation assuming that the origin of the electrons in the considered bond is defined, and therefore, to each molecular orbital the relevant atoms and their atomic orbitals are *a priory*, heuristically, associated. The *localized bonds*, formed by the pairs of atoms, are most frequently studied. Nevertheless, in the complex molecules, larger parts of the molecule, and after all, the whole molecule, can be involved in the model of formation of some bonds. The larger part of the molecule is taken into account, the results are more accurate, but the archetypal chemical picture of directly connected atoms progressively fades. The criterion of localization of the orbital is phenomenological, and only comparison to the experimental data or some more exact calculations, may justify the choice.

Application of symmetry within Rayleigh-Ritz's method is discussed previously (§ 1.7). The subspace $\mathcal{S}^{AO}$, with the projector P, in $\mathcal{S}_e(Q)$ is fixed by the choice of the relevant atoms and their atomic orbitals. Therefore, the operator $H^{AO} = PH_eP$ is defined. The set of the atoms involved in the bond becomes formally isolated by this construction, and their interaction is additionally approximated, since H_e contains only the matrix elements between the states in $\mathcal{S}^{AO}$. The chosen atomic orbitals, $\mid i\rangle$, are not orthogonal, and the overlap integrals, $S_{ij} = \langle i \mid j \rangle$, appear; finally, the variational equation (1.8) is obtained, with $h_{ij} = \langle i \mid H_e \mid j\rangle$. In this context, G is the group of symmetry of the relevant part of the molecule. To provide the invariance of $\mathcal{S}^{AO}$, for each chosen orbital $\mid i\rangle$, all the orbitals obtained by the group action on $\mid i\rangle$ are also included in $\mathcal{S}^{AO}$. Thus, the relevant representation, $D^{AO}(G)$ in $\mathcal{S}^{AO}$, can be formed analogously to the dynamical representation (§ 3.2). The j-th relevant atomic orbital of the atom α is denoted by $|\alpha, n_j l_j m_j\rangle$; the indices are the quantum numbers of the Coulomb's interaction (the angular dependance is described by the spherical harmonic $Y^{l_j}_{m_j}$). With respect to the group $\mathrm{O}(3,\mathbb{R})$ this vector is transformed according to the irreducible representation with weight l_j and parity $(-1)^{l_j}$. The product form, $|\alpha, n_j l_j m_j\rangle = |\alpha\rangle\, |n_j l_j m_j\rangle$, enables to make the action of the group transparent:

$$D^{AO}(g)\, |\alpha, n_j l_j m_j\rangle = D^{P}(g)\, |\alpha\rangle D^{(l_j,(-1)^{l_j})}(g)\, |n_j l_j m_j\rangle;$$

all the orbitals obtained in this way (from the same or different atoms) are taken in $\mathcal{S}^{AO}$.

Again, the permutational representation appears, accompanied by the action of the group in the *interior space* of the spherical harmonics. Nevertheless, for the point group $G < \mathrm{O}(3,\mathbb{R})$, the subduced representation $D^{(l,(-1)^l)}(\mathrm{O}(3,\mathbb{R})) \downarrow G$ may not be irreducible, and it is not necessary to include the whole space of the spherical harmonics with the same l (being irreducible for $\mathrm{O}(3,\mathbb{R})$); still, all these spherical harmonics are usually used, for the practical reasons. Hence, the basis of the atomic orbitals is obtained, together with the representation $D^{AO}(G)$, and the prerequisites for the standard procedure of the symmetry treatment are settled.

In this context *Hückel's approximation* is important, although very rough, as the simplest one; therefore it is frequently used as the first test of the proposed model of bonding. The chosen basis of the atomic orbitals is assumed to be orthonormal, $S_{ij} = \delta_{ij}$, meaning that the overlap integrals are completely neglected. Note that if the orbitals were really orthonormal, the matrix h would be the representative matrix of H^{AO}; thus the Hückel's approximation identifies h and H^{AO}, reducing the variational problem to the eigenproblem of h. Additionally, H^{AO} is modeled as follows: the diagonal elements are the energies of the corresponding atomic orbitals, *Coulomb's integrals*, while the remaining ones, the *resonance integrals*, are the interaction between the orbitals, and rapidly decrease with the distance between the atoms. Therefore, all of them are assumed to vanish, except those forming the bond. Crudeness of the series of approximations is partly compensated by explicit and exact application of symmetry, when the same value is given to the matrix elements corresponding to the equivalent pairs of orbitals. This can explain why the results are qualitatively good enough.

The most important are the localized bonds, involving the pairs of the atoms: they are the strongest, and firstly occupied (two electrons each); only the remaining electrons are accommodated in the less localized bonds (involving more atoms). The relevant group of symmetry is $\boldsymbol{C}_{\infty v}$ (when the atoms in the pair are different) or $\boldsymbol{D}_{\infty h}$ (the pair of identical atoms). The molecular orbitals are therefore transformed according to one-dimensional (σ-electrons) or two-dimensional (π-electrons) representations of these groups. Additionally, the parity of the mirror plane containing the ions appears as the characteristics of the σ-orbitals (A_0 for even and B_0 for odd σ states), as well as the parity of the mirror plane between the equal atoms (the superscripts $+$ and $-$ in the representations $A_0^{\pm}$, $B_0^{\pm}$, $E_{m,-m}^{\pm}$ stand for even and odd states). Obviously, the component of the angular momentum along the molecular axis, $|m|$, is good quantum number in all the cases. Each electronic level with $|m| > 0$ is twofold degenerate, $m = \pm|m|$ For the complete classification of the molecular orbitals the spin should be considered (both of the electrons and of the nuclei), and this will not be studied here; let it be mentioned only that the symmetry of the double group must be employed, and the result essentially consists in the addition of the projections of all the relevant angular moments onto the molecular axis. Clearly, the general rule, that the composition of the angular moments with the projections $|m_1|$ and $|m_2|$ gives the angular moments with the projection $|m_1| + |m_2|$ and $||m_1| - |m_2||$, easily follows from the Clebsch-Gordan's series of the relevant groups.

5.4 Electronic bands in crystals

As well as for the molecules, in the most simple treatments of the electronic system of the crystal, it is assumed that the ionic equilibrium configuration, Q, is known and fixed, and the one electron states are looked for. Only the translational group T is made use of, to enable general applicability of the results.

Regardless of the method of the construction, the one electron *crystal orbitals* are transformed according to the irreducible (one-dimensional) representations $D^{(\boldsymbol{k})}(\ I\ |\boldsymbol{z}\ ) = \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\boldsymbol{z}}$. Due to Bloch's theorem (§ 2.3.1), crystal orbital is determined by the corresponding functions $u^{(0)}_{\boldsymbol{k}t}$. In fact, the multiple irreducible subspace, $\mathcal{S}^{(\boldsymbol{k})}_{\mathrm{e}}(Q)$, of the representation $D^{(\boldsymbol{k})}(T)$, is the space $\mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{r}}\mathcal{S}^{(0)}_{\mathrm{e}}(Q)$. Therefore, for each $\boldsymbol{k}$, the functions $u^{(0)}_{\boldsymbol{k}t}$ in $\mathcal{S}^{(0)}_{\mathrm{e}}(Q)$, are to be found, such that $\mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{r}}u^{(0)}_{\boldsymbol{k}t}(\boldsymbol{r})$ are the eigenvectors of H_e. It can be directly verified that the equation for the periodical functions $u^{(0)}_{\boldsymbol{k}t}(\boldsymbol{r})$ is

$$(H_e + \frac{\hbar}{m}\boldsymbol{k}\hat{\mathbf{p}} + \frac{\hbar^2}{2m}\boldsymbol{k}^2)u^{(0)}_{\boldsymbol{k}t}(\boldsymbol{r}) = \epsilon u^{(0)}_{\boldsymbol{k}t}(\boldsymbol{r}).$$

the eigenproblem of the one electron hamiltonian in the total $\mathcal{S}_e(Q)$ is transformed into the family of the eigen problems in $\mathcal{S}^{(0)}_{\mathrm{e}}(Q)$.

Naturally, it is impossible to solve such task exactly, and different approximations are called for. The *weak binding approximation* is justified for the physical processes based on the almost free electrons; they are not bound to some specific ion in the crystal and therefore they are almost completely delocalized. At first, the potential V is neglected, and afterwards it is included perturbatively. The unperturbed electronic hamiltonian becomes T_e, and the eigenproblem reads $(\frac{\hbar^2}{2m}(\nabla + \mathrm{i}\boldsymbol{k})^2 + \epsilon)u^{(0)}_{\boldsymbol{k}}(\boldsymbol{r}) = 0$. The periodical solutions of this equation are $u^{(0)}_{\boldsymbol{k},\boldsymbol{K}}(\boldsymbol{r}) = C\mathrm{e}^{\mathrm{i}\boldsymbol{K}\boldsymbol{r}}$ (C is normalization factor), for the eigen value $\epsilon_{\boldsymbol{K}}(\boldsymbol{k}) = \frac{\hbar^2}{2m}(\boldsymbol{k}+\boldsymbol{K})^2$; here, $\boldsymbol{K}$ is the vector of the inverse lattice (note that $\boldsymbol{K}$ takes the role of t_μ in the general form of standard basis, $|\,\mu t_\mu m\rangle$). The total eigen function is $\langle\ \boldsymbol{r}\ |\ \boldsymbol{k}\boldsymbol{K}\rangle = C\mathrm{e}^{\mathrm{i}(\boldsymbol{k}+\boldsymbol{K})\boldsymbol{r}}$. This could be expected, since the approximation effectively assumes that the electrons are free (the crystal field is neglected), with the plain waves as the eigen vectors. The only remainder to the crystal field is the used crystal symmetry, manifested by the classification of the plain waves according to the vectors of the Brillouin's zone. The characteristic picture of the energy bands (one for each $\boldsymbol{K}$) is obtained by pulling back of the parabolic function $E(\boldsymbol{k}) = \frac{\hbar^2}{2m}\boldsymbol{k}^2$ (the eigenvalues of the free electron) periodically (the periods are those of the inverse lattice) into the Brillouin's zone.

