Week 3

Reciprocal Space, X-ray diffraction
Rational, Real and Complex Numbers

F. Sorin (MX)

Ecole Polytechnique Fédérale de Lausanne

Fall 2024

Reminder

- We introduced the basic notions of co-prime numbers and discussed several important concepts like the Bézout relation, or the Euclid lemma, that can be useful in understanding discrete configurations such as Bravais lattices.

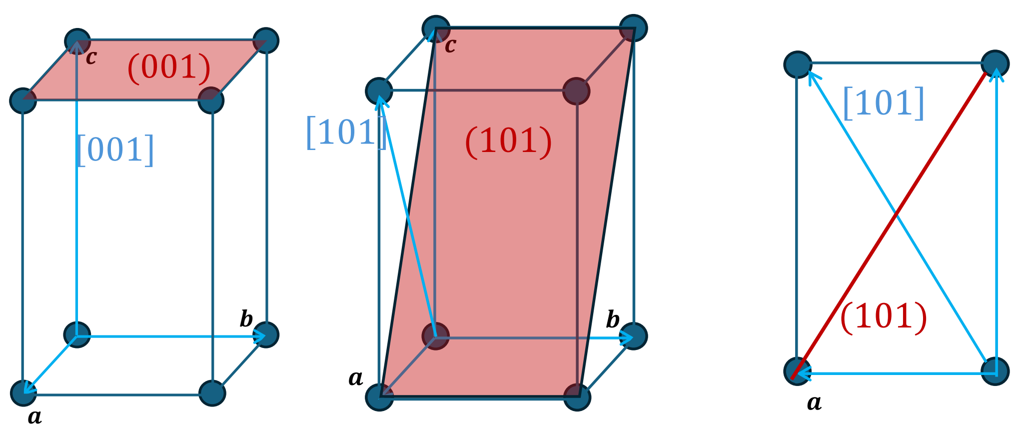
- We reminded basic objects and calculations in 3D.

- We used all these notions to review foundational aspects of crystallography including miller indices, crystal directions and planes.

- In particular, we showed that in the cubic systems, when the Miller indices are defined in the conventional cell (orthonormal basis), the planes (hkl) and directions $[hkl]$ are orthogonal.

- This is not true in other crystal structures !

    - Tetragonal structure:
        - $[001] \perp (001)$
        - But: $[101] \perp (101)$



Overview

- Reciprocal Space

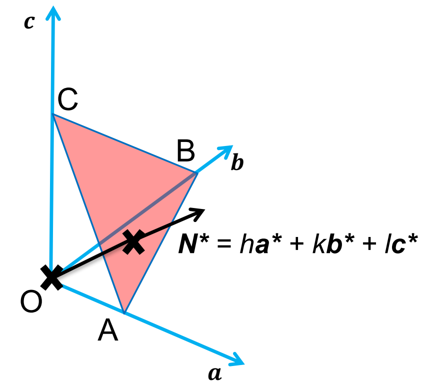
- Rational, Irrational and real numbers ($\mathbb{R}$)
- Origin of complex numbers
- Construction of $\mathbb{C}$
- Important properties of complex numbers

- Reciprocal space from X-ray diffraction (finish tomorrow)

Miller Indices and Reciprocal Space

- Can one find a new basis (O, **a***, **b***, **c***) such that a vector **N***$_{hkl}$ **=** h**a*** + k**b*** + l**c*** will be perpendicular to the plane (hkl) ?

- If A, B and C are the points of intercepts of the Bravais lattice vector basis (O, **a**, **b**, **c**) at **a**/h, **b**/k, and **c**/l respectively, we must have:



  - **AB . N***$_{hkl}$ = (-**a**/h+**b**/k).(h**a*** + k**b*** + l**c***) = 0
  - **AC . N***$_{hkl}$ = (-**a**/h+**c**/l).(h**a*** + k**b*** + l**c***) = 0

- This would work if **a*** was orthogonal to **b** and **c, b*** was orthogonal to **a** and **c,** and **c*** was orthogonal to **a** and **b**, and if **a.a* = b.b* = c.c***.

- which we can write:

$$\overrightarrow{a^*}.\ \overrightarrow{a} = 2\pi \qquad \overrightarrow{b^*}.\ \overrightarrow{a} = 0 \qquad \overrightarrow{c^*}.\ \overrightarrow{a} = 0$$
$$\overrightarrow{a^*}.\ \overrightarrow{b} = 0 \qquad \overrightarrow{b^*}.\ \overrightarrow{b} = 2\pi \qquad \overrightarrow{c^*}.\ \overrightarrow{b} = 0$$
$$\overrightarrow{a^*}.\ \overrightarrow{c} = 0 \qquad \overrightarrow{b^*}.\ \overrightarrow{c} = 0 \qquad \overrightarrow{c^*}.\ \overrightarrow{c} = 2\pi$$

- We would indeed obtain:

AB . N*$_{hkl}$ = (-**a**/h+**b**/k).(h**a*** + k**b*** + l**c***) = **-a.a*+b.b***= 0

AC . N*$_{hkl}$ = (-**a**/h+**c**/l).(h**a*** + k**b*** + l**c***) = **-a.a*+cc***= 0

$$N^*_{hkl} \perp (hkl)$$

Reciprocal space

- Reciprocal spaces are very useful in the understanding of crystals structure as well as in X-ray diffraction analysis.
- They are also a great way to approach some concepts in the band theory of electrons in solids.
- One way to see reciprocal space is to create a new basis that would mimic the orthogonal symmetry that we find in the cubic crystal structure.
- For a Direct lattice space (O,***a***,***b***,***c***), we define the Reciprocal Lattice (O,**a***,**b***,**c***) such that:

$$\begin{aligned} \overrightarrow{a^*}.\ \vec{a} &= 2\pi \\ \overrightarrow{a^*}.\ \vec{b} &= 0 \\ \overrightarrow{a^*}.\ \vec{c} &= 0 \end{aligned} \qquad \begin{aligned} \overrightarrow{b^*}.\ \vec{a} &= 0 \\ \overrightarrow{b^*}.\ \vec{b} &= 2\pi \\ \overrightarrow{b^*}.\ \vec{c} &= 0 \end{aligned} \qquad \begin{aligned} \overrightarrow{c^*}.\ \vec{a} &= 0 \\ \overrightarrow{c^*}.\ \vec{b} &= 0 \\ \overrightarrow{c^*}.\ \vec{c} &= 2\pi \end{aligned}$$

- The reciprocal lattice is: $\{P, \boldsymbol{OP} = n_1\boldsymbol{a}^* + n_2\boldsymbol{b}^* + n_3\boldsymbol{c}^*, (n_1, n_2, n_3) \in \mathbb{Z}^3\}$.
- The first important aspect is that ***a*** is orthogonal to ***b**** and ***c****: In most Bravais lattices, ***a*** is not orthogonal to ***b*** or ***c***, so the scalar product ***a.b*** and ***a.c*** cannot be ignored.

If however we consider a vector in the direct space $\boldsymbol{D} = d_1\boldsymbol{a} + d_2\boldsymbol{b} + d_3\boldsymbol{c}$ and one in the reciprocal space $\boldsymbol{N}^* = n_1\boldsymbol{a}^* + n_2\boldsymbol{b}^* + n_3\boldsymbol{c}^*$, we have:

$$\boldsymbol{D}.\boldsymbol{N}^* = d_1n_1\boldsymbol{a}.\boldsymbol{a}^* + d_2n_2\boldsymbol{b}.\boldsymbol{b}^* + d_3n_3\boldsymbol{c}.\boldsymbol{c}^* = 2\pi(d_1n_1 + d_2n_2 + d_3n_3)$$

Reciprocal space

- Why 2π ? Not defined like that in all text books. We will see that it is useful for the Diffraction of X-rays by crystal planes to have a 2π coefficient.
- How to construct the reciprocal basis from these considerations:

$$\overrightarrow{a^*} = 2\pi \frac{\vec{b} \times \vec{c}}{V} \qquad \overrightarrow{b^*} = 2\pi \frac{\vec{c} \times \vec{a}}{V} \qquad \overrightarrow{c^*} = 2\pi \frac{\vec{a} \times \vec{b}}{V}$$

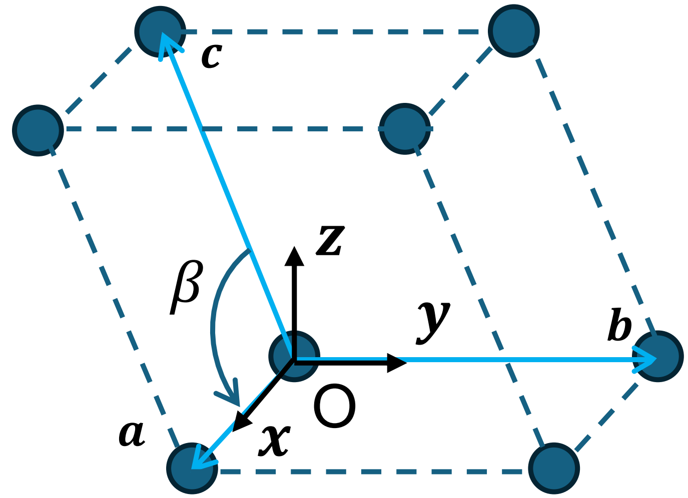
<u>A definition of Miller indices</u>:

Miller indices (hkl) represent the planes in the direct lattice that are orthogonal to the vector $h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*$ in the reciprocal lattice.

