University of Regensburg | Summer Term 2014

# Applications of Group Theory

PD Dr. Andrea Donarini
Lectures 9.2.01, Mondays, 14:15
Exercises H34, Wednesdays, 14:00

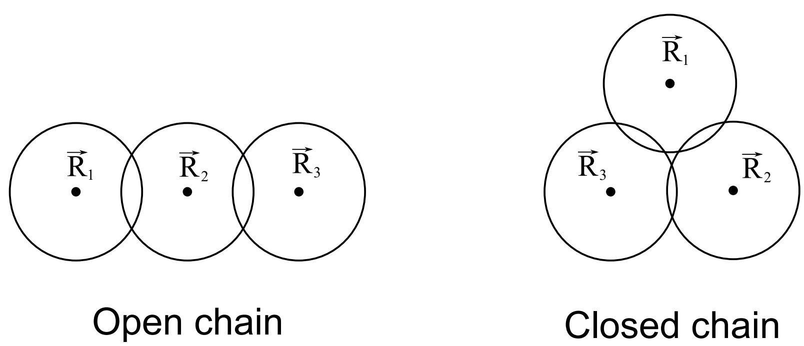
## Sheet 5

### 1. Boundary conditions

Consider the following Hamiltonians:

$$\begin{aligned} H_{\text{open}} &= t|\vec{R}_1\rangle\langle\vec{R}_2| + t|\vec{R}_2\rangle\langle\vec{R}_3| + H.c. \\ H_{\text{closed}} &= t|\vec{R}_1\rangle\langle\vec{R}_2| + t|\vec{R}_2\rangle\langle\vec{R}_3| + t|\vec{R}_3\rangle\langle\vec{R}_1| + H.c. \end{aligned} \quad (1)$$

with $t \in \mathbb{R}$, where $|\vec{R}_i\rangle$ represent spherically symmetrical $s$-type atomic orbitals located around the atomic positions $\vec{R}_i$ as illustrated below.




1. Verify that the figures above are invariant under the symmetry operations of the point groups $C_{2v}$ (for the open chain) and $C_{3v}$ (for the closed chain).
2. With the help of the two orthogonality theorems for characters construct the character tables associated to the the two point groups.
3. Consider the Hilbert spaces of the two Hamiltonians written above. Calculate the characters of the representation associated to each of the two Hilbert spaces with respect to the corresponding point groups.
4. With the help of the projection formula find the irreducible representations contained into the representations obtained at the previous point. What can we say about the degeneracies in the spectrum of the Hamiltonians?
5. Diagonalize $H_{\text{open}}$ and $H_{\text{closed}}$ and verify the degeneracies predicted at point 4.

6. Generalize the results obtained at points 3 and 4 to the case of a closed and open chain of $N$ atoms:

$$
\begin{aligned}
H_{\text{open}} &= t \sum_{i=1}^{N-1} |\vec{R}_i\rangle\langle\vec{R}_{i+1}| + H.c. \\
H_{\text{closed}} &= t \sum_{i=1}^{N} |\vec{R}_i\rangle\langle\vec{R}_{i+1}| + H.c.
\end{aligned}
\tag{2}
$$

where, for the closed case you should consider the periodic conditions $N+1=1$. Hint: Start by calculating the order of the group $C_{Nv}$ and the associated classes. Remember to distinguish the case $N$ even from $N$ odd.

**Frohes Schaffen!**