The levels $\epsilon_{\boldsymbol{K}}(\boldsymbol{k})$ are degenerated (the same energy for same $|\boldsymbol{k}+\boldsymbol{K}|$), and the perturbative corrections are obtained as the eigenvalues of the matrix $\langle \boldsymbol{k}'\boldsymbol{K}'\ |\ V\ |\ \boldsymbol{k}\boldsymbol{K}\rangle$ (indices enumerate the different vectors $\boldsymbol{k}+\boldsymbol{K}$ of the same length). Periodicity of the electron-ion interaction, included in the perturbative method, has far reaching consequences. This will be shown for one dimensional lattice, and generalization is straightforward. The degenerate levels are $\epsilon_{\boldsymbol{K}}(\boldsymbol{k})$ and $\epsilon_{-\boldsymbol{K}}(-\boldsymbol{k})$, and the corresponding matrix of perturbation is $\begin{pmatrix} \langle \boldsymbol{k}\boldsymbol{K}|\ V\ |\boldsymbol{k}\boldsymbol{K}\rangle & \langle \boldsymbol{k}\boldsymbol{K}|\ V\ |-\boldsymbol{k}-\boldsymbol{K}\rangle \\ \langle -\boldsymbol{k}-\boldsymbol{K}|\ V\ |\boldsymbol{k}\boldsymbol{K}\rangle & \langle -\boldsymbol{k}-\boldsymbol{K}|\ V\ |-\boldsymbol{k}-\boldsymbol{K}\rangle \end{pmatrix}$. The diagonal elements are equal, being

the mean values of the potential. Unless $\boldsymbol{k}$ is equivalent to $-\boldsymbol{k}$, the off diagonal elements vanish, since the Clebsch-Gordan's coefficients in the Wigner-Eckart's theorem are zero. This means that the whole band is shifted for the mean value of the potential. Nevertheless, in the special positions, when $\boldsymbol{k} = 0$ or $\boldsymbol{k} = \frac{\pi}{a}$, being equivalent to $-\boldsymbol{k}$, the off diagonal elements do not vanish, and the splitting of the energy level (§ 5.2) occurs in these points of junctions of two bands ($\boldsymbol{k} = 0$ and at the edges of the Brillouin's zone). Still, if T is only a part of the complete symmetry group of the crystal, $\boldsymbol{k}$ and $-\boldsymbol{k}$ may be in the same many dimensional irreducible representation (the signs + and − take the role of the index m in the general form of the standard basis $\mid \mu t_\mu m \rangle$), and off diagonal matrix elements vanish again, while no splitting appears.

Therefore, in general case, there are some gaps between different bands at the central and edge points of the Brillouin's zone (where are the junctions in the free electron model), and consequently there appear some intervals, called the *forbidden bands* of energy without any allowed states. The available electrons are distributed over the lowest bands (two electrons for each $\boldsymbol{k}$ in one band). In some cases the levels bellow the forbidden band are exactly fulfilled, *i.e.* the *Fermi's level* is immediately below forbidden band. To excite any electron, the jump over the gap is necessary (due to Pauli's principle), and the crystal is dielectric. If the Fermi's level is inside some energy band, the electrons are easily excited, and the crystal possesses the metallic properties.

Approximate approach to the tightly bound electrons, those from the interior shells of the atoms, is in fact the same as MOLCAO method, described for molecules. Naturally, instead of the point groups, the translational group, T, is applied, and the classification of the states is performed according to its representations. This leads to the Bloch's functions, $u^{(0)}_{\boldsymbol{k},t}(\boldsymbol{r})$. Contrary to the weak binding approximation, when the Fourier's expansion of $u^{(0)}_{\boldsymbol{k},\boldsymbol{K}}(\boldsymbol{r})$ over the vectors of the inverse lattice (§ 2.3.1) obviously contains only one term, in this, *tight binding approximation* a number of terms can appear. The functions obtained in the tight binding approximation span the subspace in $\mathcal{S}^{(0)}$. It is obvious that the states of the weakly bound electrons must be orthogonal to this subspace; thus, the *orthogonalized plane waves*, obtained by subtracting from the plane wave its projection to this subspace, are a priory better starting approximation for the tightly bound electrons then the plain waves themselves.

Appendix A

REVIEW OF GROUP THEORY

In this appendix the necessary group theoretical notions utilized in the text are reviewed briefly. The seriously interested readers are referred to the specialized literature, [5, 13, 12, 11].

A.1 General theory

A.1.1 Definition

Group is the algebraic structure defined by the non empty set G and the operation of the multiplication of its elements. This product is closed and associative, with unique identity element, e, and for each element, g in G, there is uniquely defined inverse, g^{-1}. The group is Abelian, if for each pair of its elements the equality $gh = hg$ holds.

For each element $g \in G$ the *rearrangement lemma* shows that $gG \stackrel{\text{def}}{=} \{gh|h \in G\} = G$ and $Gg = G$. The *order* of the group, $|G|$, is the number of the elements in the set G. For the finite group (the group of the finite order) there exist at least one minimal subset, the set of the *generators* of the group, such that any element of the group is a monomial over this set. On this subset, the multiplication of the group is completely defined by the *generators relations*. In the *cyclic group* all the elements are the powers of the single generator. The minimal natural number n such that $g^n = e$, is called the *order of the element* g.

A.1.2 Lie groups

Lie group is group which is also differentiable manifold, such that the multiplication and the inversion are smooth mapping from $G \times G$ and G, respectively, onto G. The *Lie algebra* of the group is the tangent space in the identity, with the defined multiplication, which is skew symmetric, bilinear and satisfies Jacobi's identity (the sum of the cyclically permuted products of any three elements vanishes). The vectors of this algebra, the *generators of the Lie group*, generate the structure of the group on the given manifold by the exponential mapping, [5, 13].

The *one parameter subgroup*, $g(t)$. of the Lie group is the subset of the elements of G, satisfying $g(0) = e$ and $g(t)g(s) = g(t+s)$, for any real t and s. The one parameter subgroups

bijectively correspond to the elements of the Lie algebra.

A.1.3 Subgroups and morphisms

The *subgroup* H is the subset of G, being itself group with the same multiplication: $G < H$. The intersection of two subgroups is subgroup again. The subgroup H is *invariant*, $H \triangleleft G$, if $gH = Hg$ for any element $g \in G$. The group G is *simple* if $\{e\}$ and G are its only invariant subgroups, and *semisimple* if its invariant subgroups are not Abelian (except $\{e\}$).

The left (right) *coset* of the subgroup H with the representative g is the set gH (Hg). The set of all the cosets, G/H, is called the *coset space*. The cosets gH and $g'H$ are equal if and only if g' is in gH, and otherwise they are disjoint (analogously for the right cosets); multiplication by $g'g^{-1}$ bijectively maps the coset gH onto $g'H$, and therefore $|gH| = |g'H|$. The *transversal* of the group with respect to the subgroup is any set of the representatives of all the different cosets, $\{t_1, t_2, \dots\}$, and, although it is not uniquely defined, it gives the partition of the group onto the cosets: $G = t_1H + t_2H + \dots$ (here, $+$ stands for the disjoint union). The order of the transversal, $\frac{|G|}{|H|}$, is called the *index* of the subgroup. Obviously, the order of the subgroup divide the order of the group (*Lagrange theorem*).

The *centralizer* of the set $S \subset G$ is the subgroup $Z(S)$, whose elements commute with elements of S. The *center of the group*, $Z(G)$, is an invariant subgroup; it is equal to the group if and only if the group is Abelian. The *normalizer* of the set $S \subset G$ is the subgroup $N(S)$, with elements commuting with set S: $N(S) = \{g \in G | \forall s \in S \quad \exists s' \in S : \quad gs = s'g\}$.

The *homomorphism* of the group G into the group G' is any mapping $G \xrightarrow{f} G'$ satisfying $f(gh) = f(g)f(h)$. While $f(G)$ is subgroup in G', the kernel of the homomorphism, $\ker f \stackrel{\text{def}}{=} \{g \in G | f(g) = e'\}$, is invariant subgroup in G. Homomorphism is called *epimorphism*, *monomorphism* and *isomorphism*, if it is surjection, injection and bijection, respectively. Homomorphism and isomorphism are called *endomorphism* and *automorphism* if $G' = G$. Isomorphism is the equivalence relation in the set of all groups.

Each element g of the group defines the *interior automorphism* or *conjugation* of the group G: $C_g a \stackrel{\text{def}}{=} gag^{-1}$. The elements a and b of the group are *conjugated* if $b = gag^{-1}$ for some $g \in G$. The conjugation is the equivalence relation, and the sets of the mutually conjugated elements are *conjugation classes*. The order of the class divides the order of the group; if it equals one, the corresponding element is in the center of the group. The product of two classes contains the complete classes.

If $H \subset G$, the conjugated set $gHg^{-1} = \{ghg^{-1} | h \in H\}$ is a subgroup if and only if $H < G$. The invariant subgroup is equal to the conjugated subgroups and contains the complete conjugation classes. The product of two cosets of the invariant subgroup $H \triangleleft G$ is the coset itself, and the coset space, G/H, is a group, known as the *factor group* (for the finite groups, its order is equal to the index of the subgroup H). The image, $f(G)$, of the homomorphism is isomorphic to the factor group $G/\ker f$, with isomorphism mapping bijectively the cosets of the subgroup $\ker f$ to the elements of $f(G)$.