- A few properties:
  - The reciprocal lattice of a reciprocal lattice is the direct lattice;
  - The reciprocal lattice of:
    - A primitive cubic lattice is primitive cubic: $\overrightarrow{a^*} = \frac{2\pi}{a^2}\vec{a}$, $\overrightarrow{b^*} = \frac{2\pi}{a^2}\vec{b}$, $\overrightarrow{c^*} = \frac{2\pi}{a^2}\vec{c}$
    - A body-centered cubic is face-centered cubic
    - A face-centered cubic is a body-centered cubic.

Example: Reciprocal lattice Monoclinic Primitive

- $\|\boldsymbol{a}\| = a, \|\boldsymbol{b}\| = b, \|\boldsymbol{c}\| = c$, and $a \neq b \neq c$ (where $\|\boldsymbol{a}\|$ is the norm of the vector $\boldsymbol{a}$);
- $\widehat{(\boldsymbol{a},\boldsymbol{c})} = \boldsymbol{\beta}$, $\widehat{(\boldsymbol{a},\boldsymbol{b})} = \widehat{(\boldsymbol{b},\boldsymbol{c})} = \frac{\pi}{2}$ (where $\widehat{(\boldsymbol{a},\boldsymbol{b})}$ is the angle between vectors $\boldsymbol{a}$ and $\boldsymbol{b}$).

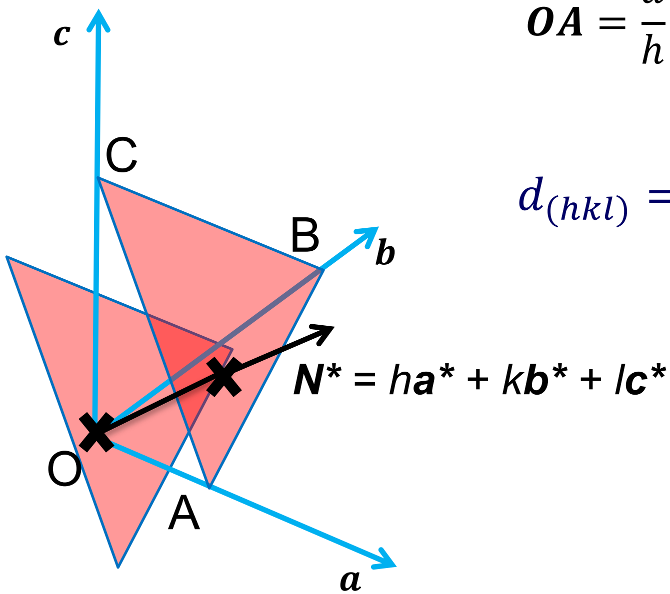


- Express the Bravais lattice vectors in the $\mathcal{B}_{(O,x,y,z)}$ Orthonormal basis;
- Calculate the volume of the primitive cell;
- Apply the formulae, which gives in $\mathcal{B}_{(O,x,y,z)}$:

$$\boldsymbol{a}^* = \frac{2\pi}{a}\begin{pmatrix} 1 \\ 0 \\ -cot\beta \end{pmatrix};\ \boldsymbol{b}^* = \frac{2\pi}{b}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix};\ \boldsymbol{c}^* = \frac{2\pi}{csin\beta}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

Distance between (hkl) planes

- The reciprical space formalism facilitates the derivation of the interplane distance of parallel (hkl) planes.



$$\boldsymbol{OA} = \frac{a}{h}\boldsymbol{x} \qquad \boldsymbol{OB} = \frac{b}{k}\boldsymbol{y} \qquad \boldsymbol{OC} = \frac{c}{l}\boldsymbol{z}$$

$$d_{(hkl)} = \boldsymbol{OA}.\frac{\boldsymbol{N}^*_{(\boldsymbol{hkl})}}{\left\|\boldsymbol{N}^*_{(\boldsymbol{hkl})}\right\|} = \boldsymbol{OB}.\frac{\boldsymbol{N}^*_{(\boldsymbol{hkl})}}{\left\|\boldsymbol{N}^*_{(\boldsymbol{hkl})}\right\|} = \boldsymbol{OC}.\frac{\boldsymbol{N}^*_{(\boldsymbol{hkl})}}{\left\|\boldsymbol{N}^*_{(\boldsymbol{hkl})}\right\|}$$

By construction:

$$\boldsymbol{OA}.\boldsymbol{N}^*_{(\boldsymbol{hkl})} = \boldsymbol{OB}.\boldsymbol{N}^*_{(\boldsymbol{hkl})} = \boldsymbol{OC}.\boldsymbol{N}^*_{(\boldsymbol{hkl})} = 2\pi$$

Demo: $\boldsymbol{OA}.\boldsymbol{N}^*_{(\boldsymbol{hkl})} = \frac{1}{h}\boldsymbol{a}.(h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*) = \boldsymbol{a}.\boldsymbol{a}^* = 2\pi$

So:

$$d_{(hkl)} = \frac{2\pi}{\left\|\boldsymbol{N}^*_{(\boldsymbol{hkl})}\right\|}$$

- Monoclinic case: $\boldsymbol{N}^*_{(\boldsymbol{hkl})} = \begin{pmatrix} 2\pi\frac{h}{a} \\ 2\pi\frac{k}{b} \\ \frac{2\pi}{sin\beta}\left(-\frac{h}{a}cos\beta + \frac{l}{c}\right) \end{pmatrix}$ and $d_{(hkl)} = \frac{1}{\sqrt{\frac{k^2}{b^2} + \frac{1}{sin^2\beta}\left(\frac{h^2}{a^2} + \frac{l^2}{c^2} - \frac{2hl}{ac}cos\beta\right)}}$

Distance between (hkl) planes

- The calculation can be made for other structures:

– Monoclinic:

$$d_{hkl} = \frac{1}{\sqrt{\left(\frac{h^2}{a^2} + \frac{l^2}{c^2} - \frac{2\,hl}{a\,c}\cos\beta\right)\frac{1}{\sin^2\beta} + \frac{k^2}{b^2}}}$$

– Orthorhombic:

$$d_{hkl} = \frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}}$$

–Tetragonal:

$$d_{hkl} = \frac{1}{\sqrt{\frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}}}$$

– Hexagonal:

$$d_{hkl} = \frac{1}{\sqrt{\frac{4}{3\,a^2}(h^2 + k^2 + hk) + \frac{l^2}{c^2}}}$$

– Cubic:

$$d_{hkl} = \frac{a_0}{\sqrt{h^2 + k^2 + l^2}}$$

Algebraic structures - Fields

The set $\mathbb{N}$ of positive integers is at the heart of the important field of enumeration. So that the sum of two numbers can be zero, the identity of the + operation, one needed to construct the set $\mathbb{Z}$ of relative integers.

Now to have a set with two operations, two identities, and the ability to have inverses for both, ie so that some elements times 2 or 3 can equal to 1 (identity for x), we must introduce the set of rational numbers $\mathbb{Q}$ based on the notion of Fields.

Since important numbers such that e and π are not rational, or the fact that there is no integers such that $2 = \left(\frac{m}{n}\right)^2$, we will have to also build the set of real numbers $\mathbb{R}$ that is the union between $\mathbb{Q}$ (rational) and $\mathbb{R}$- $\mathbb{Q}$ (irrational) numbers, which is also a Field.

- A *Field* is a set K under two operations + and × that satisfies the following:

- (K,+,x) is a Ring;
- If 0_K and 1_K are the identities for + and x respectively, $0_K \neq 1_K$
- For every $x \in K - \{0_K\}$ there is an element $y \in K$ such that $x . y = y . x = 1_K$

If x is commutative, (K,+,x) is a commutative Field (and Ring).

Examples: ($\mathbb{Z}$, +,.) is not a field but ($\mathbb{Q}$, +,.) (set of rational numbers) is !
$\mathbb{R}$ and $\mathbb{C}$ are fields for the common operations + and x.

Rational numbers - $\mathbb{Q}$

- The set of rational numbers is defined as the set $\mathbb{Q} = \left\{\frac{p}{q}, (p,q) \in \mathbb{Z}\times\mathbb{Z}^*\right\}$
- Important concepts:
  - $\mathbb{Q}$ is fully ordered;
  - Integer part: $\forall x \in \mathbb{Q}, \exists!\, n \in \mathbb{Z}$ such that $\mathrm{n} \leq x < n+1$. n is called the integer part of x.
  - $\mathbb{Q}$ is dense: $\forall (x,y) \in \mathbb{Q}^2, \exists\, z \in \mathbb{Q}$ such that $x < z < y$. (take the average of *x* and *y* for example).
  - $\mathbb{Q}$ is dense in $\mathbb{R}$: $\forall (x,y) \in \mathbb{R}^2, \exists\, z \in \mathbb{Q}$ such that $x < z < y$.

