Details about the method in our project

Master 1 Numerical Physics

Year 2022–2023

Diffraction of an electromagntic plane wave by a 2 dimensional material (graphene)

Membres du projet :

Khalis Attou

Pierre Aunay

Antoine Charvin

Tristan Goninet

Lucas Jaspard

Lidia Lappo

Morgane Lendrin

Encadrants :

Anne-Muriel Arigon

Brahim Guizal

Hervé Peyre

Diffraction of an electromagntic plane wave by a 2 dimensional material (graphene)

Khalis Attou
Pierre Aunay
Antoine Charvin
Tristan Goninet
Lucas Jaspard
Lidia Lappo
Morgane Lendrin

24 juin 2023

1 Diffraction

When a wave encounters an obstacle, the spatial distribution of its amplitude and phase can be modified. Several physical phenomena can be observed depending on the wavelength compared to the size of the obstacle. Our project consists in simulating this diffraction phenomenon. We have decided to focus on the diffraction of a plane wave by a graphene plane, as depicted below (Figure 1) :

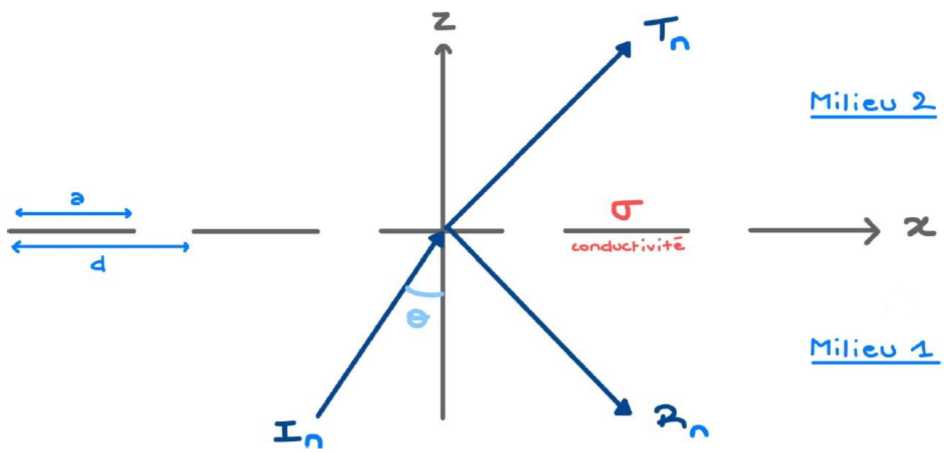

Figure 1 – Diagram of the diffraction of a plane electromagnetic wave by a plane consisting of graphene strips of width a and period d. The incident wave with amplitude I_n is sent onto the graphene plane with conductivity σ at an angle θ. It passes through medium 1 to reach the lattice, and is transmitted into medium 2 with amplitude T_n or reflected with amplitude R_n

The diffraction phenomenon is observed when the wavelength is on the order of the size of the obstacle and can be accompanied by absorption (the dielectric permittivity ϵ is complex) and dispersion (phase velocity dependent on frequency). The physical translation of this phenomenon therefore requires the use of Maxwell's equations. To simulate this phenomenon, we used the Fourier Modal Method (FMM), which involves decomposing the electric and magnetic fields into a Fourier series.

2 Principle of the Fourier Modal Method

In this section, vector quantities dependent on $\vec{r}$ and t will be written in italic uppercase letters. Vector quantities written in upright uppercase letters depend only on $\vec{r}$. This numerical method consists of determining the distribution of the electromagnetic field of a plane wave after diffraction by a periodic lattice with known geometric properties. It involves solving a problem with boundary conditions. Since we have a situation with an incidence medium, a 2D (thicknessless) material, and an outgoing medium, the problem can be divided into two parts : the incidence medium (non-dispersive) and the outgoing medium of the wave, which may be dispersive. There are then three steps to solve the latter :

- Determine the general expressions of the electromagnetic field corresponding to the physical situation in each region (here, the incidence medium and the outgoing medium).
- Apply the boundary conditions to the previously found fields. This results in a system of linear equations that allows us to find the previously unknown coefficients.
- Extract the quantities of interest.