A.1.4 Groups of transformations

Group G is *group of transformations* on the set X, if there is homomorphism of G into the group of the automorphisms of X (the permutations of the seta X, which preserve the eventual algebraic structure on X), $g \mapsto \pi(g)$; alternatively, it is told that G acts on X, or that the set X is G-space. The element x of X is a *fixed point* of the transformation g, if $\pi(g)x = x$. The *little group*(*stabilizer, isotropy group*) of the point $x \in X$ is the subgroup of all the elements of G, for which x is a fixed point: $G_x \stackrel{\text{def}}{=} \{g \in G | \pi(g)x = x\}$. The *orbit* of the point x is the set $\Omega_x \stackrel{\text{def}}{=} Gx = \{y \in X | \exists g \in G \quad \pi(g)x = y\}$. The orbits are disjoint or equal, giving the partition of the set X. All the elements of a coset of the stabilizer of x map x to the same point of the orbit. The stabilizers of the points of the same orbit are mutually conjugated, and the set of the orbits with the conjugated stabilizers is called *stratus*. The relation of the partial order among the subgroups gives the partial order of the orbits and strati. If the complete set X is one orbit (*i.e.* for any two points $x, x' \in X$ there is $g \in G$ such that $\pi(g)x = x'$), the group action is called *transitive* on X. The action is *effective* and *free*, if π is isomorphism, and if the complete X is (generic) stratus with the stabilizer $\{e\}$, respectively.

A.1.5 Products of groups

The *direct (external) product* of the groups G and G' is the Descartes's product $G \times G'$, with the multiplication $(g_1, g_1')(g_2, g_2') \stackrel{\text{def}}{=} (g_1 g_2, g_1' g_2'), \quad \forall (g_1, g_1'), (g_2, g_2') \in G \times G'$; this is the group of the order $|G \times G'| = |G||G'|$. The conjugation classes of $G \times G'$ are the direct products of one class G and one of G', and their number is the product of the numbers of the classes in G and G'.

The product of two subgroups $H, K < G$ is a subgroup itself, if and only if the subgroups commute: $HK = KH$. The group G is the *product* of its subgroups H and K, if $G = HK$. The product is *weak direct*, if $H \cap K = e$; the weak direct product is called *semidirect*, $G = H \wedge K$, and *(internal) direct*, $G = H \otimes K$, if additionally $H \lhd G$, and $H, K \lhd G$. The requirement $G = HK$ implies that for each element $g \in G$ there are factors $h \in H$ i $k \in K$, such that $g = hk$, and the condition $H \cap K = e$ provides the uniqueness of the factors.

A.2 Representations

A.2.1 Definition

The *representation of the group* G in the n-dimensional vector space $\mathcal{S}(\mathbb{F})$ is the homomorphism D of the group G into the group $\mathrm{GL}(n, \mathbb{F})$. The representation is real (complex) if $\mathbb{F} = \mathbb{R}$ ($\mathbb{F} = \mathbb{C}$). The space and the dimension of the representation are $\mathcal{S}(\mathbb{F})$ and n. The representation $D(G)$ in the space $\mathcal{S}(\mathbb{F})$ is *equivalent* to the representation $D'(G)$ in the space $\mathcal{S}'(\mathbb{F})$, if there is nonsingular operator $A : \mathcal{S}(\mathbb{F}) \to \mathcal{S}'(\mathbb{F})$, such that for each element g of the group, $D'(g) = AD(g)A^{-1}$. If D is monomorphism, the representation is called *faithful*.

If the one-parameter subgroup $g(t)$ of the Lie's group G is determined by the generator l, and $D(G)$ is a representation of G, then $D(l) \stackrel{\text{def}}{=} \frac{\partial D(g(t))}{\partial t}|_{t=0}$ is the operator corresponding to the element l of the Lie's algebra, and the set of all these operators is the representation of the algebra. The initial representation of the group can be reconstructed from this representation of the algebra by the exponential mapping, $D(g(t)) = \mathrm{e}^{tD(l)}$.

The *identity representation* of any group G is the homomorphism $I(G) = 1$. Any group of matrices represents itself faithfully by the identical automorphism, called the *identical representation*. The *regular representation* (left) of the group $G = \{g_1, \ldots, g_{|G|}\}$ is defined by the permutational matrices $D^R_{ij}(g_k) = \delta(g_i g_j^{-1}, g_k)$. The representation D is *unitary* (*orthogonal*) if $D(G)$ is a subgroup in $\mathrm{U}(n)$ ($\mathrm{O}(n, \mathbb{R})$). The Schur-Auerbach's theorem states that each representation of the compact group in euclidean (unitary) space is equivalent to an orthogonal (unitary) representation.

A.2.2 Reducibility

The representation $D(G)$ is *reducible* if in $\mathcal{S}(F)$ exists nontrivial subspace $\mathcal{S}'(F)$ invariant for all the operators of the representation. If such subspace does not exist, the representation is called *irreducible*. One-dimensional representations are obviously irreducible. The representation is *decomposable* if there is a decomposition of the space $\mathcal{S}(F)$ onto the invariant subspaces: $\mathcal{S}(F) = \oplus_i \mathcal{S}_i(F)$; then, in the adapted basis $D(g)$ is given by the block-diagonal matrix, with the blocks $D_i(g)$ being the representations of the group themselves, meaning that $D(G)$ is the direct sum $\oplus_i D_i(G)$. Each reducible representation of a compact (or finite) group is decomposable (Masche's theorem), and for these groups each reducible representation can be expressed by the irreducible ones: $D(G) = \oplus_\mu a_\mu D^{(\mu)}(G)$. The number of the nonequivalent irreducible representations of the finite group is equal to the number of the conjugation classes.

Any matrix commuting with all the matrices of an irreducible representation $D^{(\mu)}(G)$ is scalar (the first *Schur's lemma*). All the irreducible representations of the Abel's group are one-dimensional. In the irreducible representation, the scalar matrices correspond to the elements of the center of the group. If $D^{(\mu)}(G)$ and $D^{(\nu)}(G)$ are two nonequivalent irreducible representations, the rectangular matrix M, satisfying $MD^{(\mu)}(g) = D^{(\nu)}(g)M$ for each g, is zero matrix (the second Schur's lemma). The set of the vectors obtained by the action of the representation to the non vanishing vector of an irreducible subspace, spans that subspace.

For the complete set of the nonequivalent matrix unitary irreducible representations of the compact group G, the *orthogonality relations* hold:

$$\frac{1}{|G|} \sum_{g \in G} d^{(\mu)*}_{ji}(g) d^{(\nu)}_{km}(g) = \frac{1}{n_\nu} \delta_{jk} \delta_{im} \delta_{\mu\nu}.$$

A.2.3 Characters

The *character of the representation* $D(G)$ is the function on the group mapping each element g into the number $\chi(g) \stackrel{\text{def}}{=} \mathrm{Tr}(D(g))$. The dimension of the representation is the character of the identity element. Two representations are equivalent if and only if their characters are equal. The characters of the elements of the same conjugation class are equal. The orthogonality relations for the characters are:

$$\frac{1}{|G|}\sum_{g\in G}\chi^{(\mu)*}(g)\chi^{(\nu)}(g) = \delta_{\mu\nu}.$$

The character of the reducible representation $D(G)$ equals to the sum of the characters of the representations onto which $D(G)$ is decomposed: if $D(G) = \oplus_\mu a_\mu D^{(\mu)}(G)$, then $\chi(G) = \sum_\mu a_\mu \chi^{(\mu)}(G)$, and

$$a_\mu = \frac{1}{|G|}\sum_g \chi^{(\mu)*}(g)\chi(g). \tag{A.1}$$

The representation is irreducible if and only if $\frac{1}{|G|}\sum_g \chi^*(g)\chi(g) = 1$.

A.2.4 Standard basis and group projectors

The space $\mathcal{S}$ of the representation $D(G)$ can be decomposed in the form $\mathcal{S} = \oplus_\mu^s \mathcal{S}^{(\mu)}$, where $\mathcal{S}^{(\mu)} \stackrel{\text{def}}{=} \oplus_{t_\mu}^{a_\mu}\mathcal{S}^{(\mu t_\mu)}$ are multiple irreducible subspaces. The *standard basis*, $\{|\ \mu t_\mu m\ \rangle | \mu = 1,\ldots,s; t_\mu = 1,\ldots,a_\mu; m = 1,\ldots,n_\mu\}$ in $\mathcal{S}$ is the basis in which $D(G)$ is block-diagonal, with the blocks being previously given matrices of the irreducible representations of the group:

$$D(g)|\ \mu t_\mu m\ \rangle = \sum_{m'} D^{(\mu)}_{m'm}(g)\ |\mu t_\mu m'\rangle.$$

The *group operators*,

$$P^{(\mu)}_{mm'} \stackrel{\text{def}}{=} \frac{n_\mu}{|G|}\sum_{g\in G} d^{(\mu)*}_{mm'}(g)D(g) = \sum_{t_\mu} |\ \mu t_\mu m\ \rangle\langle \mu t_\mu m'\ |,$$

are for $m = m'$ the projectors onto the subspaces $\mathcal{S}^{(\mu)}_m \stackrel{\text{def}}{=} \mathrm{span}\{|\ \mu t_\mu m\ \rangle | t_\mu = 1,\ldots,a_\mu\}$. The projector onto the subspace $\mathcal{S}^{(\mu)}$ is $P^{(\mu)} \stackrel{\text{def}}{=} \frac{n_\mu}{|G|}\sum_{g\in G}\chi^{(\mu)*}(g)D(g)$.

