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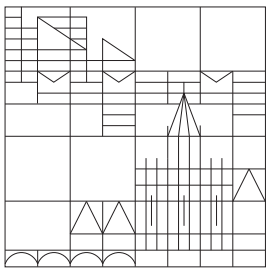

Group theory and symmetries in quantum mechanics
Summer semester 2017 - Exercise sheet 10
Distributed: 7.07.2017, Discussion: 12.07.2017 and 13.07.2017

Problem 26: Characters of the inversion and improper rotation operations in the full rotation group

In the lecture we have introduced the spherical harmonics $Y_{l,m}(\theta, \phi)$ as basis functions for the odd-dimensional representations of the full rotation group $\mathbb{R}(3)$. From their explicit form we have seen 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 27: Paramagnetic ion in a cubic crystal

In the lecture we used the point group O to describe the symmetries of the crystal field around an ion that 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 ?

Problem 28: 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 ?