First, we will focus on the media, and then we will examine the quantity necessary for implementing the material. Let's start by determining the **general equations** of the electric and magnetic fields.

The physical situation considered here allows us to use the local Maxwell's equations in a linear, homogeneous, and isotropic medium :

$$\begin{cases} r\vec{o}t(\vec{\mathcal{E}}) = -\dfrac{\partial \vec{\mathcal{B}}}{\partial t} \\ \\ r\vec{o}t(\vec{\mathcal{H}}) = \dfrac{\partial \vec{\mathcal{D}}}{\partial t} \end{cases} \tag{1}$$

with $\vec{\mathcal{B}} = \mu_0\mu_r\vec{\mathcal{H}}$ et $\vec{\mathcal{D}} = \epsilon_0\epsilon_r\vec{\mathcal{E}}$
μ_0 et ϵ_0 respectively the magnetic permeability and the dielectric permittivity.
The electric and magnetic fields ($\vec{\mathcal{E}}$ and $\vec{\mathcal{B}}$) correspond to the fields in vacuum coupled with those of the source in the medium under consideration. It is necessary to take into account the permeability and permittivity of the medium, given by μ_r and ϵ_r. Therefore, we have :

$$\begin{cases} r\vec{o}t(\vec{\mathcal{E}}) = -\mu_0\mu_r\dfrac{\partial \vec{\mathcal{H}}}{\partial t} \\ \\ r\vec{o}t(\vec{\mathcal{H}}) = \epsilon_0\epsilon_r\dfrac{\partial \vec{\mathcal{E}}}{\partial t} \end{cases} \tag{2}$$

Subsequently, we will use the harmonic Maxwell's equations, which involve representing each previously mentioned vector quantity in exponential form. Therefore, we have :

$$\begin{cases} \vec{\mathcal{E}}(\vec{r},t) = \vec{E}(\vec{r})e^{-i\omega t} \\ \vec{\mathcal{D}}(\vec{r},t) = \vec{D}(\vec{r})e^{-i\omega t} \\ \vec{\mathcal{B}}(\vec{r},t) = \vec{B}(\vec{r})e^{-i\omega t} \\ \vec{\mathcal{H}}(\vec{r},t) = \vec{H}(\vec{r})e^{-i\omega t} \end{cases} \tag{3}$$

The temporal derivatives thus have a factor of $-i\omega$, and we ultimately obtain :

$$\begin{cases} \vec{rot}(\vec{E}) = i\omega\mu_0\mu_r\vec{B}(\vec{r}) \\ \vec{rot}(\vec{H}) = -i\omega\epsilon_0\epsilon_r\vec{E}(\vec{r}) \end{cases} \tag{4}$$

Let's now develop these equations. For the electric field, we have :

$$\begin{pmatrix} \dfrac{\partial}{\partial x} \\ \\ \dfrac{\partial}{\partial y} \\ \\ \dfrac{\partial}{\partial z} \end{pmatrix} \wedge \begin{pmatrix} E_x \\ \\ E_y \\ \\ E_z \end{pmatrix} = i\omega\mu_0\mu_r\vec{H} \Longrightarrow \begin{pmatrix} \dfrac{\partial E_z}{\partial y} - \dfrac{\partial E_y}{\partial z} \\ \\ \dfrac{\partial E_x}{\partial z} - \dfrac{\partial E_z}{\partial x} \\ \\ \dfrac{\partial E_y}{\partial x} - \dfrac{\partial E_x}{\partial y} \end{pmatrix} = \begin{pmatrix} i\omega\mu_0\mu_r H_x \\ \\ i\omega\mu_0\mu_r H_y \\ \\ i\omega\mu_0\mu_r H_z \end{pmatrix} \tag{5}$$