A.2.5 Products

The direct product of the representations $D'(G)$ and $D''(G)$ is the representation $\{D(g) \stackrel{\text{def}}{=} D'(g)\otimes D''(g) | g\in G\}$ in the space $\mathcal{S}'\otimes\mathcal{S}''$; its character is $\chi(g) = \chi'(g)\chi''(g)$. The Clebsch-Gordan's series is the decomposition $D^{(\mu)}(G)\otimes D^{(\nu)}(G) = \oplus_\nu a^{\mu\nu}_\lambda D^{(\lambda)}(G)$ of the direct product of two irreducible representations onto the irreducible components, and the coefficients $a^{\mu\nu}_\lambda$ are characteristic of the group. The Clebsch-Gordan's coefficients are the elements of the transition matrix from the product of the bases $\{|\ \mu m\rangle\}$ and $\{|\ \nu n\rangle\}$ in $\mathcal{S}^{(\mu)}$ and $\mathcal{S}^{(\nu)}$,

respectively, to the standard basis $\{|\,\mu\nu\lambda t_\lambda l\rangle\}$ of the space $\mathcal{S}^{(\mu)}\otimes\mathcal{S}^{(\nu)}$. For the orthonormal initial bases, these are the scalar products $\langle\ \mu\nu\lambda t_\lambda l\,|\,\mu m,\nu n\rangle \stackrel{\text{def}}{=} \langle\ \lambda t_\lambda l\,|\,\mu m\rangle\otimes|\,\nu n\rangle$; they are uniquely (up to the phase) defined only if the coefficients of the Clebsch-Gordan's series $a_\lambda^{\mu\nu}$ are less than 2 (*i.e.* if they are equal to 0 or 1).

If $\{|\,i\rangle\}$ is the basis of the space $\mathcal{S}$ of the representation $D(G)$, the n^{th} direct power of the representation is the representation $D^n(G)$ in the space $\underbrace{\mathcal{S}\otimes\cdots\otimes\mathcal{S}}_{n}$ defined by the action onto the basis vectors: $D^n(g)(|i_1\rangle\ldots|i_n\rangle) = (D(g)\,|i_1\rangle)\ldots(D(g)\,|i_n\rangle)$. In the same space, the representation $\Delta(S_n)$ of the symmetrical group S_n is given by $\Delta(\pi)(|i_1\rangle\ldots|i_n\rangle) = |i_{\pi 1}\rangle\ldots|i_{\pi n}\rangle$. The representation Δ is not irreducible (for $n>1$), and its irreducible subspaces are invariant for the operators of $D(G)$. Therefore, $D(G)$ reduces in these subspaces; the reduced representations in the symmetrical and skew symmetrical subspaces of the group S_n (*i.e.* in the multiple irreducible subspaces of the identity and the alternative representation of S_n) are called *symmetrical* and *skew symmetrical* power of $D(G)$ (denoted by $[D^n(G)]$ and $\{D^n(G)\}$, or $[D^n(G)]_\pm$). The characters of these representations, for the powers 2, 3 and 4 are [8]:

$$[\chi^2(g)]_\pm = \frac{1}{2}\chi^2(g) \pm \frac{1}{2}\chi(g^2), \quad [\chi^3(g)]_\pm = \frac{1}{6}\chi^3(g) \pm \frac{1}{2}\chi(g)\chi(g^2) + \frac{1}{3}\chi(g^3),$$

$$[\chi^4(g)]_\pm = \frac{1}{24}\chi^4(g) \pm \frac{1}{4}\chi^2(g)\chi(g^2) + \frac{1}{8}\chi^2(g^2) + \frac{1}{3}\chi(g^3)\chi(g) \pm \frac{1}{4}\chi(g^4).$$

A.2.6 Subduction

The restriction o the representation D of the group G onto its subgroup H is the *subduced representation* of the subgroup H: $D(G)\downarrow H$. This representation may not be irreducible even if $D(G)$ is; the reductions onto the irreducible representations, $D^{(\mu)}(G)\downarrow H = \oplus a^\mu_\nu D^{(\nu)}(H)$, are called the *compatibility relations* (of the irreducible representations of the group and its subgroup).

A.2.7 Projective representations

The *projective representation* $D(G)$ with the *factor-system* (or the *multipliers*) $\{f(g,g')\in\mathbb{C}\,|\,g,g'\in G\}$, is the mapping D of the group G into the set of the operators (matrices) $D(G)=\{D(g)|g\in G\}$, such that $D(g)D(g') = f(g,g')D(gg')$.

The ordinary representations of the group are the special cases of the projective representations, with the *trivial* factor-system), $f(g,g')=1$ for each pair g i g' from G. Irreducibility, unitarity and equivalence of the projective representation are defined as for the ordinary ones. The complex numbers $\{f(g,g')\}$ are the factor-system of the group G if and only if the associativity condition, $f(g,h)f(gh,k) = f(g,hk)f(h,k)\,\forall g,h,k\in G$, is fulfilled. If $D(G)$ is a projective representation of G, and each matrix $D(g)$ is multiplied by arbitrary, non vanishing complex number $c(g)$, another projective representation, $D'(G)=\{c(g)D(g)|g\in G\}$, with the factor-system $f'(g,g') = \frac{c(g)c(g')}{c(gg')}f(g,g')$ is defined. This is an equivalence relation on the set, $F(G)$, of the all factor-systems of the group G: $f\sim f'$ if there are the complex numbers

$c(g)$, such that the last relation holds. For each factor-system there is the equivalent *standard* one: $|f(g,g')| = 1$ and $f(e,g) = f(g,e) = 1$; the corresponding projective representation is equivalent to the unitary one, with $D(e) = I$.

Since the product of two factor-systems, f and f', is another factor-system $f''(g,g') \stackrel{\text{def}}{=} f(g,g')f'(g,g')$, the set $F(G)$ is Abel's group. The equivalence class, $T(G)$, of the trivial factor-system is an invariant subgroup of $F(G)$, and the factor-group $M(G) = F(G)/T(G)$ is called the *multipliers group*.

For each equivalence class of the factor-systems the set of the nonequivalent unitary irreducible projective representations of G is constructed (their number may not be equal to the number of the conjugation classes of the group). For the standard factor-systems, the non equivalent unitary irreducible representations satisfy the orthogonality theorems for the matrix elements and characters (the characters of the conjugated elements may differ!).

If there is the homomorphism of the group G' onto G, with the kernel H, there is bijection the cosets of H in G' and the elements of G. Thus, to each element g of G the representative t_g of the coset t_gH, mapped to g, is associated. Then, by the condition $t_{g_1}t_{g_2} = t_{g_1g_2}h(g_1,g_2)$, to each pair $g_1, g_2 \in G$, corresponds the element $h(g_1,g_2) \in H$. The representation $D'(G')$ of the group G', such that the subgroup H is represented by the scalar matrices, $D'(h) = f(h)I$, defines the projective representation $D(G) = \{D(g) \stackrel{\text{def}}{=} D'(t_g)|g \in G\}$ of G, with the factor-system $f(g_1,g_2) = f(h(g_1,g_2))$. Another choice of the coset representatives, t_g, gives another, but equivalent, factor-system. If H is central, each irreducible representation of G' gives an irreducible projective representation of G. The group $\tilde{G}$ is the *covering group* for G if each projective irreducible representation of G can be derived in this way from some ordinary irreducible representation of $\tilde{G}$. There exists *universally covering* group, such that its multipliers group, $M(G)$, is isomorphic to a subgroup H of the center of $\tilde{G}$.

A.2.8 Induction

The *induced* representation [11] Δ (of the dimension n_Δ) of the subgroup H (with the transversal $\{t_1 = e, t_2, \dots\}$) to the group G, is the representation $D(G) = \Delta(H) \uparrow G$ defined by $D(g) = \sum_{pq} E_{pq} \otimes \Delta(h)\delta(t_p^{-1}gt_q, h)$, ($E_{pq}$ is the $\frac{|G|}{|H|}$-dimensional matrix $(E^{pq})_{ij} = \delta_{pi}\delta_{jq}$); its n_Δ-dimensional pq-th block is non vanishing (and equal to $\Delta(h)$) if and only if $t_p^{-1}gt_q = h \in H$. The dimension of the induced representation is the product of the index of the subgroup H and n_Δ. The representation $D^R(G) \stackrel{\text{def}}{=} I(\{e\}) \uparrow G$ is called *regular representation* of G.

If H is an invariant subgroup of G and $X = \{\Delta^{(\mu)}(H)|\mu = 1, 2, \dots\}$ is the set of all its nonequivalent irreducible representations, G defines the group of transformations on X by the action $\Delta^{(\mu)}(h) \stackrel{g}{\mapsto} \Delta^{(\mu)}(g^{-1}hg) \stackrel{\text{def}}{=} \Delta_g^{(\mu)}(h)$, yielding the partition of X onto the orbits of the representations. The irreducible representations of the same orbit induce the equivalent representations of G. The little group, G_μ, of the representation $\Delta^{(\mu)}(H)$ is supergroup of H, and among its irreducible representations, those subducing multiple representation $\Delta^{(\mu)}(H)$ onto H are called *allowable representation*, $d^{(\mu,\alpha)}(G_\mu)$. Each allowable representation induces the irreducible representation $D^{(\mu,\alpha)}(G) \stackrel{\text{def}}{=} d^{(\mu,\alpha)}(G_\mu) \uparrow G$. For fixed μ, all the representations

$D^{(\mu,\alpha)}(G)$ are non equivalent, forming the *associate set*. By choosing one representation from each orbit in X, finding all the allowable representations of their little groups, and inducing these onto G, the complete set of the nonequivalent irreducible representations of the group G is obtained.