  Hint for demo: consider $(x,y) \in \mathbb{R}^2$ & $y > x, \varepsilon = y - x > 0. \exists n \in \mathbb{N}^*$ such that $\frac{1}{n} < \varepsilon$. Consider the integer $p = E(nx) + 1$, where *E* is the integer part where $E(nx) \leq nx < E(nx)$+1. The rational $r = \frac{p}{n}$ verifies $x < r$. Also, $\mathrm{r} = \frac{E(nx)}{n} + \frac{1}{n} < x + \varepsilon = y$.

- Representation of $\mathbb{Q}$ elements as an irreducible fraction:

$$\forall x \in \mathbb{Q}, \exists!\,(p,q) \in \mathbb{Z}\times\mathbb{N}^* \text{ such that } x = \frac{p}{q} \ \& \ \gcd(p,q) = 1$$ (ie *p* and *q* are co-prime).

Proof: existence: if $x \in \mathbb{Q}, \exists (p,q) \in \mathbb{Z}\times\mathbb{N}^*$ such that $x = \frac{p}{q}$. If $\gcd(p,q) = 1$ the existence is proven. If $\gcd(p,q) = \delta > 1$, then $\exists (p',q') \in \mathbb{Z}\times\mathbb{N}^*$ such that $\mathrm{p} = \delta p'$, $\mathrm{q} = \delta q'$ and $\gcd(p',q') = 1$. p' and q' verify that $x = \frac{p'}{q'}$.
Unicity: Lets (p,q) and (u,v) $\in \mathbb{Z}\times\mathbb{N}^*$ be two representations of $x \in \mathbb{Q}$, such that $x = \frac{p}{q} = \frac{u}{v}$. We then have $pv = uq$. So p$|uq$ and from Gauss, p$|u$. But also, $u|pv$ and so $u|p$. Hence $p = u$, and so $q = v$.

Real numbers -ℝ

- The set of real numbers ℝ is characterized by the following important properties:

- (ℝ,+,x) is a commutative Field;
- ≤ is a total order relation in ℝ.
- $\forall(a,b,c) \in \mathbb{R}^3, (a \leq b \Longrightarrow a + c \leq b + c)$ & $(a \leq b \text{ and } c \geq 0 \Longrightarrow \text{ac} \leq bc)$
- Any non-empty set of real numbers that has an upper bound must have a least upper bound in real numbers.

- Important notions used in engineering problems:
  - Absolute value:
    - $\forall x \in \mathbb{R}, |x| = (x \text{ if } x \geq 0, -x \text{ if } x \leq 0).$
    - $\forall(x,y) \in \mathbb{R}^2, |xy| = |x||y|$
    - $\forall x \in \mathbb{R}^*, \left|\frac{1}{x}\right| = \frac{1}{|x|}$
    - $\forall(x,y) \in \mathbb{R}^2, |x+y| \leq |x| + |y|$, and $\big||x| - |y|\big| \leq |x - y|$

  - The common distance in ℝ between two points is usually defined as
    $\forall(x,y) \in \mathbb{R}^2, d(x,y) = |x - y|$
    - $\forall(x,y) \in \mathbb{R}^2, d(x,y) = 0 \Leftrightarrow x = y$; $\forall(x,y) \in \mathbb{R}^2, d(x,y) = d(y,x)$;
    - $\forall(x,y,z) \in \mathbb{R}^3\ d(x,z) \leq d(x,y) + d(y,z)$

  - Inequality of Cauchy-Schwartz:

$$\left(\sum_{i=1}^{n} x_i y_i\right)^2 \leq \left(\sum_{i=1}^{n} {x_i}^2\right)\left(\sum_{i=1}^{n} {y_i}^2\right)$$

  - Inequality of Minkowsky: $\sqrt{\sum_{i=1}^{n}(x_i+y_i)^2} \leq \sqrt{\sum_{i=1}^{n} {x_i}^2} + \sqrt{\sum_{i=1}^{n} {y_i}^2}$

Real numbers -$\mathbb{R}$

- Nth root: $\forall (y,n) \in \mathbb{R}_+ \times \mathbb{N}^*, \exists! \, x \in \mathbb{R}$ tel que $x^n = y$.
- Notation: we call *y* the nth root and write: $x = \sqrt[n]{y}$, or $x = y^{1/n}$
- It is called a nth root because it is the root of the polynomial of degree n: $P(x) = x^n - y$
- Hint of demonstration:

First, one can consider the set $E = \{x \in \mathbb{R}_+, x^n \leq y\}$. E is not empty ($0 \in E$) and is bounded, so E admits a least upper bound *b*.
Then one shows that if $b^n < y$, then $\exists \varepsilon \in \mathbb{R}$ such that $(b+\varepsilon)^n < y$ which is a contradiction.
Similarly, one shows that if $b^n > y$, then $\exists \varepsilon \in \mathbb{R}$ such that $(b-\varepsilon)^n > y$ which is a contradiction.

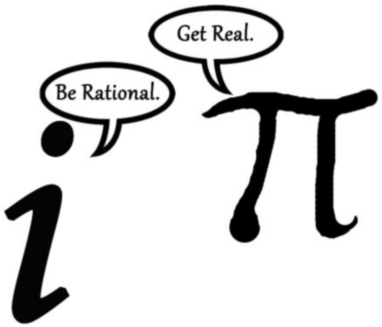
- Root of a second degree polynomial
  - For $(a,b,c) \in \mathbb{R}^3, a \neq 0$ we consider the trinomial for $x \in \mathbb{R}$, $T(x) = ax^2 + bx + c$ and its discriminant $\Delta = b^2 - 4ac$:
    - If $\Delta < 0$, $\forall x \in \mathbb{R}$, $aT(x) > 0$
    - If $\Delta = 0$, T has one root $-\frac{b}{2a}$, and $aT(x) \geq 0$
    - If $\Delta > 0$, T has two roots x' and x'' with $x' + x'' = -\frac{b}{2a}$ and $x'x'' = \frac{c}{a}$
    - $x' = \frac{-b-\sqrt{\Delta}}{2a}$ and $x'' = \frac{-b+\sqrt{\Delta}}{2a}$
- Hint of demonstration:

$$T(x) = ax^2 + bx + c = a\left[\left(x + \frac{b}{2a}\right)^2 - \frac{b^2}{4a^2} + \frac{c}{a}\right] = a\left[\left(x + \frac{b}{2a}\right)^2 - \frac{\Delta}{4a^2}\right]$$

The birth of complex numbers

- Complex numbers were invented to address the need of solving cubic equations, or of finding roots to polymers of degree 3.
- In this search, The solution put forward by Girolamo Cardano (1501 – 1576) made appear the square root of negative numbers. These strange square roots cancelled out, but still showed up and no one could make sense of them.
  What is $\sqrt{-1}$?

Cardano 1501-1576



- They were also already considered although not explicitly, in the fact of finding numbers when multiply by themselves give a negative number, i.e. $x \in ? \ldots such\ that\ x^2 < 0$.
- Descartes used such square root, but since they made no sense mathematically he called them imaginary numbers.

- For equations of the second degree, it is also very useful to consider non real solutions (imaginary ones) when the discriminant is negative.

Complex numbers in Materials Science

- Complex numbers are a great tool to manipulate angles and magnitudes.
- They are extremely useful to deal with phases and losses / dissipation phenomena in physics, materials science and engineering in general.
- They are also essential in the theoretical framework of modern physics such as in quantum mechanics.

$$i\hbar\frac{\partial}{\partial t}\left|\Psi\right\rangle = \hat{H}\left|\Psi\right\rangle$$

- Are complex numbers "real" in the sense that they represent real physical values, objects and phenomena ?

This is still debated !