Concerning the magnetic field, we have :

$$\begin{pmatrix} \dfrac{\partial}{\partial x} \\ \\ \dfrac{\partial}{\partial y} \\ \\ \dfrac{\partial}{\partial z} \end{pmatrix} \wedge \begin{pmatrix} H_x \\ \\ H_y \\ \\ H_z \end{pmatrix} = -i\omega\epsilon_0\epsilon_r\vec{E} \Longrightarrow \begin{pmatrix} \dfrac{\partial H_z}{\partial y} - \dfrac{\partial H_y}{\partial z} \\ \\ \dfrac{\partial H_x}{\partial z} - \dfrac{\partial H_z}{\partial x} \\ \\ \dfrac{\partial H_y}{\partial x} - \dfrac{\partial H_x}{\partial y} \end{pmatrix} = \begin{pmatrix} -i\omega\epsilon_0\epsilon_r E_x \\ \\ -i\omega\epsilon_0\epsilon_r E_y \\ \\ -i\omega\epsilon_0\epsilon_r E_z \end{pmatrix} \tag{6}$$

By isolating the y components of each field, we obtain the so-called transverse components, which correspond to the two types of polarization. This refers to the orientation of the electric and magnetic fields with respect to the plane of incidence (here, the xOz plane, which is the plane of symmetry for the structure).
Polarization is often denoted by the letters s or p, with s representing the electric transverse polarization and p representing the magnetic transverse polarization.
In the case being studied here, we have an invariance along the $\mathbf{u}_y$ direction, and the incident wavevector belongs to the plane of symmetry. As a result, all derivatives with respect to y are zero, leading to two subsystems, one for each type of polarization :

TE	TM
$-\dfrac{\partial E_y}{\partial z} = i\omega\mu_0\mu_r H_x$	$-\dfrac{\partial H_y}{\partial z} = -i\omega\epsilon_0\epsilon_r E_x$
$\dfrac{\partial H_x}{\partial z} - \dfrac{\partial H_z}{\partial x} = -i\omega\epsilon_0\epsilon_r E_y$	$\dfrac{\partial E_x}{\partial z} - \dfrac{\partial E_z}{\partial x} = i\omega\mu_0\mu_r H_y$
$\dfrac{\partial E_y}{\partial x} = i\omega\mu_0\mu_r H_z$	$\dfrac{\partial H_y}{\partial x} = -i\omega\epsilon_0\epsilon_r E_z$

(7)

In each of these polarization cases (TE and TM), a fundamental component (E_y and H_y) appears from which the other components can be easily obtained (through derivation). Therefore, we focus on these components by writing the partial differential equation that they obey. The similarity between the two systems of equations allows us to set $u(x, z) = E_y(x, z)$ for TE and $H_y(x, z)$ for TM. By performing a substitution in one of the two systems, we obtain the following propagation equation, known as the Helmholtz equation :

$$\frac{\partial^2 u(x,z)}{\partial x^2} + \frac{\partial^2 u(x,z)}{\partial y^2} + \frac{\partial^2 u(x,z)}{\partial z^2} + \frac{\omega^2}{c^2}\epsilon_r\mu_r u(x,z) = 0 \tag{8}$$

The solutions of this equation are plane waves of the form $u(x,z) = u_0 e^{i\vec{k}.\vec{r}}$ with $|\vec{k}| = k = \alpha x + \beta y + \gamma z$. By substituting these solutions into the Helmholtz equation, we obtain the dispersion equation :

$$\alpha^2 + \beta^2 + \gamma^2 = \frac{\omega^2}{c^2}\epsilon_r \mu_r \tag{9}$$

Here, $\beta = 0$, thus we have :

$$\boxed{\alpha^2 + \gamma^2 = \frac{\omega^2}{c^2}\epsilon_r \mu_r} \tag{10}$$

We can now consider the geometry of the problem to obtain a new simplified system of equations.
Equation 10, coupled with the quasi-periodic characteristics of our problem, allows us to deduce that the desired solution is periodic up to an exponential factor. These solutions are called pseudo-periodic solutions.
The Floquet-Bloch theorem enables us to expand the solutions in terms of generalized Fourier series :

$$u(x,z) = \sum_{n\in\mathbb{Z}} u_n(z) e^{i\alpha_n x} \quad avec \quad \alpha_n = \alpha_0 + n\frac{2\pi}{d},\ \alpha_0 = k_i\ sin(\theta) \tag{11}$$