To each element k of the factor-group $K = G_\mu/H$, the element t_k is associated when choice of the coset representatives is fixed (H is invariant subgroup of $G_\mu = \sum_k t_i H$). Since the coset representatives are the elements of the little group, the representations $\Delta^{(\mu)}_{t_k}(H)$ and $\Delta^{(\mu)}(H)$ are equivalent, and there is unitary operator, $C(k)$, establishing the equivalence: $\Delta^{(\mu)}_{t_k}(H) = C^{-1}(k)\Delta^{(\mu)}(H)C(k)$. In this way to each element $k \in K$ the operator $C(k)$ is associated. The operators $f(k,k') = C(kk')\Delta(t_{kk'})C(k')^{-1}C(k)^{-1}$ commute with $\Delta^{(\mu)}(H)$, and being scalars therefore, define a factor-system of the group K (§ A.2.7). For each projective irreducible representation $d^{(\alpha)}(K)$ of this factor-system, one allowable representation of the little group: $d^{(\mu,\alpha)}(t_k h) = (C(k)\Delta^{(\mu)}(h)) \otimes d^{(\alpha)}(k)$; these are all the allowable representations of the orbit. Alternatively, the covering group may be used, and its irreducible representations for the same factor-system. Two important special cases will be considered in detail.

If $G = H + sH$, the halving subgroup H is invariant, while $s^2 \in H$. The orbits of its irreducible representations contain one or two representations. In the first case, such a representation, $\Delta^{(\mu)}(H)$, gives two nonequivalent associated irreducible representations:

$$D^{(\mu\pm)}(G) = \{D^{(\mu\pm)}(g) \stackrel{\text{def}}{=} \begin{cases} \Delta(\mu)(h), & \text{for } h \in H, \\ \pm Z\Delta(\mu)(h), & \text{for } h \in sH, \end{cases}\}$$

where Z is the operator satisfying $Z^{-1}\Delta^{(\mu)}(h)Z = \Delta^{(\mu)}(s^{-1}hs)$ and $Z^2 = \Delta^{(\mu)}(s^2)$. In the second case, both of the representations of the orbit, $\Delta^{(\mu)}(H)$ and $\Delta^{(\mu)}_s(h)$, induce the same irreducible representation of the group G:

$$D^{(\mu)}(h) = \begin{pmatrix} \Delta^{(\mu)}(h) & 0 \\ 0 & \Delta^{(\mu)}_s(h) \end{pmatrix}, \quad D^{(\mu)}(sh) = \begin{pmatrix} 0 & \Delta^{(\mu)}(s^2)\Delta^{(\mu)}_s(h) \\ \Delta^{(\mu)}(h) & 0 \end{pmatrix}, \quad h \in H.$$

If the group G is semidirect product, $G = N \wedge H$, with Abel's invariant subgroup N, the irreducible representations, $\Delta^{(\mu)}(N)$, are one-dimensional, and their little groups are $G_\mu = N \wedge H_\mu$, where H_μ is subgroup in H. All the allowable representations $d^{(\mu,\alpha)}(G_\mu)$ are $d^{(\mu,\alpha)}(nh) = \Delta^{(\mu)}(n)d^{(\alpha)}(h)$ ($n \in N$, $h \in H_\mu$), where $d^{(\alpha)}(H_\mu)$ are all the irreducible representations of H_μ.

Finally, for $G = H \otimes K$, all the irreducible representations of G are the direct products of the representations $\{\Delta^{(\mu)}(H)\}$ and $\{\delta^{(\nu)}(K)\}$: $\Delta^{(\mu,\nu)}(h,k) = \Delta^{(\mu)}(h) \otimes \delta^{(\nu)}(k)$.

A.3 Complex conjugation

A.3.1 Conjugation

The representation $D(G)$ in $\mathcal{S}$, defines in the dual space $\mathcal{S}^*$ the *contragredient representation* $\phi(x) = (D'(g)\phi)(D(g)x)$, which is in the biorthogonal basis represented by the contragredient matrices. In the same space the *conjugated (dual) representation*, $D^*(g)\phi_x = \phi_{D(g)x}$, is in the

dual orthonormal basis represented by the conjugated matrices (ϕ_x is the functional dual to the vector x). These two representations are equivalent.

A.3.2 Corepresentations

If any element of G is in the representation $D(G)$ represented by anti unitary operator, then there is the halving subgroup, H, represented by the unitary operators, while its coset, sH, corresponds to anti unitary operators $D(sh) = \theta D(h)$, with $\theta = D(s)$. The choice of the basis determines the matrix form $\theta = K_0 D_c(s)$ and $D(sh) = K_0 D_c(sh) = K_0 D_c(s) D_(h)$, where K_0 is the operator of the complex conjugation of the columns in this basis (anti unitary, $K_0^2 = I$). The homomorphism condition satisfied for the operators $D(g)$, yields for the matrices $D_c(G) \stackrel{\text{def}}{=} \{D(h), D_c(sh) | h \in H\}$, called the *corepresentation* of the group, [12], the relations $D(hh') = D(h)D(h')$, $D_c(shh') = D_c(sh)D(h')$, $D_c(hsh') = D^*(h)D_c(sh')$ and $D(shsh') = D_c^*(sh)D_c(sh)$. Also, the equivalence of the representations, $D(g) = AD'(g)A^{-1}$ for each g from G, for the corepresentation reads $D(h) = AD'(h)A^{-1}$ and $D(s) = A^* D_c'(s) A^{-1}$, and reduces to the equivalence of the subduced representations $D(H)$ and $D'(H)$.

The irreducible corepresentations of the group G are constructed from the irreducible representations of the subgroup H, by the $*$-induction method. The $*$-s-conjugated representation to the representation $\Delta(H)$ is defined as $\Delta_s^*(h) \stackrel{\text{def}}{=} \Delta^*(s^{-1}hs)$. If $\Delta_s^*(H) \sim \Delta(H)$ (the one member orbit) and $\Delta_s^*(H) = Z\Delta(H)Z^{-1}$, then $ZZ^* = c_Z \Delta(s^2)$, where $c_Z > 0$ for the representations of the *first kind* and $c_Z < 0$ for the representations of the *second kind*. If $\Delta_s^*(H) \not\sim \Delta(H)$, then the orbit is with two representations of the *third kind*. The irreducible representation $\Delta(H)$ is of the I, II and III kind for the $*$-s-conjugation if

$$\frac{1}{|H|} \sum_{h \in H} \chi((sh)^2) = 1, -1, 0,$$

respectively. For $\Delta(H)$ of the I kind, there is the unitary matrix Z, such that $\{\Delta(h), D_c(sh) = Z\Delta(h)\}$ is irreducible corepresentation of G. In other cases the matrices of the corresponding irreducible corepresentation are given by:

$$D(h) = \begin{pmatrix} \Delta(h) & 0 \\ 0 & \Delta^*(s^{-1}hs) \end{pmatrix}, D_c(sh) = \begin{pmatrix} 0 & \Delta(s^2) \\ I & 0 \end{pmatrix} D(h)$$

(I is the identity matrix of the dimension n_Δ). Applying these procedures to all the orbits of the $*$-s-conjugation, the complete set of the nonequivalent irreducible corepresentations of the group G is found (one corepresentation from each orbit).

In the special case, when $G = H \otimes \{e, s\}$ (s commutes with all the elements of H, and $s^2 = e$), the $*$-s-conjugation is reduced to the ordinary conjugation. The representation $\Delta^{(\mu)}(H)$ is of the I kind if it is equivalent to the real representation (and to $\Delta^{(\mu)^*}(H)$), of the II kind if it is equivalent to $\Delta^{(\mu)^*}(H)$, but not to any real representation, and of the III kind if it is not equivalent to $\Delta^{(\mu)^*}(H)$. The irreducible representation $\Delta^{(\mu)}(H)$ is of the I (II,III) kind if and only if $\frac{1}{|H|}\sum_h \chi^{(\mu)}(h^2)$ equals to 1 (-1, 0). The sum of the numbers of

the representations of the I and II kind is equal to the number of the ambivalent classes. If in the basis $\{x_1, \ldots, x_n\}$ of the space $\mathcal{S}(\mathbb{C})$ the group is represented by the matrices $\Delta(h) = \Delta_r(h) + \mathrm{i}\Delta_i(h)$ (real and imaginary parts of the matrix), in the basis $\{x_1, \ldots, x_n, ix_1, \ldots, ix_n\}$ of the decomplexified $2n$-dimensional real space $\mathcal{S}_R$ the matrices $\Delta_R(h) \stackrel{\text{def}}{=} \begin{pmatrix} \Delta_r(h) & -\Delta_i(h) \\ \Delta_i(h) & \Delta_r(h) \end{pmatrix}$ of the *decomplexified representation* are found. If $\Delta(H)$ is the representation of the first kind, $\Delta_R(H)$ is reducible over the real (and complex) field in the form $\Delta_R(H) = 2\Delta(H)$. In the case of the representations of the II or III kind, $\Delta_R(H)$ is reduced over the complex field in the form $\Delta_R(H) = \Delta(H) + \Delta^*(H)$, while the irreducibility of $\Delta(H)$ implies the irreducibility of $\Delta_R(H)$ over reals. Therefore, the set of the *real* or *physical* irreducible representations is consisted of the representations of the I kind, and the decomplexified representations of the II and III kind (for each representation of the II kind, and each pair of the conjugated representations of the III kind, one real irreducible representation, equivalent to $D^{(\mu)}(G) \oplus D^{(\mu)*}(G)$ is obtained).

The real matrix representation $D(G)$, in the complex space $\mathcal{S}$, is equivalent to the orthogonal sum of the real irreducible representations; therefore the complex irreducible representations of the II and III kinds appear as the components of $D(G)$ in the conjugated pairs: each real irreducible component of $D(G)$ is either irreducible or equivalent to $D^{(\mu)}(G) \oplus D^{(\mu)*}(G)$.

Appendix B

WIGNER'S THEOREMS

This appendix is devoted to some mathematical details, which in the main part have been important for the applications of the symmetry in quantum mechanics. The physical background is examined at first, to emphasize the basic assumptions involved in the formulations and proofs of the Wigner's and Wigner-Eckart's theorem.