Nature: https://doi.org/10.1038/s41586-021-04160-4

Article

Quantum theory based on real numbers can be experimentally falsified

https://doi.org/10.1038/s41586-021-04160-4
Received: 28 January 2021
Accepted: 18 October 2021
Published online: 15 December 2021
Open access

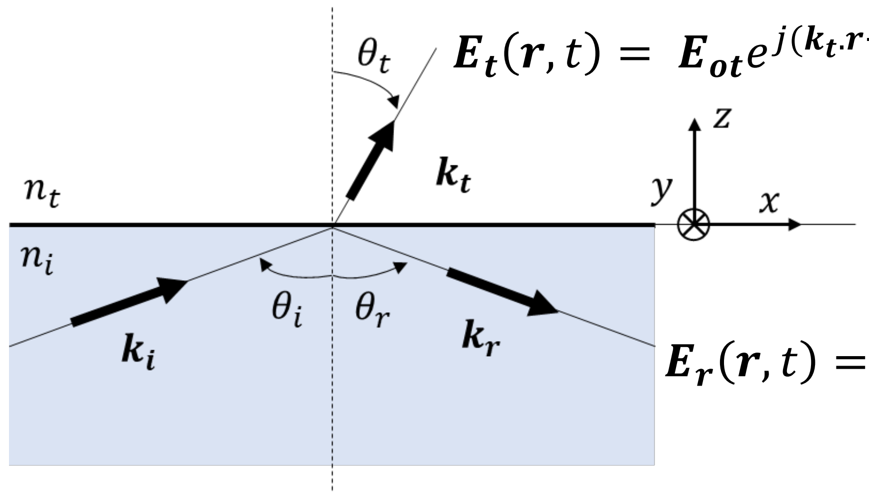
Marc-Olivier Renou[1], David Trillo[2], Mirjam Weilenmann[2], Thinh P. Le[2], Armin Tavakoli[2,3], Nicolas Gisin[4,5], Antonio Acín[1,6] & Miguel Navascués[2]✉

Although complex numbers are essential in mathematics, they are not needed to describe physical experiments, as those are expressed in terms of probabilities, hence real numbers. Physics, however, aims to explain, rather than describe, experiments

Plane wave at interfaces

- Complex formalism is a powerful tool to apprehend many phenomena in materials science and engineering.
- An important one relates to the propagation of light at the interface of two materials:

$$\boldsymbol{E_t}(\boldsymbol{r},t) = \boldsymbol{E_{ot}}e^{j(\boldsymbol{k_t}.\boldsymbol{r}-\omega t)}$$



$$\boldsymbol{E_i}(\boldsymbol{r},t) = \boldsymbol{E_{oi}}e^{j(\boldsymbol{k_i}.\boldsymbol{r}-\omega t)}$$

$$\boldsymbol{E_r}(\boldsymbol{r},t) = \boldsymbol{E_{or}}e^{j(\boldsymbol{k_r}.\boldsymbol{r}-\omega t)}$$

- At the interface, the tangential electric field must be continuous:

$$\boldsymbol{E_{i,T}}(\boldsymbol{r_{interface}},t) + \boldsymbol{E_{r,T}}(\boldsymbol{r_{interface}},t) = \boldsymbol{E_{t,T}}(\boldsymbol{r_{interface}},t)$$

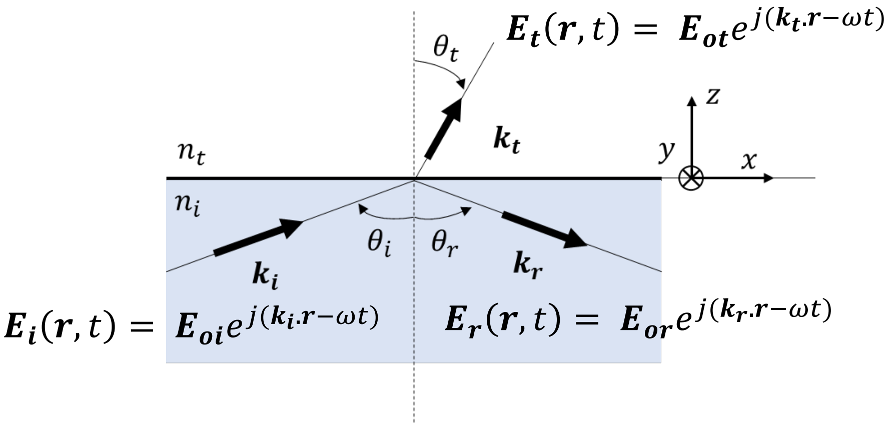
- This leads to: $k_{ix} = k_{rx} = k_{tx}$
- And hence Snell's law: $\theta_r = \theta_i$ and $k_t \sin(\theta_t) = k_i \sin(\theta_i)$
- Where, inside a material: $k_r = n_i \frac{\omega}{c}$ and $k_t = n_t \frac{\omega}{c}$

Plane wave at interfaces

- In waveguides and optical fibers, $n_i > n_t$ so that there is a critical angle θ_c such as:

$$\forall\theta_i \geq \theta_c \text{ ,} \sin(\theta_t) = \sin(\theta_i)\frac{n_i}{n_t} \geq \sin(\theta_c)\frac{n_i}{n_t} = 1$$

So there is no real solution for θ_t, and we have a total internal reflection.



- The complex numbers formalism enable to express this differently and have a deeper physical interpretation of this result.

- $k_t = n_t\frac{\omega}{c} = \sqrt{{k_{tx}}^2 + {k_{tz}}^2}$ which we can re-write: $k_{tz} = \sqrt{{k_t}^2 - {k_{tx}}^2}$, or:

$$k_{tz} = n_t\frac{\omega}{c}\sqrt{1 - \frac{{n_i}^2}{{n_t}^2}\sin^2(\theta_i)}$$

- So, when $\theta_i \geq \theta_c$, $k_{tz} = jn_t\frac{\omega}{c}\sqrt{\frac{{n_i}^2}{{n_t}^2}\sin^2(\theta_i) - 1}$
- No propagation in the cladding material ! $\boldsymbol{E_t}(\boldsymbol{r},t) = \boldsymbol{E_{ot}}e^{-zn_t\frac{\omega}{c}\sqrt{\frac{{n_i}^2}{{n_t}^2}\sin^2(\theta_i)-1}}e^{j(\boldsymbol{k_{tx}}.\boldsymbol{x}-\omega t)}$

The electric field decays exponentially in the z direction, carrying no energy.

Construction of $\mathbb{C}$

- One way to build the set of complex numbers is to define two operations over $\mathbb{R}^2$, + and x, such that:

$$\forall (x,y)\&(x',y') \in \mathbb{R}^2, (x,y)+(x',y') = (x+x', y+y')$$
$$(x,y)\times(x',y') = (xx'-yy', xy'+x'y)$$

- One can easily show that $(\mathbb{R}^2,+,\times)$ is a commutative Field that is called $\mathbb{C}$.

- $\forall x \in \mathbb{R}$, $(x,0)$ is a sub field of $(\mathbb{R}^2,+,\times)$ since the addition and product are also of the form *(y,0)*. $\mathbb{R}\times\{0\}$ and $\mathbb{R}$ are hence interchangeable, and the element $(x,0)$ can be referred to as x.

- We can define $i = (0,1)$, which verifies $i^2 = (-1,0) = -1$

- We also have: $i = \sqrt{-1}$ which allows to express the square root of negative numbers.

Example: $\sqrt{-5} = i\sqrt{5}$

- With these conventions, one can write:

$$\forall (x,y) \in \mathbb{R}^2, (x,y) = (x,0)(1,0) + (y,0)(0,1) = x + iy$$

- The form $\mathrm{z} = x + iy$ constitutes the algebraic form of a complex number z.

- x is called the real part and written $x = Re(z)$, and y is the Imaginary part with $y = Im(z)$.

- One can easily show that $\mathbb{C}$ is a $\mathbb{C}$-vectorial space of dimension 1, and a $\mathbb{R}$-vectoral space of dimension 2

Manipulations and relations in $\mathbb{C}$

- For $z = x + iy$ and $z' = x' + iy'$ we hence have, using algebraic calculation and the fact that $i^2 = -1$

$$z + z' = x + x' + i(y + y')$$

- So *Re(z+z')* = *Re(z)* + *Re(z')* and *Im(z+z')* = *Im(z)* + *Im(z')*
- A complex number *z* = *0* if and only if *Re(z)* = *Im(z)* = *0*.
- This directly means that for two complex numbers *z* and *z'*:

z = *z'* if and only if *Re(z)* = *Re(z')* and *Im(z)* = *Im(z')*

- Conjugate: $z^* = x - iy$. Also noted $\bar{z}$.
- The modulus of a complex number $z = x + iy$ is given by: $|z| = \sqrt{zz^*} = \sqrt{x^2 + y^2}$
- For $(z, z') \in \mathbb{C}^2$, the multiplication proceeds as follow:

$$z \times z' = (x + iy) \times (x' + iy') = (xx' - yy') + i(x'y + xy')$$

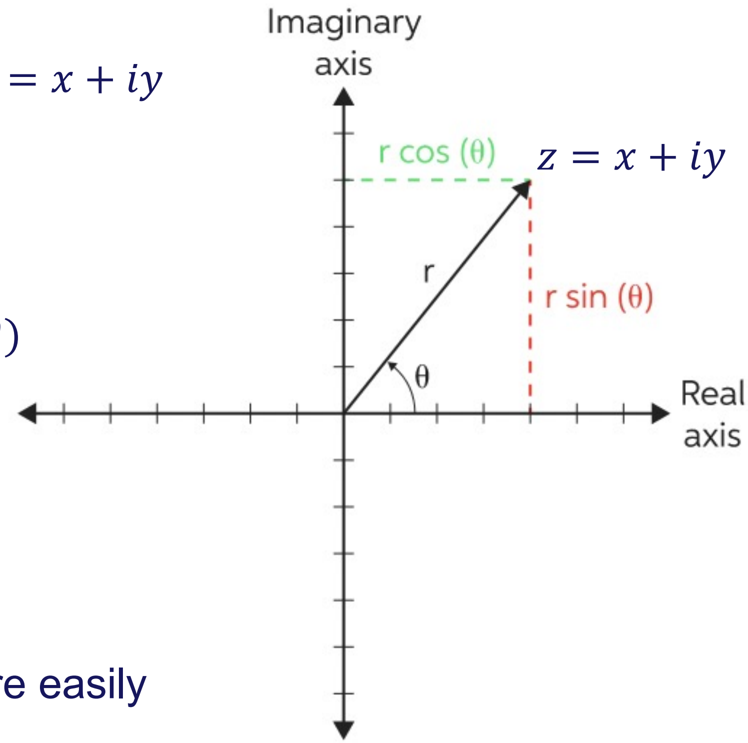
- The division: $\frac{z}{z'} = \frac{x+iy}{x'+iy'} = \frac{(x+iy)(x'-iy')}{|z'|^2} = \frac{xx'+yy'}{x'^2+y'^2} + i\,\frac{x'y-xy'}{x'^2+y'^2}$

Polar form of complex numbers

- The polar form comes quite naturally when looking at the graphical representation. It is very similar to cylindrical coordinates in 2D.

- In the orthonormal plane, it is straightforward that, for $z = x + iy$ if we call *r* the magnitude of the depicted vector, then :

$$x = rcos\theta\ , y = rsin\theta$$



Hence one can write : $z = rcos\theta + irsin\theta = r(cos\theta + isin\theta)$

r is called the modulus and θ is the argument.

$r = \sqrt{x^2 + y^2}$ and $\tan\theta = \frac{y}{x}$

- The multiplication of complex numbers can now be more easily interpreted on the graphical representation.

Remember that:

$$\sin(\alpha + \beta) = \sin\alpha\ \cos\beta + \cos\alpha\ \sin\beta$$
$$\cos(\alpha + \beta) = \cos\alpha\ \cos\beta - \sin\alpha\ \sin\beta$$
$$\sin(\alpha - \beta) = \sin\alpha\ \cos\beta - \cos\alpha\ \sin\beta$$
$$\cos(\alpha - \beta) = \cos\alpha\ \cos\beta + \sin\alpha\ \sin\beta$$

- For $z = r(cos\theta + isin\theta)$ and $z' = r'(cos\theta' + isin\theta')$

$$zz' = rr'(\cos(\theta + \theta') + isin(\theta + \theta'))$$

$$\frac{z}{z'} = \frac{r}{r'}(\cos(\theta - \theta') + isin(\theta - \theta'))$$

Exponential form of complex numbers

- There is a very convenient way to write the polar form :

$$z = rcos\theta + irsin\theta = re^{i\theta}$$

- The relation $e^{i\theta} = cos\theta + isin\theta$ is called the **Euler relation**

- Does it make sense to bring a real number to the power of a complex number ?

- We will review that, for $x \in \mathbb{C}$:

$$e^x = \sum_{k=0}^{\infty} \frac{x^k}{k!}$$

$$\cos(x) = \sum_{k=0}^{\infty} (-1)^k \frac{x^{2k}}{(2k)!} \quad \text{and.} \quad \sin(\mathrm{x}) = \sum_{k=0}^{\infty} (-1)^k \frac{x^{2k+1}}{(2k+1)!}$$

- For $\mathrm{z} \in \mathbb{C}, z = re^{i\theta}, z^* = re^{-i\theta}$
- Note also that:

$$\cos(x) = \frac{e^{ix} + e^{-ix}}{2}$$

$$\sin(x) = \frac{e^{ix} - e^{-ix}}{2i}$$

Exponential form of complex numbers

- With the exponential form, all the product of division of complex numbers study above become easier to establish
- $z, z' \in \mathbb{C}, z = re^{i\theta}, z' = re^{i\theta'}$

$$zz' = rr'e^{i\theta}e^{i\theta'} = rr'e^{i(\theta+\theta')} \quad \text{so} \quad zz' = rr'\left(\cos(\theta+\theta') + isin(\theta+\theta')\right)$$

$$\frac{z}{z\prime} = \frac{re^{i\theta}}{r'e^{i\theta'}} = \frac{r}{r\prime}e^{i(\theta-\theta')} \qquad \text{so} \quad \frac{z}{z\prime} = \frac{r}{r\prime}(\cos(\theta-\theta') + isin(\theta-\theta'))$$

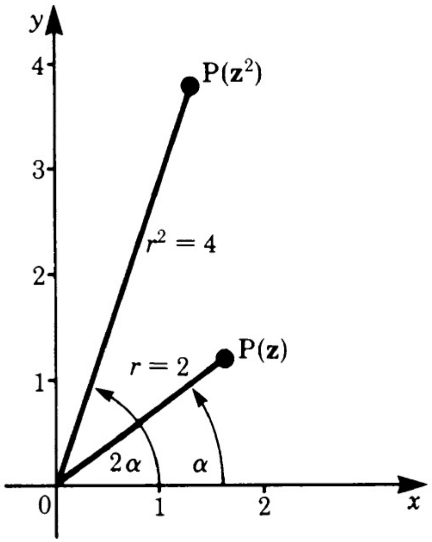
- Raising to a power: for $z = re^{j\alpha}$, $z^n = (re^{j\alpha})^n = r^n e^{jn\alpha}$

(remember that in engineering, "i" is sometimes written "j")`

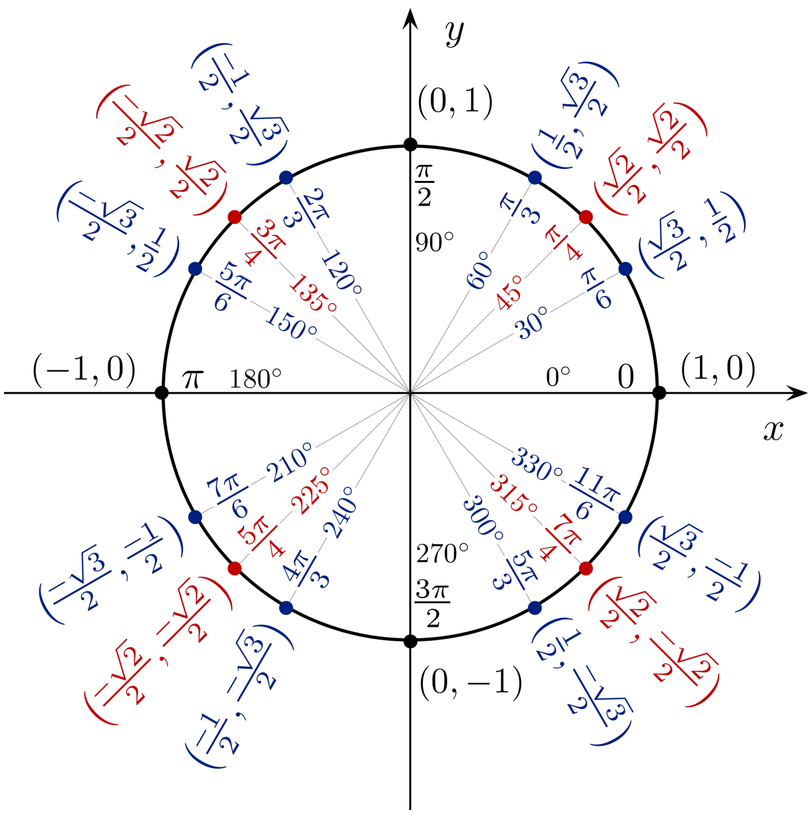
- Link with the algebraic form:

$$r = \sqrt{x^2 + y^2} \text{ and } \tan\theta = \frac{y}{x}$$

$$cos\theta = \frac{x}{\sqrt{x^2+y^2}} \text{ and } \sin\theta = \frac{y}{\sqrt{x^2+y^2}}$$



Complex numbers: the unit circle



- Remember that $e^{i\theta}$ is periodic ! So:

$$e^{i\theta} = e^{i(\theta+2p\pi)}, p \in \mathbb{Z}$$

- $\left|e^{i\theta}\right| = 1 = \sqrt{x^2 + y^2}$, with

$x = cos\theta$ and y= $sin\theta$

So the x coordinate are the cosine of the angle;
The y coordinates are the sine of the angle.