named Rayleigh developpment.
Using this developpment in the input medium *in* (called i) and th eoutput one *out* (o), we obtain :

$$u_i(x,z) = \sum_{n\in\mathbb{Z}} e^{i\alpha_n x}(I_n e^{i\gamma_{i,n}z} + R_n e^{-i\gamma_{i,n}z}) \tag{12}$$

$$u_o(x,z) = \sum_{n\in\mathbb{Z}} e^{i\alpha_n x}(T_n e^{i\gamma_{o,n}z} + I'_n e^{-i\gamma_{o,n}z}) \tag{13}$$

T_n and R_n correspond to the transmitted and reflected waves, respectively.
α and γ are constants, k is the wave number, and $n_{i/o}$ represents the refractive index, given by :

$$\begin{cases} k_{i/o} = k_0 n_{i/o}\ ,\ k_0 = \dfrac{\omega}{c}; \\ \alpha_n = \alpha_0 + \dfrac{2\pi}{d}\ ,\ \alpha_0 = k_i sin(\theta) \\ \gamma_{i/o,n} = \sqrt{k^2_{i/o,n} - \alpha_n^2} \end{cases}$$

When coupling the equations obtained with the geometry of our problem, we can now deduce and use the **boundary conditions**, which depend on the polarization.

Let's consider the **electric transverse** case first. The geometry of the problem gives us the continuity of the field at $z = 0$. Additionally, we have $-\partial_z E_y = i\omega\mu_0\mu_r H_x$, thus :

$$E_{yi}(x,0) = E_{yo}(x,0) \tag{14}$$

$$H_{xo}(x,0) - H_{xi}(x,0) = \sigma_g(x) E_y(x,0) \tag{15}$$

Using equation 14 on equations 12 et 13, we obtain :

$$u_i(x,0) = \sum_{n\in\mathbb{Z}} e^{i\alpha_n x}(I_n e^{i\gamma_i 0} + R_n e^{i\gamma_i 0}) \tag{16}$$

and

$$u_o(x,0) = \sum_{n\in\mathbb{Z}} e^{i\alpha_n x}(T_n e^{i\gamma_i 0} + I'_n e^{i\gamma_i 0}) \tag{17}$$

Thus we have :

$$\sum_{n\in\mathbb{Z}} e^{i\alpha_n x}(I_n e^{i\gamma_i 0} + R_n e^{i\gamma_i 0}) = \sum_{n\in\mathbb{Z}} e^{i\alpha_n x}(T_n e^{i\gamma_i 0} + I'_n e^{i\gamma_i 0}) \tag{18}$$

and finally obtain :

$$I_n + R_n = T_n + I'_n \qquad \forall n \in \mathbb{Z} \tag{19}$$

Using :

$$-\frac{\partial E_y(x,z)}{\partial z} = i\omega\mu_0\mu_r H_x \tag{20}$$

we deduce :

$$\begin{aligned} H_{x,o} &= -\frac{1}{i\omega\mu_0\mu_r}\sum_{n\in\mathbb{Z}} e^{i\alpha_n x}(i\gamma_{o,n}T_n - i\gamma_{o,n}I'_n) \\ &= \frac{i^2}{i\omega\mu_0\mu_r}\sum_{n\in\mathbb{Z}} e^{i\alpha_n x}(i\gamma_{o,n}T_n - i\gamma_{o,n}I'_n) \\ &= \frac{i}{\omega\mu_0\mu_r}\sum_{n\in\mathbb{Z}} e^{i\alpha_n x}(i\gamma_{o,n}T_n - i\gamma_{o,n}I'_n) \end{aligned} \tag{21}$$

As $\epsilon_0\mu_0 c^2 = 1 \Longrightarrow c = \dfrac{1}{\sqrt{\epsilon_0\mu_0}} \Longrightarrow c = z_0\epsilon_0$ and $w = k_0 c$ so $\omega = k_0 z_0 \epsilon_0$, thus we have :

$$H_{x,o} = \frac{i}{k_0 z_0 \mu_r}\sum_{n\in\mathbb{Z}} e^{i\alpha_n x}(i\gamma_{o,n}T_n - i\gamma_{o,n}I'_n) \tag{22}$$