B.1 Quantum states and vectors

One of the usual statements in the quantum mechanics is that the states (here only the pure states are thought of, to differ from the mixed ones) are the elements of some vector space. This is followed by the remark that all the collinear vectors defines the same state, and furthermore, a postulate, necessary for the statistical analysis the states are restricted to the normalized vectors. Therefore, the set of the states is not really vector space, $\mathcal{S}$, but the structure called projective space, $P(\mathcal{S})$. Still, partly due to the tradition, and mostly by the pure technical reasons (projective spaces are more complicated to deal with), the quantum mechanics explicitly uses the complete space $\mathcal{S}$; the physical requirements, related to the probabilistic interpretation, and realized by the various normalizing conditions, tacitly correct such approach.

Nevertheless, it is clear that the symmetries must be defined as the groups of the transformations on the projective space. The concept of symmetry itself imposes the condition that the observable parameters of the system cannot be changed in the course of such transformations. The measurable quantities, being related to the probabilities, remain invariant if the moduli of the scalar products are invariant. Thus, the transformation T cannot be the symmetry, unless $|(TX, TY)| = |(X, Y)|$, for $X, Y \in P(\mathcal{S})$ (since $P(\mathcal{S})$ is derived from the unitary space $\mathcal{S}$, the scalar product is understood as the scalar product of the normalized ray representatives; since the moduli do not depend on the choice of the representatives, the whole expression is a function on the rays only).

On the other hand, most of the general principles of the application of the symmetry (§ 1) are elaborated treating the symmetry as the operator in the vector space. Therefore, the relation between the symmetry transformations in $P(\mathcal{S})$ and $\mathcal{S}$ must be established, to

enable the transition from $P(\mathcal{S})$ to $\mathcal{S}$ (manifested in the utilization of the linear combinations of the elements of $P(\mathcal{S})$). This procedure can be understood as the widening of the domain of transformation T, and the condition that the moduli of the scalar products are conserved partly remove the ambiguities.

B.2 Wigner's theorem

The operators in $\mathcal{S}$ and the transformations in $P(\mathcal{S})$ are connected by the following theorem, [5, 15].

Teorem 3 *Let T be the symmetry transformation in $P(\mathcal{S})$, i.e. the transformation satisfying $|(TX,TY)| = |(X,Y)|$, for any pair of the rays $X,Y \in P(\mathcal{S})$. Then, there is the operator U extending the action of T onto $\mathcal{S}$. This operator is unitary or anti unitary.*

Proof. Let $\{x\} = \{x_1, x_2, \dots\}$ be orthonormal basis in $\mathcal{S}$. The vectors x_i are considered as the representatives of the corresponding rays, X_i. When the symmetry T act on these rays, the new rays $TX_i = Y_i$, are obtained, with the normalized representatives y_i. Let U^0 be any operator in $\mathcal{S}$ such that $U^0 x_i = y_i$ (no assumption on the linearity of U^0 is not introduced, and therefore U^0 is neither uniquely nor completely defined; in addition, the representatives y_i are arbitrarily chosen). The condition of the scalar products conservation gives $|(y_i, y_j)| = |(U^0 x_i, U^0 x_j)| = |(x_i, x_j)| = \delta_{ij}$, showing that $\{y_i\}$ is the orthonormal basis in $\mathcal{S}$, irrespectively on the choice of the representatives and complete definition of U^0 on $\mathcal{S}$.

For $x = \sum_i \alpha x_i$, the vector $y \stackrel{\text{def}}{=} U^0 x = \sum_i \beta_i y_i$ satisfies $|\beta_i| = |\alpha_i|$ (since for the symmetries $|(y_i, y)| = |(x_i, x)|$ hold). Consequently, if x is from the subspace spanned by a part of the basis $\{x\}$, then y is from the subspace spanned by the corresponding elements of the basis $\{y\}$ (*e.g.* $x \in \text{span}\{x_1, \dots, x_p\}$ implies $y \in \text{span}\{y_1, \dots, y_p\}$).

After these general study of the operators acting compatibly with T on some basis only, the possibility of implementation of some linear properties will be considered. At first the action on the sum of the vectors have to be in accordance with action of T. It follows from the previous conclusions that $U^0(x_1 + x_i) = \beta_1^i y_1 + \beta_i y_i = \beta_1^i (y_1 + \gamma_i y_i)$, where β_1^i, β_i and γ_i are phase factors. If another choice of the ray representatives, $z_1 = y_1, z_i = \gamma_i y_y$ $(i = 2, 3, \dots)$, is taken, then among the possible operators U^0 that one, U, satisfying $U x_i = z_i$ i $U(x_1 + x_i) = \beta_1^i U^0(x_1 + x_i) = z_1 + z_i$, obviously is homomorphism with respect to the addition of the basis vectors.

The definition of the operator U has to completed by determination of its action on the arbitrary vector $x = \sum_i \alpha x_i$, *i.e.* by fixing the coefficients in $Ux = \sum_i \beta_i z_i$. The derived condition, $|\alpha_i| = |\beta_i|$, has to be regarded. It turns out that fixing β_1 either by $\beta_1 = \alpha_1$ or by $\beta_1 = \alpha_1^*$ consistently determines the other coefficients. In the first case, $|(x_1 + x_i, x)| = |(z_1 + z_i, Ux)|$ yields $|\alpha_1 + \alpha_i| = |\alpha_1 + \beta_i|$. Expanding the square of the last expression, one obtains the equation $\alpha_1^* \beta_i^2 - (\alpha_1^* \alpha_i + \alpha_1 \alpha_i^*)\beta_i + \alpha_1 |\alpha_i|^2 = 0$ over β_i, with the solutions $\beta_i = \alpha_i$ and $\beta_i = \alpha_i^* \frac{\alpha_1}{\alpha_1^*}$. The first one gives the linear operator: $U(\sum_i \alpha_i x_i) = \sum_i \alpha_i U x_i$. Analogously,

in the second case there are also two solutions, $\beta_i = \alpha_i^*$ i $\beta_i = \alpha_i \frac{\alpha_1^*}{\alpha_1}$, and the first of them defines the anti linear operator $U(\sum_i \alpha_i x_i) = \sum_i \alpha_i^* U x_i$.

Finally, the initial condition on the scalar products directly implies that the (anti)linear solution is also (anti)unitary. *QED*

Depending on the physical contents of the concrete transformation, the unitary or the anti unitary action of the symmetry operator in $\mathcal{S}$ is taken. Thus, it turned out that the time reversal is necessary represented by anti unitary operator (§ 2.6.1). As for the Lie's groups, due to the continuity, all the elements of the same connected component of the group must be represented in the same way; especially, this means that the component of the identity, being itself Lie's group, is unitary represented. Consequently, referring to the complete Euclid's group (including time reversal), the rotations and translations are unitary operators in $\mathcal{S}$.

B.3 Wigner-Eckart's theorem

If the coefficients in the Clebsch-Gordan's series of the group G satisfy the requirement $a_\lambda^{\mu\nu} = 0, 1$, then for this group holds

Teorem 4 *The matrix element* $\langle\ \alpha t_\alpha a \mid A_m^{(\mu t_\mu)} \mid \beta t_\beta b\ \rangle$ *is product of the Clebsch-Gordan's coefficient* $\langle\ \mu\beta\alpha a \mid \mu m, \beta b\ \rangle$ *with* reduced matrix element, $(\alpha t_\alpha \mid\mid A^{(\mu t_\mu)} \mid\mid \beta t_\beta)$, *being the same for all* a, b *and* m*:*

$$\langle\ \alpha t_\alpha a \mid A_m^{(\mu t_\mu)} \mid \beta t_\beta b\ \rangle = \langle\ \mu\beta\alpha a \mid \mu m, \beta b\ \rangle (\alpha t_\alpha \mid\mid A^{(\mu t_\mu)} \mid\mid \beta t_\beta).$$

Proof. Let $\mathcal{S}^{(\mu)}$ and $\mathcal{S}^{(\beta)}$ be the irreducible subspaces of the corresponding representations $D^{(\mu)}(G)$ and $D^{(\beta)}(G)$. When the standard basis in $\mathcal{S}^{(\mu)} \otimes \mathcal{S}^{(\beta)}$ is looked for, some vector, v, is projected by the one-dimensional projector $P_{aa}^{(\alpha)}$ (for $a_{\mu\beta\alpha=1}$), and the normalized projection (if it does not vanish) is chosen as $|\mu\beta\alpha a\rangle$. The other standard vectors are $|\mu\beta\alpha a'\rangle = P_{a'a}^{(\alpha)} |\mu\beta\alpha a\rangle$. If $\{|\ \mu t_\mu m\ \rangle\}$ and $\{|\ \beta t_\beta b\ \rangle\}$ are the standard bases in $\mathcal{S}^{(\mu)}$ and $\mathcal{S}^{(\beta)}$, respectively, then $\{|\ \mu t_\mu m\ \rangle \otimes |\ \beta t_\beta b\ \rangle \stackrel{\text{def}}{=} |\ \mu m, \beta b\rangle\}$ is (uncorrelated) basis in $\mathcal{S}^{(\mu)} \otimes \mathcal{S}^{(\beta)}$. Some of its vectors certainly have non vanishing projections by $P_{aa}^{(\alpha)}$; therefore, $|\ \mu\beta\alpha a\rangle = C P_{aa}^{(\alpha)} |\ \mu m, \beta b\rangle$, with C being normalizing constant, and expansion of the uncorrelated basis over the standard one, reads

$$|\ \mu\beta\alpha a\rangle = C P_{aa}^{(\alpha)} \sum_{\alpha' a'} \langle\ \mu\beta\alpha' a' | \mu m, \beta b\ \rangle\ |\ \mu\beta\alpha' a'\rangle = C \langle\ \mu\beta\alpha a \mid \mu m, \beta b\ \rangle\ |\ \mu\beta\alpha a\rangle,$$

i.e. $\frac{1}{C} = \langle\ \mu\beta\alpha a \mid \mu m, \beta b\ \rangle$. The remaining vectors of the standard basis are:

$$|\ \mu\beta\alpha a'\rangle = C \frac{n_\alpha}{|G|} \sum_{g \in G} d_{a'a}^{(\alpha)^*}(g) D^{(\mu)}(g) \otimes D^{(\beta)}(g)\ |\ \mu m, \beta b\rangle =$$

$$\sum_{m', b'} C \frac{n_\alpha}{|G|} \sum_{g \in G} d_{a'a}^{(\alpha)^*}(g) d_{m'm}^{(\mu)}(g) d_{b'b}^{(\beta)}(g)\ |\ \mu m', \beta b'\rangle.$$

