GROUP TUTORING SESSIONS

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Contents

1 Problem Set on Numerical Methods

1.1 Using Mathematica® in Optics: an introduction

The following is a list of resources available to help you navigate the software:

- Mathematica basics, by James Stewart from *CalcLabs with Mathematica: single variable calculus*. This book chapter describes many of the most important and basic elements of Mathematica® and discuss a few of the more common technical issues related to using Mathematica®.
  This Mathematica® text is suggested for first-time users.

- Mathematica tutorial, by Mark S. Gockenbach. To accompany *Partial differential equations: analytical and numerical methods* [1].
  This tutorial is my suggested text for students who have minor experience using Mathematica®.

- Comprehensive documentation for Mathematica® and the Wolfram Language, which includes details and examples for functions, symbols, and workflows.

- Wolfram demonstrations project. Explore thousands of free applications across science, mathematics, engineering, technology, and more.

- Wolfram library archive has thousands of downloadable resources for Mathematica, collected over the full history of Wolfram.

This is a list of resources available in Spanish:

- Guía rápida para el nuevo usuario de Mathematica 5.0®, by Eugenio M. Fedriani Martel and Alfredo García Hernández-Díaz.

- Breve manual de Mathematica 5.1, by Robert Ipanaqué Chero and Ricardo Velesmoro León.

- Docencia con Mathematica, by Javier Pérez (Departamento de Análisis Matemático, Universidad de Granada).

1.1.1 Plotting scalar and vector wave fields

Consider the electric field of a time-harmonic plane wave propagating along the z axis in a vacuum. The electric field $\mathbf{E}(z,t) = \mathrm{Re}[\vec{E}(z,t)]$ can be determined by means of its analytical representation $\vec{E}(z,t) = \hat{\sigma}E(z,t)$, where $E(z,t) = E_0 \exp(ik_0 z - i\omega t)$. Here, $k_0 = \omega/c$ is the vacuum wavenumber, and the unit vector $\hat{\sigma} = \sigma_x\hat{x} + \sigma_y\hat{y}$ gives the state of polarization (here, $\hat{\sigma}$ is equivalent to the Jones vector), where $|\sigma_x!^2 + |\sigma_y|^2 = 1$. For numerical purposes, set the amplitude $E_0 = 1$ V/m and the vacuum wavelength $\lambda_0 = 500$ nm (where $k_0 = 2\pi/\lambda_0$), and $c = 3\ 10^8$m/s.

First, consider a linearly-polarized plane wave, $\hat{\sigma} = \hat{\sigma}^*$. In practical terms, the electric field can be represented by the scalar wave function $E(z,t)$.

1. Plot $\mathrm{Re}[E(z,t)]$ and $|E(z,t)|^2$ within the range $0 \le z \le 2\lambda_0$ at the instants $t = 0$ and $t = T/4$, where T is the period of the oscillation, that is, $\omega = 2\pi/T$.
   Hint: use the built-in symbol `Plot[]`.

2. Plot $\mathrm{Re}[E(z,t)]$ within the range $0 \le z \le 2\lambda_0$ and $0 \le t \le 2T$.
   Hint: use the built-in symbols `Plot3D[]` and `ContourPlot[]`.

Next, consider a circularly-polarized plane wave with $\hat{\sigma} = (\hat{x} + i\hat{y})/\sqrt{2}$.

3. Show the locus traced by the tip of the electric field $\text{Re}[\vec{E}(z,t)]$ at a given point of the plane $z = 0$ through one cycle, for instance within $0 \le t \le T$, by using a two-dimensional (2-D) plot, which generates the so-called *ellipse of polarization*.
   Hint: use the built-in symbol `ParametricPlot[]`.