Example: $\cos\left(\frac{\pi}{3}\right) = \frac{1}{2}$; $\sin\left(\frac{\pi}{3}\right) = \frac{\sqrt{3}}{2}$

- Roots:

$$(\cos\alpha + \mathrm{j}\sin\alpha)^n = [\cos(\alpha + 2\pi k) + \mathrm{j}\sin(\alpha + 2\pi k)]^n$$
$$= \cos(n\alpha + 2\pi nk) + \mathrm{j}\sin(n\alpha + 2\pi nk)$$

where $k = 0, \pm 1, \pm 2, \pm 3, \cdots$

- Exemple:

$$z^4 = \cos\frac{2\pi}{3} + \mathrm{j}\sin\frac{2\pi}{3}$$

$$\sqrt[n]{x + jy} = \sqrt[n]{r}\left[\cos\left(\frac{\alpha}{n} + \frac{2\pi}{n}k\right) + \mathrm{j}\sin\left(\frac{k}{n} + \frac{2\pi}{n}k\right)\right]$$

where $k = 0, \pm 1, \pm 2, \cdots$

Complex Functions

- **Polynomials**
  - Fundamental theorem: every polynomial in $\mathbb{C}$ admits at least one root.
  - It is obvious for a polynomial of degree 1.
  - For degree 2, remember that:

$$T(x) = ax^2 + bx + c = a\left[\left(x + \frac{b}{2a}\right)^2 - \frac{b^2}{4a^2} + \frac{c}{a}\right] = a\left[\left(x + \frac{b}{2a}\right)^2 - \frac{\Delta}{4a^2}\right]$$

  - If $\Delta < 0, \sqrt{\Delta} = i\sqrt{-\Delta}$ so the polynomial has two roots: $x = \frac{-b \pm i\sqrt{-\Delta}}{2a}$
  - Polynomial in $\mathbb{C}$ of any degree are split, i.e. $\alpha_i, \beta_i \in \mathbb{N}$ such that $P(X) = \prod_i (X - \alpha_i)^{\beta_i}$

- **Logarithmic**
  - For $(x, y) \in \mathbb{R}^2, y = e^x > 0$. So $x = lny$ defined with $y \in \mathbb{R}_+^*$
  - What is then the meaning of ln(-5) ? Make sense with a new set of numbers !
  - $\ln(-5) = 2\ln(i) + \ln(5) = i\pi + \ln(5) \in \mathbb{C}$

Complex numbers - summary

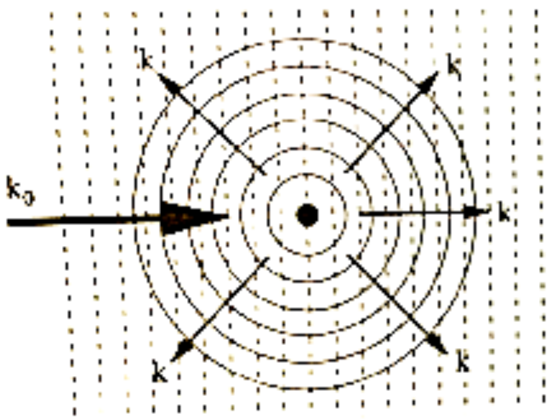
Designation	Formulae
Imaginary unit j Imaginary number η	$j^2 = -1$ $\eta = \mathrm{j}y$ (y real)
Complex number z in arithmetic form Complex conjugate	$z = x + \mathrm{j}y$ (x, y real) $x =$ real part $y =$ imaginary part $z^* = x - \mathrm{j}y$
Complex numbers in polar form	$z = r(\cos\alpha + \mathrm{j}\sin\alpha)$
Transformation $(x, y) \leftrightarrow (r, \alpha)$	$\left.\begin{array}{l} x = r\cos\alpha \\ y = r\sin\alpha \end{array}\right\\} \quad \left.\begin{array}{c} r = \sqrt{x^2 + y^2} \\ \tan\alpha = y/x \end{array}\right\\}$
Complex number in exponential form Euler's formula	$z = r\mathrm{e}^{\mathrm{j}\alpha}$ $\mathrm{e}^{\mathrm{j}\alpha} = \cos\alpha + \mathrm{j}\sin\alpha$
Exponential form for cosine and sine functions	$\cos\alpha = \frac{1}{2}(\mathrm{e}^{\mathrm{j}\alpha} + \mathrm{e}^{-\mathrm{j}\alpha}) = \cosh \mathrm{j}\alpha$ $\sin\alpha = \frac{1}{2\mathrm{j}}(\mathrm{e}^{\mathrm{j}\alpha} - \mathrm{e}^{-\mathrm{j}\alpha}) = \frac{1}{\mathrm{j}} \sinh \mathrm{j}\alpha$
Periodicity of complex numbers	$z = r\,\mathrm{e}^{\mathrm{j}\alpha}$ $= r\,\mathrm{e}^{\mathrm{j}(\alpha + 2k\pi)} \quad (k = \pm 1, \pm 2, \pm 3, \cdots)$

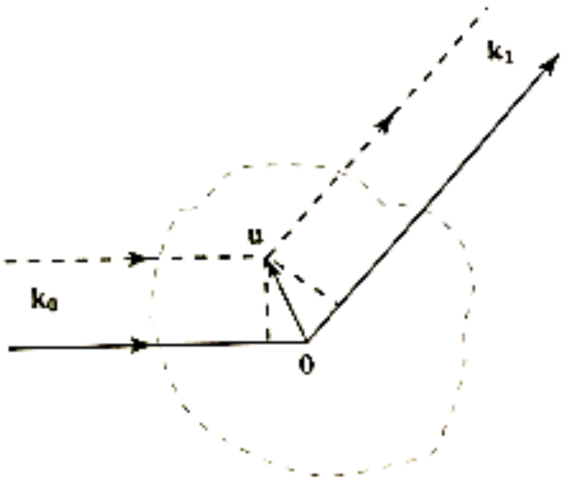
Complex numbers - summary

Designation	Formulae
Multiplication and division in exponential form	$z_1 = r_1 \mathrm{e}^{\mathrm{j}\alpha_1}, z_2 = r_2 \mathrm{e}^{\mathrm{j}\alpha_2}$ $z_1 z_2 = r_1 r_2 \mathrm{e}^{\mathrm{j}(\alpha_1+\alpha_2)}$ $\frac{z_1}{z_2} = \frac{r_1}{r_2} \mathrm{e}^{\mathrm{j}(\alpha_1-\alpha_2)}$
Raising to a power and extracting roots in exponential form	$z = r\mathrm{e}^{\mathrm{j}\alpha}$ $z^n = r^n \mathrm{e}^{\mathrm{j}n\alpha}$ $\sqrt[n]{z} = \sqrt[n]{r}\mathrm{e}^{\mathrm{j}[(\alpha+2\pi k)/n]}\ (k = 0, \pm 1, \pm 2, \cdots)$
Multiplication and division in polar form	$z_1 = r_1(\cos\alpha_1 + \mathrm{j}\sin\alpha_1)$ $z_2 = r_2(\cos\alpha_2 + \mathrm{j}\sin\alpha_2)$ $z_1 z_2 = r_1 r_2[\cos(\alpha_1+\alpha_2) + \mathrm{j}\sin(\alpha_1+\alpha_2)]$ $\frac{z_1}{z_2} = \frac{r_1}{r_2}[\cos(\alpha_1-\alpha_2) + \mathrm{j}\sin(\alpha_1-\alpha_2)]$
Raising to a power and extracting roots in polar form	$z = r(\cos\alpha + \mathrm{j}\sin\alpha)$ $z^n = r^n[\cos n\alpha + \mathrm{j}\sin n\alpha]$ $\sqrt[n]{z} = \sqrt[n]{r}\left[\cos\left(\frac{\alpha}{n} + \frac{2\pi k}{n}\right) + \mathrm{j}\sin\left(\frac{\alpha}{n} + \frac{2\pi k}{n}\right)\right]$ $(k = 0, \pm 1, \pm 2, \cdots)$

Reciprocal Space and Bragg condition

- The properties of complex numbers reviewed here find a great application in the continuation of the study of reciprocal space.
- Consider a plane wave of k vector $\boldsymbol{k_0}$ impingent on a crystal.
- Each atom/motif acts like an independent source that scatters the incoming light in different directions.