The orthonormality of the standard basis yields

$$\langle\ \mu m', \beta b' | \mu\beta\alpha a'\ \rangle\langle\ \mu\beta\alpha a \mid \mu m, \beta b\ \rangle = \frac{1}{C}\langle\ \mu m', \beta b' | \mu\beta\alpha a'\ \rangle = \frac{n_\alpha}{|G|}\sum_{g\in G} d^{(\alpha)^*}_{a'a}(g) d^{(\mu)}_{m'm}(g) d^{(\beta)}_{b'b}(g).$$

The last relation, when $I = D^{-1}(g)D(g)$ is written in front and behind the operator in the matrix element, and the unitarity of the representation is employed, is summed over the group elements into

$$\langle\ \alpha t_\alpha a \mid A^{(\mu t_\mu)}_m \mid \beta t_\beta b\ \rangle = \sum_{a'm'b'} d^{(\alpha)^*}_{a'a}(g) d^{(\mu)}_{m'm}(g) d^{(\beta)}_{b'b}(g) \langle\ \alpha t_\alpha a' \mid A^{(\mu t_\mu)}_{m'} \mid \beta t_\beta b'\ \rangle.$$

Introducing

$$(\alpha t_\alpha \mid\mid A^{(\mu t_\mu)} \mid\mid \beta t_\beta) \stackrel{\text{def}}{=} \frac{1}{n_\alpha}\sum_{a'm'b'} \langle\ \mu\beta\alpha a' \mid \mu m', \beta b'\ \rangle\langle\ \alpha t_\alpha a' \mid A^{(\mu t_\mu)}_{m'} \mid \beta t_\beta b'\ \rangle,$$

the relation of the theorem is achieved. *QED*

Appendix C

Modified Group Projector Technique

Finding energy spectrum is the corner stone for analysis of physical systems. It is well known that symmetry facilitates this and, providing eigenbases labeled by conserved quantum numbers, afterward considerations of the properties and processes. Particularly fruitful and widespread is implementation of symmetry in the quantum mechanical state spaces which are of inductive structure, when each atom (site) contributes by its own (usually low-dimensional) subspace to the total state space being the sum of all these. Such space is shared characteristic of tight-binding electronic (TBA), harmonic lattice dynamics (LDH) and classical magnetism approximations (CAM), the three basic techniques for the main ingredients of the physical systems. Utilizing translational symmetry, Bloch theorem exactly reduces considerations to the elementary cell of the crystals only, and the goal of the modified group projector technique (MGPT) is to generalize this to arbitrary symmetry. Generally, full symmetry group generates the system from a minimal part, *symcell*, with usually only a few atoms, and it is intuitively clear that all the properties of the system are determined by the properties of this part and full symmetry. Thus, MGPT realization of this task consists of using full symmetry and minimal set of input ingredients, i.e. symcell only to find SAEB in the inductive spaces. In two- and three-dimensional crystals the translational group is a subgroup of the space group of the order up to 32, and from the technical point of view this is an estimate of the efficiency rate with respect to pure Bloch theorem. However, in quasi one-dimensional systems, like nanotubes and polymers, this may be much greater. In molecular physics there is no other general prescription for application of symmetry.

C.1 Geometry and State Space

To introduce convenient notation, some of the well known notions will be revisited. Let the considered system X (with $|X|$ atoms, e.g. molecule, crystal, etc.), with dynamics governed by the hamiltonian operator H in the state space $\mathcal{S}$, has group of symmetry G (point, line, diperiodic, space group) acting in $\mathcal{S}$ by the representation $D(G)$, i.e. the triple $(\mathcal{S}, H, D(G))$ is fixed. This has geometrical, kinematical and dynamical contents.

Geometrically, permuting the atoms, group decomposes system into orbits X^P ($P =$

$1,\dots,$), with the same type atoms, and generates X acting on the symcell: the set X_0 of the orbit representatives x_0^P. The elements leaving x_0^P fixed form stabilizer or fixing subgroup, F^P; transverzal $Z^P = \{z_0 = e, z_1, \cdots, |Z^P|\}$ of the coset partition $G = F^P + z_1^P F^P + \cdots$ is not unique, but its order, $|Z^P| = |G|/|F^P|$, is the number of atoms in the orbit. The atoms are counted by orbit (type) and transverzal indices, $x_p^P = z_p^P x_0^P$. As g maps each atom x_p^P of the orbit X^P into another one $gx_p^P = x_t^P$, it establishes bijection $g^P(p) = t$ (shortly, $gp = t$, assuming context defined P) of the transverzal Z^P:

$$gz_p^P = z_{gp}^P f^P(g,p), \quad \text{i.e.} \forall g,p,\exists!(f,gp) \text{ such that } g = z_{gp}^{P^{-1}} f^P(g,p) z_p^P \tag{C.1}$$

where $f^P(g,p)$ is unique element of F^P.

As for quantum kinematics, to each atom the space $\mathcal{S}_p^P$ is associated; it is characterized by the atom type, $\mathcal{S}_p^P \cong \mathcal{S}^P$ (dimension $|\mathcal{S}^P|$) and depends on the studied physical property: in CAM and LDH it is $\mathbb{R}^3$, with vectors (site spins and displacements) given in the fixed *exterior* Cartesian basis; in TBA it is spanned by the relevant orbitals transformed along the orbit by the group action, to make convenient *interior* basis. Thus, $\mathcal{S}_p^P = \mathcal{S}_{ip}^P \otimes \mathcal{S}_{ep}^P$, and the state space is the direct sum of the atomic ones: $\mathcal{S} = \oplus_{Pp} \mathcal{S}_p^P$, with the basis $|\,Pp;\psi\rangle = |\,Pp;\psi_{\rm i}\psi_{\rm e}\rangle$, where ψ counts bases in the atomic (interior and exterior) spaces. The group acts in $\mathcal{S}$ by unitary representation $D(G)$ (all the involved representations are unitary):

$$D(g) = \sum_{Pp} E_{Pp}^{P,gp} \otimes \delta^P(f^P(g,p)) \otimes d^P(g). \tag{C.2}$$

Here, basis matrices E_{Qq}^{Pp} have all zeros except 1 at the intersection of the row Pp and column Qq. Thus, $E_{Pp}^{P,gp}$ emulates group action on the sites, and (as it is easily checked) that $\sum_{Pp} E_{Pp}^{P,gp}$ is permutational representation of G (mentioned in Chapter 3); also, it $\mathbb{1}(F \uparrow G)$ induced identity representation of stabilizer to group, being in a sense is a prototypical (thus known as *ground* representation) for induction as seen from (C.2): the first factor is interior part, representation $\delta^P(F^P \uparrow G)$ of G induced from the representation $\delta^P(F^P)$ of the stabilizer. Exterior part is $d^P(G)$. The representation $D(G)$ is reduced to the ($|\mu|$-dimensional) irreducible components $D^{(\mu)}(G)$ as $D(G) = \sum_\mu a^\mu D^{(\mu)}(G)$; frequency numbers a^μ following orbit decomposition of $D(G)$, satisfy $a^\mu = \sum_P a_P^\mu$.

Dynamically, hamiltonian matrix elements $\langle Pp;\psi_{\rm i}\psi_{\rm e} \mid H \mid Qq;\psi_{\rm i}\psi_{\rm e}\rangle$ are groupped into $|\delta^P||d^P| \times |\delta^P||d^Q|$ blocks $H_{Pp}^{Qq} = \chi_{Pp}^{Qq} \otimes h_{Pp}^{Qq}$, modeling interaction of the atoms x_q^Q and x_p^P in the interior and exterior spaces: $H = \sum_{PpQq} E_{Qq}^{Pp} \otimes H_{Qq}^{Pp}$. As H is hermitean, blocks satisfy $H_{Pp}^{Qq} = H_{Qq}^{Pp\dagger}$ (as well as h and χ). Finally, manifesting symmetry, hamiltonian commutes with group: $[D(g), H] = 0$ for each g, or equivalently $\delta^P(f^P(g,p))\chi_{Qq}^{Pp}\delta^{Q\dagger}(f^P(g,q)) = \chi_{Q,gq}^{P,gp}$ and $d^P(g)h_{Qq}^{Pp}d^{Q\dagger}(g) = h_{Q,gq}^{P,gp}$. In particular, taking $g = z_q^{Q^{-1}}$ interaction is expressed through the atoms interacting with orbit representatives, i.e. their relevant neighbors only:

$$\chi_{Qq}^{Pp} = \chi_{Pp}^{Qq\dagger} = \delta^{P\dagger}(f^P(z_q^{Q^{-1}},p))\chi_{Q0}^{P,z_q^{Q^{-1}}p}, \quad h_{Qq}^{Pp} = h_{Pp}^{Qq\dagger} = d^P(z_q^Q)h_{Q0}^{P,z_q^{Q^{-1}}p}d^{Q\dagger}(z_q^Q). \tag{C.3}$$

