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## Introduction to group theory for molecules and solids

### Academic year 2020/2021

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### Problem : Point co-group of a $\mathbf{k}$ point

The little group of a  $\mathbf{k}$  point of the Brillouin zone is a subgroup of the space group of the solid  $\{(S_i, \boldsymbol{\tau}_i)\}$  ( $S_i$  is a rotation and  $\boldsymbol{\tau}_i$  a translation) that contains all the operations for which the rotational part satisfies the equation:

$$S_i \mathbf{k} = \mathbf{k} + \mathbf{G}_{S_i}, \quad (1)$$

where  $\mathbf{G}_{S_i}$  is a reciprocal lattice vector. The point group formed by the operations  $\{S_i\}$  that satisfy this relation is called small point group of  $\mathbf{k}$  or point co-group of  $\mathbf{k}$ .

- Consider the  $\mathbf{k}$  points  $\Gamma$ ,  $X$ ,  $M$ ,  $R$  of the Brillouin zone of the cubic lattice. For each of these points find the point co-group of  $\mathbf{k}$  assuming a monatomic solid with one atom per cell.
- Same problem for the  $\mathbf{k}$  points  $\Gamma$ ,  $X$ ,  $K$ ,  $W$ ,  $U$ , and  $L$  of the Brillouin zone of the face-centered cubic lattice.
- Same problem for the  $\mathbf{k}$  points  $\Gamma$ ,  $H$ ,  $N$ ,  $P$ , of the Brillouin zone of the body-centered cubic lattice.
- Same problem for the  $\mathbf{k}$  points  $\Gamma$ ,  $K$ ,  $M$ ,  $A$ ,  $H$ ,  $L$  of the Brillouin zone of the hexagonal lattice.
- Write a code that receives in input the rotation matrices of the space group of a solid, the primitive vectors of the reciprocal lattice, and the coordinates of a  $\mathbf{k}$  point and gives as output the list of rotation matrices that belong to the point co-group of  $\mathbf{k}$ . Check the correctness of your code on some of the  $\mathbf{k}$  points analyzed in the previous questions.

Hint: The definition of the  $\mathbf{k}$  points can be found in the file `brillouin_zones.pdf` in the Quantum ESPRESSO documentation.