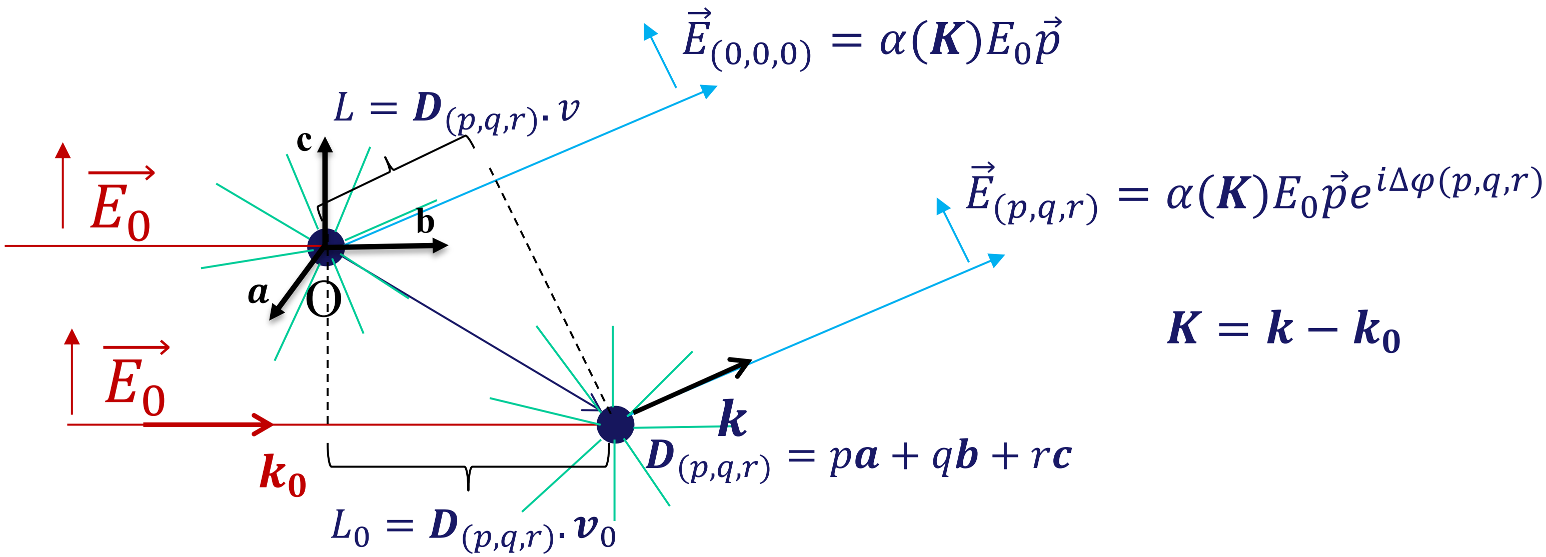




- If we first consider two atoms, the incident wave : $\vec{E} = \overrightarrow{E_0} e^{i(\boldsymbol{k}.\boldsymbol{r} - \omega t)}$
- Along the $\boldsymbol{k_1}$ direction, interference will give: $\vec{E} = \overrightarrow{E_0} e^{i(\boldsymbol{k_0}.\boldsymbol{u} - \omega t)} + \overrightarrow{E_0} e^{i(\boldsymbol{k_1}.\boldsymbol{u} - \omega t)}$
- Which gives:

$$|\vec{E}| = 2|\overrightarrow{E_0}| cos \left(\frac{\boldsymbol{u}.(\boldsymbol{k_1} - \boldsymbol{k_0})}{2} \right)$$

Reciprocal Space and Laue's condition

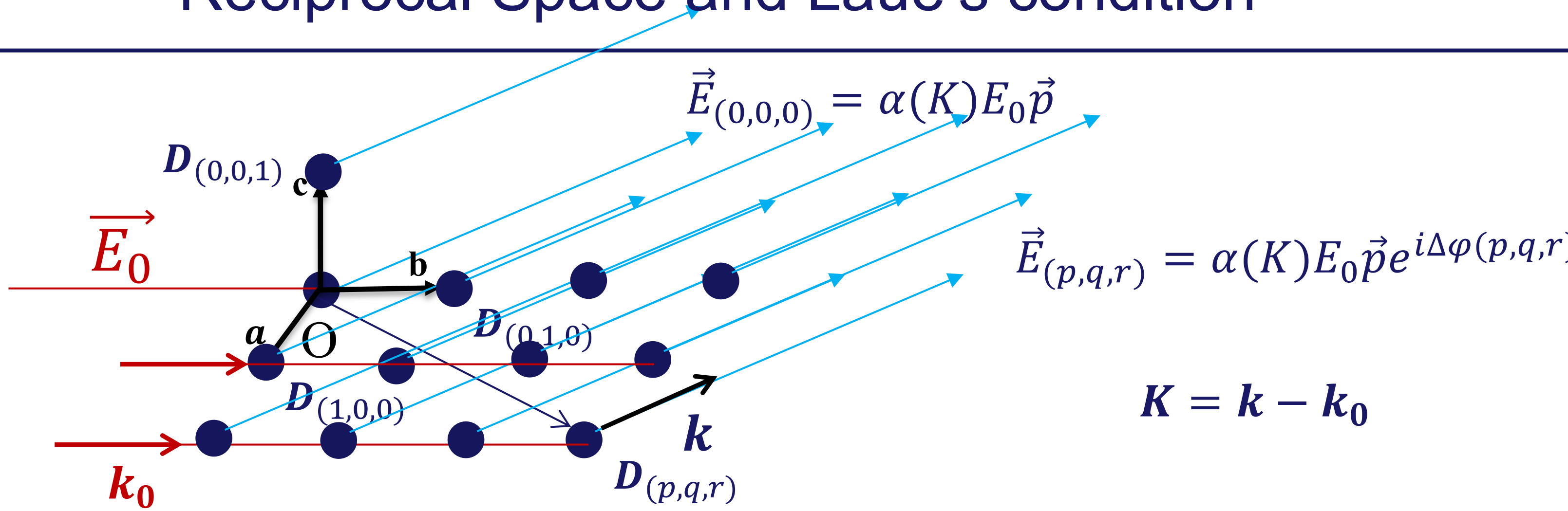


$\boldsymbol{k_0} = \frac{2\pi}{\lambda}\boldsymbol{v}_0$, with $\|\boldsymbol{v}_0\| = 1$; $\boldsymbol{k} = \frac{2\pi}{\lambda}\boldsymbol{v}$, with $\|\boldsymbol{v}\| = 1$.

- We can fix the phase to 0 on the origin of the crystal O. We only need to then consider the part of the field that is scattered in the $\boldsymbol{K} = \boldsymbol{k} - \boldsymbol{k_0}$ direction: $\vec{E}_{(0,0,0)} = \alpha(K)E_0\vec{p}$
- For another arbitrary motif in the crystal at position $\boldsymbol{D}_{(p,q,r)} = p\boldsymbol{a} + q\boldsymbol{b} + r\boldsymbol{c}$ (with $(p,q,r) \in \mathbb{Z}^3$, we have a phase shift that builds up as the wave travels. This phase shift is the wave vector $\mathrm{k} = \frac{2\pi}{\lambda}$ times the differences of optical path $\Delta L_{(p,q,r)}$:

$$\Delta L_{(p,q,r)} = L_0 - L$$
$$\Delta L_{(p,q,r)} = \boldsymbol{D}_{(p,q,r)}.\,\boldsymbol{v}_0 - \boldsymbol{D}_{(p,q,r)}.\,\boldsymbol{v}$$

Reciprocal Space and Laue's condition



- The scattered field in the **K** direction by this motif is then given by: $\vec{E}_{(p,q,r)} = \alpha(\boldsymbol{K})E_0\vec{p}e^{i\Delta\varphi(p,q,r)}$
- The phase shift being:

$$\Delta\varphi(p,q,r) = \frac{2\pi}{\lambda}\Delta L_{(p,q,r)}$$

$$\Delta\varphi(p,q,r) = \boldsymbol{D}_{(p,q,r)}.\frac{2\pi}{\lambda}\boldsymbol{v}_0 - \boldsymbol{D}_{(p,q,r)}.\frac{2\pi}{\lambda}\boldsymbol{v} = \boldsymbol{D}_{(p,q,r)}.(\boldsymbol{k_0} - \boldsymbol{k}) = -\boldsymbol{K}.\boldsymbol{D}_{(p,q,r)}$$

- The detector will mesaure the intensity diffracted at the distal end along the direction **K**, that is the module of the total electric field, with:

$$\vec{E}_{total}(\boldsymbol{K}) = \vec{E}_{(0,0,0)} + \vec{E}_{(p,q,r)}$$

$$\vec{E}_{total}(\boldsymbol{K}) = \sum_{p=-\infty}^{p=+\infty}\sum_{q=-\infty}^{q=+\infty}\sum_{r=-\infty}^{r=+\infty}\vec{E}_{(p,q,r)} = \alpha(K)E_0\vec{p}\sum_{p,q,r} e^{i\Delta\varphi(p,q,r)}$$

Reciprocal Space and Laue's condition

- Which we can re-write:

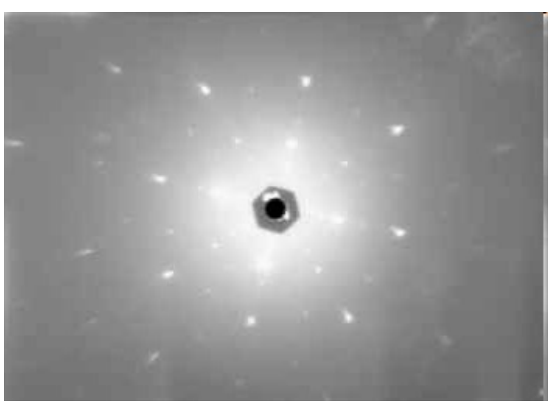
$$\vec{E}_{total}(\boldsymbol{K}) = \alpha(\boldsymbol{K})E_0\vec{p}\sum_{p,q,r} e^{-i\boldsymbol{K}.\boldsymbol{D}_{(p,q,r)}} = D(\boldsymbol{K})E_0\vec{p}$$

