4.4   The Hamiltonian and its symmetry operations

To calculate the commutator relation of Eq. (4.10) we used the (lattice) translational invariance of the Hamiltonian. The Bloch theorem and the use of the reciprocal lattice for the description of a solid are therefore a direct consequence of the translational invariance.

The calculation of Eq. (4.10) using Eq. (4.9) is valid for every operator S which describes a symmetry-operation of the Hamiltonian. Consequently we find

$$[S, H] = 0 \qquad , \tag{4.23}$$

and the Eigenvector system of S is simultaneously a Eigenvectorsystem of H:

$$\begin{aligned} H\psi_s &= E\psi_s \\ S\psi_s &= s\psi_s \end{aligned} \tag{4.24}$$

Searching for all Operators (measurable quantities and Quantum numbers) which commutate with the Hamiltonian can be interpreted as the search for all symmetry operations which leave the Hamiltonian invariant.

This is a quite constructive way to classify a quantum mechanical system completely and to quantify the state.
Knowing the complete set of symmetry operators S_i of a Hamiltonian, each Eigenstate ψ can be written as

$$\psi = \psi_{s_1}\psi_{s_2}...\psi_{s_N} \qquad . \tag{4.25}$$

Every state can be evaluated into these Eigenvectors:

$$\xi = \sum_{s_1, s_2, ..., s_N} \psi_{s_1}\psi_{s_2}...\psi_{s_N} \qquad . \tag{4.26}$$

This is the adequate description of the state of a system described by the Hamiltonian H. This representation allows to calculate the time evolution easily.

REMARK: This is just one example in natural science where discussing the symmetries serve fundamental information on the system. The search for symmetries in nature and the formulation of mathematical models based on sometimes quite abstract symmetries are the very successful way of modern science.

Considering this new approach of quantum mechanics we will discuss the results of the last chapter again.

- The time dependent Schrödinger equation reflects the invariance in time of the system. Only if the Schrödinger equation is not explicitly time dependent, a linear combination of Eigenvectors of the time independent Schrödinger equation is a solution. Only in this case the energy E is conserved and a quantum number of the system.

- For a free particle the momentum is a Quantum number. This reflects the translation invariance of the Hamiltonian. The $\vec{k}$-vectors are continuous since in contrast to a solid each translation leaves the system invariant.

- For the Hydrogen atom the rotational invariance causes the conservation of rotational momentum and the quantum numbers l.

- The magnetic quantum numbers m just reflect the mirror symmetry of the Coulomb potential.

Symmetry-Operations and solids

In addition to the lattice translation invariance we find several symmetry operations of the Hamiltonian of a solid which depend on the type of the lattice and the basis of atoms:

- mirror symmetry for several planes

- rotations with several angles around several axis

The treatment of these space groups (classification, characterization calculation of Eigenvalues and Eigenfunctions) is the task of the group theory. Using this Eigenvectors for each symmetry operation, all Eigenvectors and Eigenvalues of the Hamiltonian can be calculated according to Eq. (5.26). The Schrödinger equation is needed "only" for the calculation of the Energy Eigenvalues which belong to the Eigenvectors. The diagonalization and calculation of the unitary transformation is not necessary any more.

Crystallographs and theoretical physicists therefore do often not think in the categories "lattice + basis" which allows to describe a crystal quite simply and elegantly, but in the categories of space groups which allows the solid to be calculated quite simply and elegantly.