UNIVERSITY OF KONSTANZ
Department of Physics
Dr. Andor Kormányos, Prof. Dr. Guido Burkard

Group theory and symmetries in quantum mechanics
Summer semester 2016 - Exercise sheet 9
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Problem 24: Characters of the inversion and improper rotation operations in the full rotation group

The spherical harmonics $Y_{l,m}(\theta,\phi)$ are basis functions for the odd-dimensional representations of the full rotation group $SO(3)$ ($\mathbb{R}(3)$) . From their explicit form one can see that they are a product of a simple complex exponential function and an associated Legendre polynomial $P_l^m(\cos\theta)$.

(a) Using e.g., Mathematica, Wikipedia, or some handbook on special functions, learn about the properties of the function $P_l^m(x)$. Is it an odd or even function of x ?

(b) Consider the *inversion* operation i, which acts an the Cartesian coordinates in the following way: $(x,y,z)\to(-x,-y,-z)$. Using $Y_{l,m}(\theta,\phi)$ as a basis, what is the character of i in $\mathbb{R}(3)$?

(c) Now consider the following symmetry operations:

- $\sigma_h=\sigma_{xy}$ mirror reflection with respect to the xy plane: $(x,y,z)\to(x,y,-z)$
- $\sigma_v=\sigma_{xz}$ mirror reflection with respect to the xz plane: $(x,y,z)\to(x,-y,z)$

Write these operations is terms of the inversion and a rotation around an appropietly chosen axis and using $Y_{l,m}(\theta,\phi)$ as a basis calculate their character!

(d) Improper rotations are defined as a σ_h operation followed by a rotation C_n around the z-axis by $2\pi/n$, $n=2,3,4,5,6$ and we use the notation S_n to denote them. What is the character of S_n in $\mathbb{R}(3)$? How can one express S_n in terms of a rotation and a inversion operation ?

Problem 25: Paramagnetic ion in a cubic crystal

Consider a paramagnetic ion with a single electron in its highest occupied orbital. In the lecture we used the point group O to describe the symmetries of the crystal field around this ion when it is placed into a substitutional lattice site of a cubic crystal. In fact, the symmetry is higher, and is described by the group O_h, which can be viewed as a direct product of two groups: $O\otimes S_2$, where $S_2=\{E,i\}$ contains the identity E and the inversion i.

(a) Using the character tables of O and S_2, construct the character table of O_h!

(b) Do our results regarding the crystal field splitting of the $l=2$ energy levels change if we use the group O_h instead of O ?

(c) Consider now the case when the paramagnetic ion has a single electron in an orbital state described by angular momentum quantum number l. Assume that we would like to investigate this ion using dipole excitations of its electron into other orbital states $l'\neq l$. Formulate the selection rule for the dipole transitions in terms of the change Δl in the angular momentum quantum number l !

Problem 26: Paramagnetic ion in a strained cubic crystal.

Suppose that a paramagnetic ion is placed into a substitutional lattice site of a cubic crystal and then strain is applied along the (110) direction of the crystal.

(a) What is the symmetry of the crystal field around the ion? What are the symmetry operations in the point group $\mathcal{G}_{strain}$ of the crystal field?

(b) Considering the irrep $\Gamma_{rot}^{l=2}$ for $\mathbb{R}(3)$ as a reducible representation of $\mathcal{G}_{strain}$, find the irreps of $\mathcal{G}_{strain}$ contained in $\Gamma_{rot}^{l=2}$!

(c) How are the T_2 and E levels corresponding to $\Gamma_{rot}^{l=2}$ in the cubic group O split by the strain along the (110) direction ? Are there new allowed dipole transitions with respect to the case, when the strain acts in the (001) direction ?