UNIVERSITETET I TRONDHEIM
NORGES TEKNISKE HØGSKOLE
INSTITUTT FOR FYSIKK

Faglig kontakt under eksamen:
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Eksamen i fag 74984 Fysiske grupperepresentasjoner
Tirsdag 19.12.89
Tid: 0900-1300

Use of calculator forbidden. Printed or handwritten notes not permitted.

Problem 1

a) Define the class concept in group theory. Show that the characters of elements in the same class are identical.

b) The symmetry of the linear molecule CO_2 is described by the product group $D_{\infty h} = C_{\infty v} \otimes S_2$. (The character table of $C_{\infty v}$ is given below and S_2 stands for the inversion group.) Verify that the two symmetry operations C_ϕ and $C_{-\phi}$ are in the same class by means of geometric reasoning.

c) Work out a representation Γ of the CO_2 symmetry by means of Cartesian displacement vectors. Reduce the representation and identify the translational and rotational modes.

d) The operator

$$P^i_{mn} = \sum_r \Gamma^i(A_r)^*_{mn} A_r$$

projects out functions that belong to the mth row of the irreducible representation Γ^i. Find the total-symmetric vibration mode of CO_2 by means of this operator. Is it possible to determine the eigenfrequency of this state by means of absorption/emission spectroscopy?

$C_{\infty v}$			E	$2C_\phi$	σ_v
x^2+y^2, z^2	z	$A_1(\Sigma^+)$	1	1	1
	R_z	$A_2(\Sigma^-)$	1	1	−1
(xz, yz)	(x, y) (R_x, R_y)	$E_1(\Pi)$	2	$2\cos\phi$	0
(x^2-y^2, xy)		$E_2(\Delta)$	2	$2\cos 2\phi$	0
		...	...	...	...

Problem 2.

a) Term configurations of free atoms and ions are specified through the use of the symbol ^{2S+1}L, where S and L are total spin and orbital quantum number, respectively. The spherical harmonic Y^M_L describes the spatial symmetry of a term. Representations of the three-dimensional rotation group R(3) have Y^M_L as basis functions. The characters are

$$\chi_L(\alpha) = \frac{\sin((L+\frac{1}{2})\alpha)}{\sin(\frac{\alpha}{2})}$$

where α denotes an arbitrary rotation. Derive this formula.

b) A Ti^{+++} ion with a single electron in a 3d-orbital is put into an octahedral complex. (See figure and character table for O_h below.) Assume the validity of crystal-field theory and show that the state is split into two sub-levels.

c) In the same figure the surrounding atoms, which act as sources of electrostatic potential, are shown as black points. Explain with reference to the figure why you expect a three-fold degeneracy for one of the two sub-levels. (See b)).

d) The lowest and second lowest term energies in a free Ti^{++} ion with $[\cdots 3d^2]$ configuration are ^3F and ^3P, respectively. These levels split as $^3P = {}^3T_{1g}$ and $^3F = {}^3A_{2g} \oplus {}^3T_{2g} \oplus {}^3T_{1g}$ in a cubic environment. A detailed analysis shows that the energies fullfill the inequalities $^3T_{1g} < {}^3T_{2g} < {}^3T_{1g} < {}^3A_{2g}$. Plot a correlation diagram for the energy, i.e. curves showing energy levels as functions of increasing field strength. Why is the spin quantum number S conserved in the diagram?

O		E	$8C_3$	$3C_2 = 3C_4^2$	$6C_2$	$6C_4$
	A_1	1	1	1	1	1
	A_2	1	1	1	−1	−1
$(x^2 - y^2, 3z^2 - r^2)$	E	2	−1	2	0	0
(R_x, R_y, R_z), (x, y, z)	T_1	3	0	−1	−1	1
(xy, yz, zx)	T_2	3	0	−1	1	−1

$O_h = O \times i$