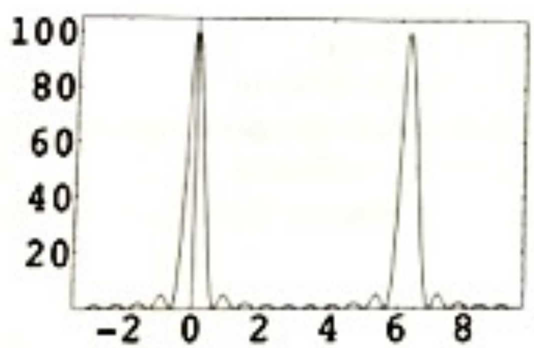
$$D(\boldsymbol{K}) = \alpha(\boldsymbol{K})\sum_{p,q,r} e^{-i\boldsymbol{K}.\boldsymbol{D}_{(p,q,r)}}$$

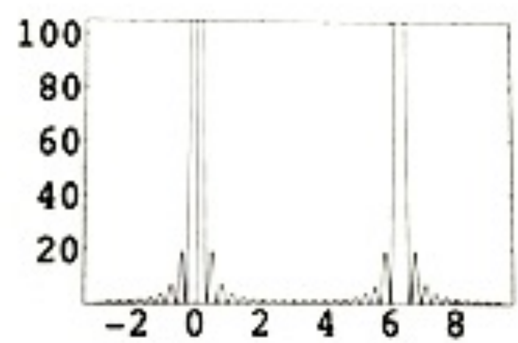
- This scattering is maximum for

$$\forall(p,q,r) \in \mathbb{Z}^3, e^{-i\boldsymbol{K}.\boldsymbol{D}_{(p,q,r)}} = 1$$

condition from which we built the reciprocal basis (O, **a***,**b***,**c***) that is the same as the one built from the geometric argument.







Reciprocal Space and Laue's Condition

This is a more general Bragg condition.

- If we define a basis of vectors (**a***,**b***,**c***) in which we can define $\boldsymbol{K} = x_1\boldsymbol{a}^* + x_2\boldsymbol{b}^* + x_3\boldsymbol{c}^*$ with $(x_1, x_2, x_3) \in \mathbb{R}^3$, and since $\boldsymbol{D_n}$ is a lattice vector in the direct space, we have $(d_1, d_2, d_3) \in \mathbb{Z}^3$ such that $\boldsymbol{D_n} = d_1\boldsymbol{a} + d_2\boldsymbol{b}. + d_3\boldsymbol{c}$, we must have:

$$(x_1\boldsymbol{a}^* + x_2\boldsymbol{b}^* + x_3\boldsymbol{c}^*).(d_1\boldsymbol{a} + d_2\boldsymbol{b}. + d_3\boldsymbol{c}) = 2p\pi \text{ with } p \in \mathbb{Z}$$

- This works with:

$$\begin{array}{lll} \vec{a^*}.\ \vec{a} = 2\pi & \vec{b^*}.\ \vec{a} = 0 & \vec{c^*}.\ \vec{a} = 0 \\ \vec{a^*}.\ \vec{b} = 0 & \vec{b^*}.\ \vec{b} = 2\pi & \vec{c^*}.\ \vec{b} = 0 \\ \vec{a^*}.\ \vec{c} = 0 & \vec{b^*}.\ \vec{c} = 0 & \vec{c^*}.\ \vec{c} = 2\pi \end{array}$$

- Which forms the same reciprocal basis (**a***,**b***,**c***) we defined earlier !

- And we get:

$$\forall(d_1, d_2, d_3) \in \mathbb{Z}^3, \qquad x_1d_1 + x_2d_2 + x_3d_3 \in \mathbb{Z}$$

which imposes that $(x_1, x_2, x_3) \in \mathbb{Z}^3$.

Hence we have formed the reciprocal lattice !

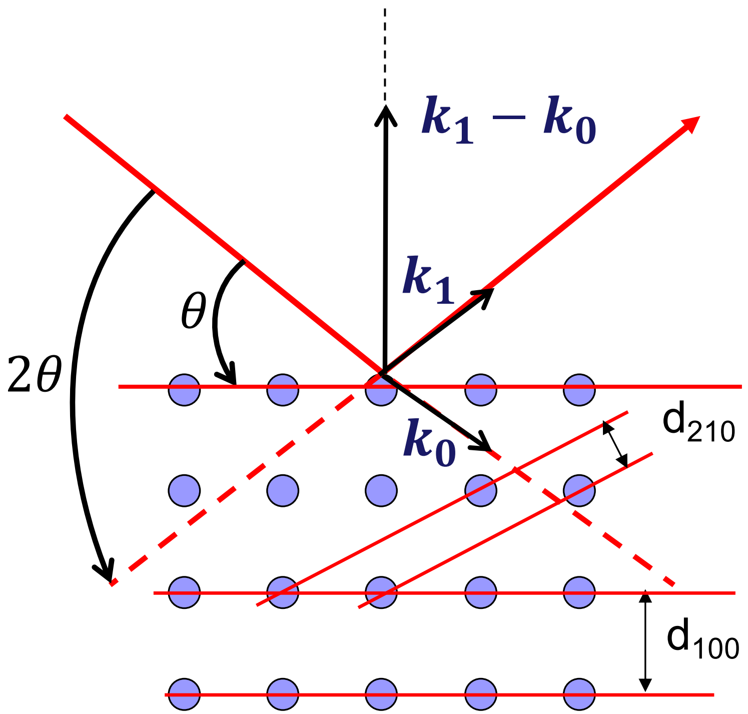
$$\mathcal{R} = \{P, \boldsymbol{OP} = n_1\boldsymbol{a}^* + n_2\boldsymbol{b}^* + n_3\boldsymbol{c}^*, (n_1, n_2, n_3) \in \mathbb{Z}^3\}$$

The condition of interference: $\boldsymbol{K} = \boldsymbol{k_1} - \boldsymbol{k_0} \in \mathcal{R}$ is called commonly **the condition of Laue.**

This condition is equivalent to the commonly known Bragg law.

Bragg Law and Laue's condition

- Laue's condition does not constraint on the diffracted direction. As long as the difference of the incoming wave vector, and the diffracted one, belongs to the reciprocal space, constructive interference from the Bravais Lattice should occur.
- Bragg's law is a particular case where the diffracted direction is only considered at an angle 2θ.



- Laue condition: $\boldsymbol{K} = \boldsymbol{k_1} - \boldsymbol{k_0} \in \mathcal{R}$, the Reciprocal space;
- Bragg condition: Diffraction measured when $\boldsymbol{K} = \boldsymbol{k_1} - \boldsymbol{k_0}$ is orthogonal to the diffracting plane (hkl)
- So: $\exists \alpha \in \mathbb{R}, \boldsymbol{K} = \alpha \boldsymbol{N}^*_{(\boldsymbol{hkl})} = \alpha h \boldsymbol{a}^* + \alpha k \boldsymbol{b}^* + \alpha l \boldsymbol{c}^*$
- And we must have $\boldsymbol{K} \in \mathcal{R}$, so $\alpha h \in \mathbb{Z} \Longrightarrow \alpha \in \mathbb{Z}$
- Hence $\exists n \in \mathbb{Z}$, $\boldsymbol{K} = n \boldsymbol{N}^*_{(\boldsymbol{hkl})}$
- $\|\boldsymbol{K}\| = 2k sin(\theta) = \frac{4\pi}{\lambda} sin(\theta)$ and $\left\|\boldsymbol{N}^*_{(\boldsymbol{hkl})}\right\| = \frac{2\pi}{d_{(hkl)}}$
- So: $\frac{4\pi}{\lambda} sin(\theta) = n \frac{2\pi}{d_{(hkl)}} \Rightarrow$ $\boxed{2d_{(hkl)} sin(\theta) = n\lambda}$

SUMMARY

- We reviewed reciprocal spaces.
- We introduced rational and real numbers with a few important properties.
- We reviewed the application of complex numbers and how one can construct the field of complex numbers.
- We defined the algebraic form (sometimes also called the arithmetic) form of complex number $z = x + iy$, and the polar form $z = rcos\theta + irsin\theta$
- We finally defined the polar form $z = re^{i\theta}$ and express the relationship between the different ways of expressing and manipulating complex numbers.
- We reviewed the unit circle, and show examples on how complex numbers can extend the use of common functions that become complex functions.
- We showed a direct application of complex numbers in how one handles the propagation of waves, and how ones construct the reciprocal space for deriving the Bragg condition for X-rays probing a crystal lattice.
- <u>Next Week</u>
  - Linear Algebra