Taking $\gamma'_{o,n} = \dfrac{\gamma_{o,n}}{\mu_r}$, we obtain :

$$-\gamma'_{o,n}(T_n - I'_n) + \gamma'_{i,n}(I_n - R_n) = k_0 Z_0 \sum_{p\in\mathbb{Z}^{\neq}} \sigma_{n-p}(T_n + I'_n) \qquad \forall n \in \mathbb{Z} \tag{23}$$

with Z_0 the electromagnetic impedance of the void.
Using matrix notation [?] we obtain :

$$-\gamma'_{\mathbf{o}}\{T - I'\} + \gamma'_{\mathbf{i}}\{I - R\} = k_0 Z_0.\mathbf{\Lambda}.(T + I') \tag{24}$$

with I or I', R and T the column vectors of the incident, reflected and transmitted waves, respectively.
$\gamma'_{\mathbf{i}}$ and $\gamma'_{\mathbf{o}}$ correspond to the matrixes of the coefficient γ in medium *in* and *out* and $\mathbf{\Lambda}$ is the Toeplitz matrix, filled with σ values that we'll see later.
Now, we have :

$$\begin{cases} -\gamma'_{\mathbf{o}}\{T - I'\} + \gamma'_{\mathbf{i}}\{I - R\} = k_0 Z_0.\mathbf{\Lambda}.(T + I') \\ I + R = T + I' \end{cases} \tag{25}$$

As seen in Figure 1, we only consider an incident wave from the lower-left quarter, denoted as I, thus we have $I' = 0$, which leads to :

$$-\gamma'_{\mathbf{o}}T + \gamma'_{\mathbf{i}}I - \gamma'_{\mathbf{i}}R = k_0 Z_0.\mathbf{\Lambda}.T \tag{26}$$

$$T = I + R \tag{27}$$

Injecting 27 in the equation 26, we obtain :

$$\begin{aligned} &-\gamma_{\mathbf{o}}'I - \gamma_{\mathbf{o}}'R + \gamma_{\mathbf{i}}'I - \gamma_{\mathbf{i}}'R = k_0 Z_0 \mathbf{\Lambda} I + k_0 Z_0 \mathbf{\Lambda} R \\ &\Longrightarrow (-\gamma_{\mathbf{o}}' + \gamma_{\mathbf{i}}' - k_0 Z_0 \mathbf{\Lambda}) I = (k_0 Z_0 \mathbf{\Lambda} + \gamma_{\mathbf{o}}' + \gamma_{\mathbf{i}}') R \end{aligned} \tag{28}$$

Thus we have :

$$\boxed{R = (k_0 Z_0 \mathbf{\Lambda} + \gamma_{\mathbf{o}}' + \gamma_{\mathbf{i}}')^{-1} (-\gamma_{\mathbf{o}}' + \gamma_{\mathbf{i}}' - k_0 Z_0 \mathbf{\Lambda}) I} \tag{29}$$

and

$$\boxed{T = I + R} \tag{30}$$

These vectors will allow us to deduce all the quantities of interest for s polarization. We now need to redo these calculations for p polarization.

For **magnetic transverse** polarization, we have $\partial_z H_y = -i\omega\epsilon_0\epsilon_r E_x$, and the boundary conditions are given by :

$$E_{xi}(x,0) = E_{xo}(x,0) \tag{31}$$

$$H_{yo}(x,0) - H_{yi}(x,0) = -\sigma_g(x).E_{yi/o}(x,0) \tag{32}$$

Following the same method as before, we have :

$$\sum_{n\in\mathbb{Z}} \gamma_{i,n} e^{i\alpha_n x} (I_n e^0 - R_n e^0) = \sum_{n\in\mathbb{Z}} \gamma_{o,n} e^{i\alpha_n x} (T_n e^0 - I_n' e^0) \tag{33}$$

Thus we obtain :

$$\gamma_{i,n}(I_n - R_n) = \gamma_{o,n}(T_n - I_n') \qquad \forall n \in \mathbb{Z} \tag{34}$$