C.2 Concept of MGPT

Within MGPT [47] for each irreducible component $D^{(\mu)}(G)$ of $D(G)$, the state space is expanded by the irreducible space $\mathcal{S}^{(\mu^*)}$ (with basis $|\,\mu^* m\rangle$ $(m = 1, \ldots, |\mu|)$, of the conjugated representation $D^{(\mu^*)}(G)$, to get space $\mathcal{S}^{\mu} = \mathcal{S} \otimes \mathcal{S}^{(\mu^*)}$. The fixed points of the representation $\Gamma^{\mu}(G) = D(G) \otimes D^{(\mu)^*}(G) = \oplus_P \Gamma^{P\mu}(G)$ span a_μ dimensional subspace, with the projector $G(\Gamma^{\mu})$, and its arbitrary basis $|\mu t_\mu\rangle$ $(t_\mu = 1, \ldots, a_\mu)$ gives a SAB by the partial scalar product:

$$|\,\mu t_\mu m\rangle = \langle\, \mu^* m \mid \mu t_\mu \,\rangle \quad t_\mu = 1, \ldots, a_\mu;\ m = 1, \ldots, |\mu|. \tag{C.4}$$

To get SAEB, the chosen vectors have to be eigenvectors of the auxiliary hamiltonian $H_\mu = H \otimes \mathbb{1}_\mu$ in the auxiliary space $\mathcal{S}^{\mu}$. All this is easily seen directly from the standard group projector technique. One of the advantages is that to get the subspace of the fixed points of a representation, it is enough to find the intersection of the fixed points subspaces of the generators only, thus avoiding summation over the group. Therefore, the method is applicable to infinite, even noncompact Lie groups.

C.3 MGPT in Inductive Spaces

For the inductive representation (C.2), the task is reduced to the symcell space $\mathcal{S}_0 = \oplus_P \mathcal{S}_{P0}$. To see this the modified projector (in the auxiliary space) $\mathcal{S}^{\mu} = \mathcal{S} \otimes \mathcal{S}^{(\mu^*)}$

$$G(\Gamma^{\mu}) = \sum_P \frac{1}{|G|} \sum_{g,p} E^{Pgp}_{Pp} \otimes \delta^P(f^P(g,p)) \otimes d^P(g) \otimes D^{(\mu)^*}(g)$$

is to be calculated. Using (C.1), and the transverzal pool-up operators

$$\hat{Z}^{P\mu} = \frac{1}{\sqrt{|Z^P|}} \sum_p E^{Pp}_{P0} \otimes \zeta^{P\mu}_p, \quad \zeta^{P\mu}_p = \mathbb{1}_\delta \otimes d^P(z^P_p) \otimes D^{(\mu)^*}(z^P_p), \tag{C.5}$$

it becomes: $G(\Gamma^{\mu}) = \sum_P \hat{Z}^{P\mu} \left[E^{P0}_{P0} \otimes F^P(\delta^P \otimes d^P \otimes D^{(\mu)^*})\right] \hat{Z}^{P\mu^\dagger}$. Finally, as all the operators above are block-diagonal (within orbit spaces, following independent group action over orbits), introducing subduced to stabilizer representations

$$\gamma^{P\mu}(F^P) = \delta^P(F^P) \otimes d^P(F^P) \otimes D^{(\mu)^*}(F^P), \tag{C.6}$$

the result is:

$$G(\Gamma^{\mu}) = \hat{Z}^{\mu} G^{\downarrow}(\Gamma^{\mu}) \hat{Z}^{\mu^\dagger}, \quad G^{\downarrow}(\Gamma^{\mu}) = \sum_P E^{P0}_{P0} \otimes F^P(\gamma^{P\mu}), \quad \hat{Z}^{\mu} = \sum_P \hat{Z}^{P\mu}. \tag{C.7}$$

The operator $\hat{Z}^{\mu}$ is a partial isometry on the range of the modified projector $G^{\downarrow}(\Gamma^{\mu})$: it maps this subspace in $\mathcal{S}_0$ onto the range of $G(\Gamma^{\mu})$, i.e. fixed points of $\Gamma^{\mu}(G)$. Its adjoint $\hat{Z}^{\mu^\dagger}$ is its inverse on the fixed points of $\Gamma^{\mu}(G)$ (Fig. C.1). In this sense $G(\Gamma^{\mu})$ is pulled-up operator

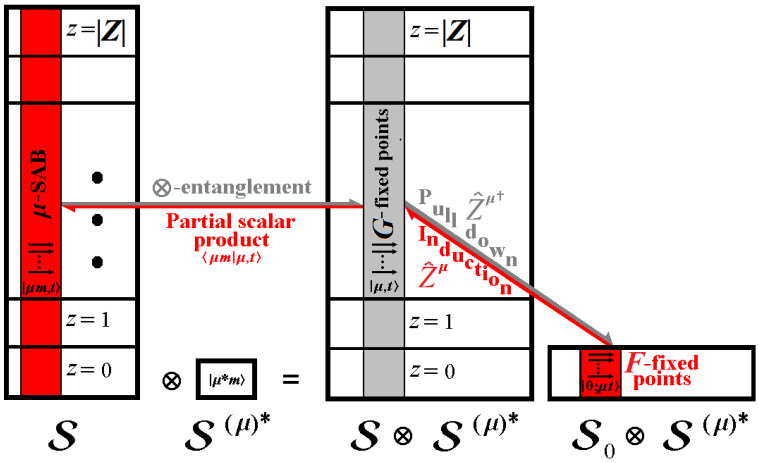

Figure C.1: Scheme of the modified group projector technique in the induced spaces. The symmetry adapted basis $|\,\mu t_\mu m\rangle$ looked for in the state space $\mathcal{S}$ is effectively found in the symcell space $\mathcal{S}_0$: the fixed points $|0;\mu t_\mu\rangle$ of the stabilizer group F in this space are induced to auxiliary space $\mathcal{S}\otimes\mathcal{S}^{(\mu)*}$ (where they are fixed points $|\,\mu t_\mu\rangle$ of the whole group G), and then by the partial trace mapped to $|\mu m,t\rangle$

of $G^{\downarrow}(\Gamma^\mu)$, and oppositely, $G^{\downarrow}(\Gamma^\mu)=\hat{Z}^{\mu\dagger}G(\Gamma^\mu)\hat{Z}^\mu$ is pulled-down to $\mathcal{S}_0^\mu$ modified projector $G(\Gamma^\mu)$. As within MGPT just the fixed points of $\Gamma^\mu(G)$ are looked for, it turns out that it is sufficient to work with the symcell space (thus low-dimensional) representations $\gamma^{P\mu}$ using only stabilizers. Any basis $|\mu t_\mu\rangle^0$ of the range of $G^{\downarrow}(\Gamma^\mu)$ is mapped by $\hat{Z}^\mu$ to the basis in the range of $G(\Gamma^\mu)$, giving multiplet $|\mu t_\mu m\rangle$ of SAB by (C.4):

$$|\mu t_\mu\rangle_p^P=\mathbb{1}_{\delta^P}\otimes d^P(z_p^P)\otimes D^{(\mu)^*}(z_p^P)\,|\mu t_\mu\rangle_0^P,\quad |\mu t_\mu m\rangle=\langle\mu^* m|\,(Z^\mu\,|\mu t_\mu\rangle^0). \tag{C.8}$$

To find SAEB, it remains to pull-down the auxiliary hamiltonian $H_\mu=H\otimes\mathbb{1}_\mu$ to $\mathcal{S}_0^\mu$:

$$H_\mu^{\downarrow}=Z^{\mu\dagger}H_\mu Z^\mu=\sum_{PQ}E_{Q0}^{P0}\otimes\frac{1}{\sqrt{|Z^P||Z^Q|}}\sum_p\left(\sum_q\gamma^{P\mu}(f^P(z_q^Q,p))\right)\zeta_p^{P\mu\dagger}(H_{Q0}^{Pp}\otimes\mathbb{1}_\mu). \tag{C.9}$$

It commutes with $G^{\downarrow}(\Gamma^\mu)$, and the vectors $|\mu t_\mu\rangle^0$ are the eigenvectors of $H_\mu^{\downarrow}$ from the range of $G^{\downarrow}(\Gamma^\mu)$, i.e. those satisfying both $G^{\downarrow}(\Gamma^\mu)\,|\mu t_\mu\rangle^0=|\mu t_\mu\rangle^0$ and $H_\mu^{\downarrow}\,|\mu t_\mu\rangle^0=H_\mu^{\downarrow}G^{\downarrow}(\Gamma^\mu)\,|\mu t_\mu\rangle^0=\epsilon_{\mu t_\mu}\,|\mu t_\mu\rangle^0$. Rearrangement lema for the stabilizers gives for the operator reduced to the range of $G^{\downarrow}(\Gamma^\mu)$:

$$H_{0\mu}^{\downarrow}=G^{\downarrow}(\Gamma^\mu)H_\mu^{\downarrow}=\sum_{PQ}E_{Q0}^{P0}\otimes\sqrt{\frac{|F^P|}{|F^Q|}}F^P(\gamma^{P\mu})H_{PQ}^\mu,\quad H_{PQ}^\mu=\sum_p\zeta_p^{P\mu\dagger}H_{Q0}^{Pp}. \tag{C.10}$$

Its eigenvectors from the range of $G^{\downarrow}(\Gamma^\mu)$, are $|\mu t_\mu\rangle^0$, giving SAEB site components:

$$|\mu t_\mu m\rangle^{Pp}=d^P(z_p^P)\sum_{m'}D_{mm'}^{(\mu)^*}(z_p^P)\,|\mu t_\mu m'\rangle^{P0}. \tag{C.11}$$

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