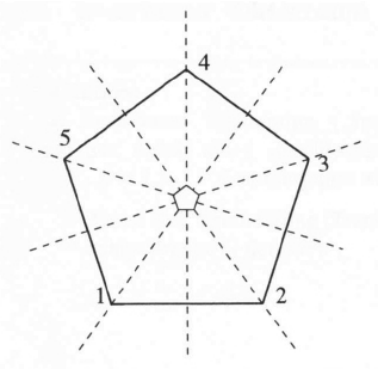
Universität Bielefeld	Symmetrien in der Physik	Prof. Dr. Jürgen Schnack
Fakultät für Physik	WS 2014/2015	jschnack@uni-bielefeld.de

Problem sheet 10

10.1 C_{5v}



The regular pentagon possesses the symmetry C_{5v}. This group contains 10 elements.

a. Identify the group elements.

b. How many conjugacy classes does the group possess and how many elements are contained in each of the classes?

c. How many irreducible representations do exist?

d. Look up the character table from literature.

10.2 Two-dimensional coordinate vector in C_{5v}

The vector $\vec{r}$ shall be transformed according to C_{5v} in a two-dimensional space $\mathbb{R}^2$ with carthesian coordinates.

a. Represent the group operations by 2×2–matrices.

b. Set up the character table for this representation.

c. Is this representation reducible or not?

10.3 LCAO using point group symmetry

The construction of trial states from atomic orbitals is termed *Linear Combination of Atomic Orbitals* (LCAO).
A fictitious molecule of five atoms possesses C_{5v} symmetry. The $1s$ wave function of one atom is known. Construct the symmetry-adapted wave functions for the charged molecule (5 cores, 1 electron) using first C_5 and then C_{5v}. Start by considering how the symmetry operations act on the $1s$ wave function. Then construct an invariant subspace and apply the *basis function generating machine*.

10.4 Extra problem: $3d$–orbitals in a ligand field

If atoms or ions of a chemical compound are surrounded by other atoms or ions, their atomic levels can be modified according to the symmetry of the environment. Such is statement is meant in a perturbation theory sense, since in full beauty the many-body problem does not allow to speak of atomic levels of the central ion.
In a perturbation theory approach in atomic and molecular physics as well as in chemistry one studies which basis sets of irreducible representations of a point group can be formed of the eigenfunctions belonging to a certain angular momentum quantum number.

a. Study how the following five real functions can be constructed from the spherical harmonics of $l = 2$:

$$\frac{1}{\sqrt{2}}\left(3\cos^2\theta - 1\right) \ , \sqrt{6}\sin\theta\ \cos\theta\ \cos\phi \ , \sqrt{6}\sin\theta\ \cos\theta\ \sin\phi \ , \tag{1}$$

$$\sqrt{\frac{3}{2}}\sin^2\theta\ \cos(2\phi) \ , \sqrt{\frac{3}{2}}\sin^2\theta\ \sin(2\phi) \ . \tag{2}$$

b. Study which irreducible basis functions can be build up in case of D_4 (z-axis as rotational axis).

c. Several chemical environments are octahedral, the respective point group is O_h. From the d orbitals one can form functions belonging to the irreducible representations E_g and T_{2g}. What does this mean? How many functions belong to each irreducible representation if E_g and T_{2g} are the only ones?