Using :

$$\partial_z H_y = -i\omega\epsilon_0\epsilon_r E_x \tag{35}$$

and taking $\gamma_{i/o,n}' = \dfrac{\gamma_{i/o,n}}{\epsilon_{ri/o}}$, we obtain :

$$(T_n + I_n') - (I_n + R_n) = -\frac{z_0}{k_0} \sum_{p\in\mathbb{Z}^{\not\in}} \sigma_{n-p} \gamma_{o,n}' (T_n - I_n') \qquad \forall n \in \mathbb{Z} \tag{36}$$

Thus, using the matrix notation, we have :

$$(T + I') - (I + R) = -\frac{Z_0}{k_0} . \mathbf{\Lambda} . \gamma_{\mathbf{o}}' (T - I') \tag{37}$$

As $I' = 0$, we finally obtain :

$$\boxed{R = ({\gamma_{\mathbf{o}}}^{-1}\gamma_{\mathbf{i}} + \mathbb{1} + \mathbf{\Lambda}\gamma_{\mathbf{o}}{\gamma_{\mathbf{o}}}^{-1}\gamma_{\mathbf{i}})^{-1} \left({\gamma_{\mathbf{o}}}^{-1}\gamma_{\mathbf{i}} - \mathbb{1} + \frac{Z_0}{k_0} \mathbf{\Lambda} \gamma_{\mathbf{o}}' {\gamma_{\mathbf{o}}}^{-1}\gamma_{\mathbf{i}} \right) I} \tag{38}$$

and :

$$\boxed{T = {\gamma_{\mathbf{o}}}^{-1}\gamma_{\mathbf{i}}(I - R)} \tag{39}$$

We now have the expressions for the vectors R and T in both types of polarization, which will allow us to deduce all the quantities of interest.

To complete the model, we need to incorporate the material by considering its **conductivity** $\sigma_g(x)$. This conductivity is determined by the sum of the conductivities of the graphene bands as well as the "empty" region between the bands.

$$\begin{cases} \sigma_g = \sigma_{intra} + \sigma_{inter} \\ \sigma_{vide} = 0 \end{cases}$$

σ_{intra} comes from the energy exchange in the valence band and σ_{inter} represents the energy transfert between the different energy levels of an electron [?], given by :

$$\boxed{\sigma_{intra} = \frac{2ie^2 k_B T}{\pi\hbar^2(\omega + i\gamma)} ln\left(2cosh\left(\frac{\mu_c}{2k_B T}\right)\right)} \tag{40}$$

and

$$\boxed{\sigma_{inter} = \frac{e^2}{4\hbar}\left[\frac{1}{2} + \frac{1}{\pi}arctan\left(\frac{\hbar(\omega + i\gamma) - 2\mu_c}{2k_B T}\right) - \frac{i}{2\pi}ln\left(\frac{[\hbar(\omega + i\gamma) + 2\mu_c]^2}{[\hbar(\omega + i\gamma) - 2\mu_c]^2 + (2k_B T)^2}\right)\right]} \tag{41}$$

with :

- e the elementary charge ;
- $\hbar = \dfrac{h}{2\pi}$ with h the Plack constant ;
- μ_c the chemical potential, which describes the way that the system's energy vanishes, depending on the number of particles ;
- k_B the Boltzman's constant ;
- T the temperature ;
- Γ the damping factor ($\hbar\Gamma = 0.658meV$), which represents the temporal decay of the oscillations.

Thus the conductivity is a periodic function with a shape and characteristics as followed :

$$\begin{cases} \sigma(x) = \sigma_g, & x \in [0\ ;\ a] \\ \sigma(x) = 0, & x \in [a\ ;\ d] \end{cases}$$

The Toeplitz' matrix is given by :

$$\sigma_0 = \frac{1}{d}\int_0^d \sigma_g(x)dx \tag{42}$$

and :

$$\sigma_{p\neq 0} = \frac{i\sigma_g}{2p\pi}(e^{-iKpa} - 1) \tag{43}$$

with $K = \dfrac{2\pi}{d}$