# Applications of Group Theory

PD Dr. Andrea Donarini Lectures

Exercises

H33, Mondays, 14:15 H34, Thursdays, 14:15 5.0.21, Wednesdays, 13:15

#### Sheet 2

#### 1. Group of the Hamiltonian

Consider the linear hermitian operator  $\hat{H}$  (in practice the Hamiltonian!) that maps a given Hilbert space  $\mathcal{H}$  into itself. Prove that the set of all linear, regular operators  $\hat{R}$  defined on the same Hilbert space and with the property  $[\hat{R}, \hat{H}] = 0$  form a group. Take as binary composition the usual multiplication between operators.

#### 2. Conservation of the norm

Consider a vectorial space V on which a scalar product is defined as a bilinear function by the relation  $\langle e_i, e_j \rangle = \delta_{ij}$ , where  $\delta_{ij}$  is the Kronecker function, and  $i(j) = 1, \ldots, n$  labels the n elements  $e_{i(j)}$  of a complete basis for V. Prove that each linear transformation f in V which conserves the scalar product between vectors, *i.e.*  $\langle f(v), f(w) \rangle = \langle v, w \rangle$  is represented by a unitary matrix *i.e.*  $M_f M_f^{\dagger} = M_f^{\dagger} M_f = \mathbf{1}$ , where  $\mathbf{1}$  represents the identity matrix.

### 3. Matrix representations

In the lecture we have introduced the homomorphism connecting point groups to groups of 3x3 matrices generating linear mappings of  $\mathbb{R}^3$  into itself. Moreover we related the latter to a group of functionals which can eventually be mapped back into a matrix group once a vectorial space of functions left invariant under the group of functionals is introduced. Let us now make a concrete example:

- 1. Construct the matrix that generates, in  $\mathbb{R}^3$ ,  $C_4^+$ , *i.e.* the anticlockwise rotation of  $\pi/2$  with respect of the z axis.
- 2. Construct the associated function operator  $\hat{R}_{C_4^+}$  and find the transformed function for each of the 5 d atomic orbitals. Find the associated matrix representation of the point symmetry operation in the Hilbert space generated by such orbitals.
- 3. Repeat the first two steps for all the elements of the cyclic group  $C_4$ . Is the representation reducible or irreducible?
- 4. Analogously, find the matrix representation of the group  $D_4$  in the same Hilbert space.

## Frohes Schaffen!