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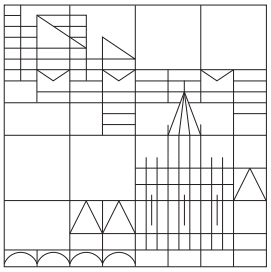
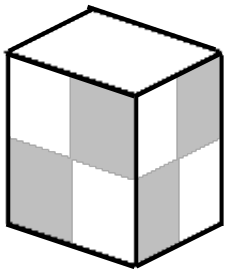
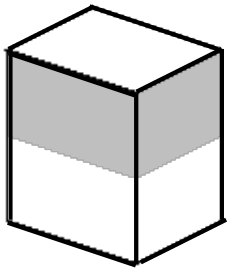
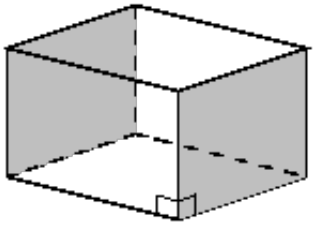


Group theory and symmetries in quantum mechanics
Summer semester 2016 - Exercise sheet 10
Distributed: 04.07.2016, Discussion: 08.07.2016

Problem 27: The double groups $\bar{D}_2$, $\bar{C}_{2v}$ and $\bar{C}_{2h}$







Objects with D_2, C_{2v} and C_{2h} symmetries are shown in the left, middle and right figures, respectively. The single group character table for D_2 reads:

			E	C_2	C_2'	C_2''
x^2, y^2, z^2		A_1	1	1	1	1
xy	R_z, z	B_1	1	1	-1	-1
xz	R_y, y	B_2	1	-1	1	-1
yz	R_x, x	B_3	1	-1	-1	1

while for C_{2v} it is given by

			E	C_2	σ_v	σ_v'
x^2, y^2, z^2	z	A_1	1	1	1	1
xy	R_z	A_2	1	1	-1	-1
xz	R_y, x	B_1	1	-1	1	-1
yz	R_x, y	B_3	1	-1	-1	1

Here σ_v and σ_v' denote mirror reflections.
(a) Consider the character table of D_2 and C_{2v}. Using the Frobenius-Schur criterion find out whether individual irreps are of a), b) or c) type, as discussed in the lecture !

(b) Try to construct the double group character table for $\bar{D}_2$ and $\bar{C}_{2v}$! How many new classes and representations are there in these double groups?

(c) Now consider the group C_{2h}. The character table is given below. How many new classes and representations are there in $\bar{C}_{2h}$? What are the dimensions of the new representations?

			E	C_2	σ_h	i
x^2, y^2, z^2	R_z	A_g	1	1	1	1
	z	A_u	1	1	-1	-1
xz, yz	R_y, x	B_g	1	-1	-1	1
	x, y	B_u	1	-1	1	-1

Table 1: Character table of C_{2h}. i denotes inversion.

Problem 28: Splitting of an erbium ion Er^{3+} in a cubic enviroment

Let us consider the erbium ion Er^{3+} in a host crystal. This ion is important for applications of amplification capabilities in optical fibres. Erbium is a rare earth element where the atomic spin-orbit coupling is stronger than the crystal field. In the ground state of the ion the total angular momentum is $j = 15/2$.

(a) How would this state split in a crystal field which has octahedral symmetry?

(b) Let us assume that the presence of this ion strains the host crystal and therefore the symmetry of the crystal field is lowered to D_4. How many new classes are in the double group $\bar{D}_4$ in comparison to D_4? Consider now the effect of the crystal field on the energy levels found in (a). Would the strain lift some of the degeneracies ?

Problem 29: Energy states of the nitrogen vacancy center (NV^-) defect in diamond

Point defects in crystals can lead to well-resolved bound states in the band gap of the host crystal. These states can be thought of as if they belonged to an artifical atom which has discrete spectrum, but the symmetries of the energy levels are determined by the local enviroment of the defect. One well-known example is the nitrogen vacancy center (NV^-) defect in diamond, which has attracted a lot of interest recently, because e.g., it can be used as a basic unit of a quantum computer. The local symmetry of the NV^- center is C_{3v}, whose character table is given below. The ground state

			E	$2C_3$	$3\sigma_v$
x^2+y^2, z^2	z	A_1	1	1	1
	R_z	A_2	1	1	-1
$\{x^2-y^2, xy\}$	(x, y)	E	2	-1	0

of the NV^- center has E symmetry and is occupied by two electrons.

(a) Consider first the spinor representation $D_{1/2}$ introduced in the lecture. What are the possible spin-states of two electrons? How are they related to $D_{1/2}$?

(b) Using the symmetries of the possible wave functions of two spins, find the effect of the spin-orbit coupling on the doubly-degenerate ground state of the NV^- center! Do we need the double group representations of C_{3v} to answer this question?