

Weeks of September 8th and 15th

**Algebraic structures, \mathbb{N} and \mathbb{Z} , prime numbers
Crystals and Symmetries**

Additional Exercises

Exercise 1: Sub-groups (more abstract, just for fun)

Let's consider a group G for an operation $*$, and two subgroups A and B of G . Show that $A \cup B$ is a subgroup of G if and only if $A \subseteq B$ or $B \subseteq A$.

Hint on notations: $A \cup B$, or A union B , is a set that gathers all the elements of both groups. $A \subseteq B$, or A included in B means that all the elements of A also belong to B .

Exercise 2: The Fibonacci sequence

The Fibonacci sequence first appears in his Liber Abaci (The Book of Calculation, 1202) where he calculates the growth of rabbit populations. Assume that:

- A newly born breeding pair of rabbits are put in a field at month 1;
- Each breeding pair mates at the age of one month, and at the end of their second month they always produce another pair of rabbits;
- Rabbits never die, but continue breeding forever.

At month $n \in \mathbb{N}$, we call F_n the number of pairs of rabbits ($F_0 = 0$ & $F_1 = 1$).

2a. How many pairs of rabbit will there be at months two, three and four?

2b. For $n \geq 2$, explain why: $F_n - F_{n-1} = F_{n-2}$

2c. For $n \in \mathbb{N}$, find the two real solutions $\varphi > 0$ and $\psi < 0$ of the equation:

$$x^{n+2} = x^{n+1} + x^n.$$

2d. We define the sequence $u_n = a\varphi^n + b\psi^n$, with $(a, b) \in \mathbb{R}^2$. Show that:

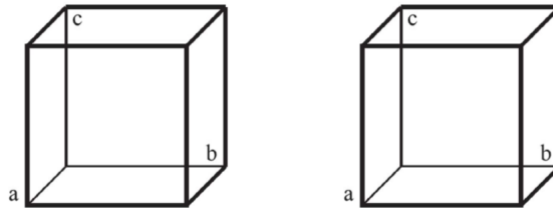
$$\forall n \in \mathbb{N}, u_{n+2} = u_{n+1} + u_n$$

2e. Express $(a, b) \in \mathbb{R}^2$ as a function of φ and ψ such that $u_0 = 0$ and $u_1 = 1$

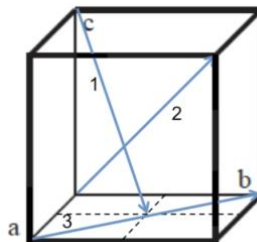
2f. Conclude that $\forall n \in \mathbb{N}, F_n = \frac{\varphi^n - \psi^n}{\varphi - \psi} = \frac{\varphi^n - \psi^n}{\sqrt{5}}$

Exercise 3: Miller indices

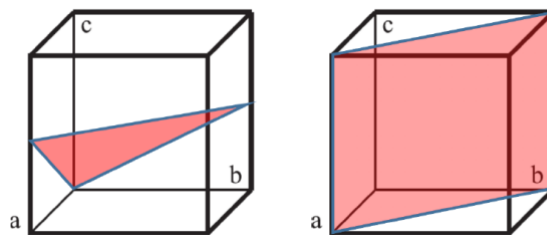
3a. Draw the crystal directions $[101]$, $[\bar{1}\bar{1}2]$ in the cubes to the right representing the cubic structure:



3b. Find the Miller indices of the directions (1, 2 and 3) shown in the cube on the right. What is the angle between directions 1 and 3 ? To which plan do directions 1 and 3 both belong ?



2c. What are the Miller indices of the crystal planes below:



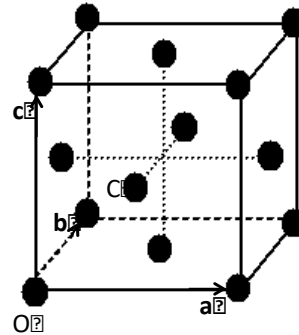
Exercise 4: Diamond structure

The diamond structure shown below consists of tetrahedra of carbon atoms arranged in space to form the crystal. This arrangement turns out to be represented by a motif of two carbon atoms translated in the face-centered cubic Bravais lattice. The atoms can be represented by a sphere of radius R . In the motif, one atom has its center at one corner of the cube that could be an origin $O(0,0,0)$, and the other one is shifted along the diagonal at position $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$. The two spheres representing the two atoms are in contact with each other (to the contrary of what is shown on the schematic below for clarity).

- 4a. Is the point of coordinate $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ a lattice point ?
- 4b.
 - (i) How many atoms are in the conventional FCC cell for Diamond ?
 - (ii) What is the coordination number ?
- 4c. Deduce the packing fraction of the Diamond structure.
- 4d. Find a condition on mutually prime relative integers (h,k,l) so that the plan (hkl) goes through the point $P(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$.

Exercise 5 : Primitive cell of the FCC structure

Consider the Face-centered cubic conventional cell shown to the right with the origin marked as O and the three orthogonal axis of length the cube edge a .



- 5a. In the basis $(O, \mathbf{a}, \mathbf{b}, \mathbf{c})$, what are the coordinate of the point C at the center of a face of the cube ? Is this basis a Bravais lattice for the FCC cubic structure ?

- 5b. We consider the same origin O and three new vectors \mathbf{a}' , \mathbf{b}' and \mathbf{c}' such that :

$$\mathbf{a}' = \frac{1}{2}(\mathbf{b} + \mathbf{c}) ; \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{c}) ; \mathbf{c}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

- (i) Show that for all point M of the FCC lattice, one can find relative integers n, p and q , such that: $\overrightarrow{OM} = \frac{n}{2}\mathbf{a} + \frac{p}{2}\mathbf{b} + \frac{q}{2}\mathbf{c}$, with (n,p,q) either all even numbers, or 1 is odd and 2 are even numbers.

- (ii) Express the **OM** vector in the $(O, \mathbf{a}', \mathbf{b}', \mathbf{c}')$ basis and conclude whether this basis is indeed a primitive basis for the FCC structure.

5c. Calculate the volume occupy by the FCC primitive cell in two ways:

- (i) Using the vectorial formula seen in class;
- (ii) Making an argument regarding the number of motifs should be present in the primitive and conventional cells of the FCC.