Universität Regensburg | Winter Semester 09/10

Mesoscopic Physics

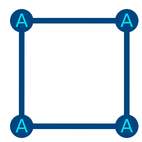
Dr. Andrea Donarini
Dr. Miriam del Valle

Room 5.01.01
Wednesdays at 15:30

Sheet 5

Analysis of the molecule A_4 by means of Group Theory

Consider a schematic molecule A_4, built by positioning all A-atoms at the corners of a square, as seen in the figure:



1. Prove that the molecule is invariant with respect to the D_{4h} symmetry point group.

2. Prove that D_4 and C_4 are two subgroups of D_{4h} and find for each of the groups all the classes of symmetry.

3. • Consider the Hamiltonian

$$H = \sum_{\alpha\sigma} \varepsilon c^\dagger_{\alpha,\sigma} c_{\alpha,\sigma} + b \sum_{\alpha\sigma} \left(c^\dagger_{\alpha,\sigma} c_{\alpha+1,\sigma} + c^\dagger_{\alpha+1,\sigma} c_{\alpha,\sigma} \right) \tag{1}$$

where $c^\dagger_{\alpha,\sigma}$ creates an electron in the $1\,s$ atomic orbital centered in atom α, and $b < 0$. The index $\alpha = 1, ..., 4$ should be consider with periodic boundary conditions: $\alpha + 4 = \alpha$. Which is the group of this Hamiltonian? Why? Construct explicitly one element of the group of operators which leaves the Hamiltonian invariant.

4. • Construct the representation corresponding to the single particle Hilbert space associated to states with total spin in the z-direction of $1/2$.

   Hint: There is no need of calculating all matrix representatives. The characters are enough.

5. By means of the reduction formula and of the character tables for C_4 and D_4 (see Tables **??**, **??**), determine whether the representation constructed at point 4 is reducible or not and the irreducible components calculated with respect of the two groups. What can you say about the single particle spectrum of the Hamiltonian H?

6. • By means of the projection operator technique, calculate the eigenvectors of the Hamiltonian H. To which eigenvalues do they correspond? Check the expected degeneracies of the spectrum.

7. Consider the case of the two electron problem. How would you proceed?

Table 1: Character table for group C_4

C_4	E	C_4^+	C_2	C_4^-
Γ_1	1	1	1	1
Γ_2	1	-1	1	-1
Γ_3	1	$-i$	-1	i
Γ_4	1	i	-1	$-i$

Table 2: Character table for group D_4

D_4	E	$2C_4$	C_2	$2C_2'$	$2C_2''$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
B_1	1	-1	1	1	-1
B_2	1	-1	1	-1	1
E	2	0	-2	0	0

Frohes Schaffen!