4. Show again the locus traced by the tip of $\text{Re}[\vec{E}(z,t)]$ at $z = 0$ within the interval $0 \le t \le 3T$, however using a 3-D plot, for the same circularly-polarized plane wave. Can you infer from this figure the polarization handedness of the light: right circular or left circular? Also, create a 3-D graph of the locus traced by the tip of $\text{Re}[\vec{E}(z,t)]$, now set at the instance $t = 0$ and evaluated along the z axis, within the interval $0 \le z \le 3\lambda_0$.
   Hint: use the built-in symbol `ParametricPlot3D[]`.

5. Plot the time evolution of the vector field $\text{Re}[\vec{E}(z,t)]$ at different points of the plane $z = 0$ (for instance, in the domain $|x|, |y| \le 1$ mm) for the same circularly-polarized plane wave.
   Hint: use the built-in symbol `VectorPlot[]` to generate a vector plot of the vector field $\text{Re}[\vec{E}]$ as a function of x and y, and the built-in symbol `Animate[]` to generate an animation where t varies continuously from 0 to T.

1.1.2 Solving second-order linear homogeneous ODEs

Consider a half-space $z < 0$ filled with an isotropic, homogeneous, lossless, dielectric material of index of refraction n_1. Also, in the half-space $z > 0$ the medium is isotropic and homogeneous with index of refraction n_2, which is not necessarily real valued but $\text{Re}[n_2] \ge 0$ is assumed without loss of generality. Finally, the photonic system is free of charges and currents.

In the semi-space $z < 0$, a 1-D time-harmonic electric field $\vec{E}(z)\exp(-i\omega t)$ satisfies the following second-order linear homogeneous ordinary differential equation (ODE) with constant coefficients,

$$\left[\frac{\partial^2}{\partial z^2} + k_1^2\right]\vec{E}(z) = 0, \tag{1.1.1}$$

which is the so-called *Helmholtz equation*, where $k_1 = n_1 k_0$ ($k_0 = \omega/c$) is the wavenumber in the medium. Furthermore, one may show that $\vec{E}(z) = \hat{\sigma}E(z)$, where

$$E(z) = E_0\left[\exp(ik_1 z) + r\exp(-ik_1 z)\right], \tag{1.1.2}$$

is a solution of the 1-D Helmholtz equation in $z < 0$, where $\hat{\sigma}$ is a complex, unitary ($\hat{\sigma}\cdot\hat{\sigma}^* = 1$), transverse ($\hat{\sigma}\cdot\hat{z} = 0$) vector denoting the state of polarization of the wave field, and E_0 and r are complex-valued constants. The electric field given in Eqs. (1.1.2) represents a superposition of two counter-propagating plane waves: the *incident* wave has an electric field with amplitude E_0, and thus intensity $n_1 S_0 = \frac{1}{2}n_1|E_0|^2/Z_0$ ($Z_0 = \sqrt{\mu_0/\epsilon_0}$ is the intrinsic impedance of a vacuum), which propagates along the z axis in direction to the interface set at $z = 0$, whereas the *reflected* wave propagates back from the interface having an amplitude rE_0. In fact, r is the well-known reflection coefficient, which can be estimated by means of

$$r = \frac{E(0)}{E_0} - 1, \tag{1.1.3}$$

and $R = |r|^2$ gives the wave reflectance. Furthermore, the complex Poynting vector, $\vec{S}(z) = \frac{1}{2}\vec{E}(z)\times\vec{H}^*(z) = \hat{z}S_z(z)$, has its real part, as measured at $z = 0$, given by $\text{Re}[S_z(0)] = n_1 S_0(1-|r|^2)$.

In the half-space $z > 0$, the 1-D electric field satisfies the Helmholtz equation, $\left(\partial_z^2 + k_2^2\right)\vec{E}(z) = 0$, where $k_2 = n_2 k_0$ is the wave number in this medium. One may verify the validity of the solution $\vec{E}(z) = \hat{\sigma}E(z)$ to the Helmholtz equation, where

$$E(z) = E_0 t \exp\left(ik_2 z\right), \quad z > 0. \tag{1.1.4}$$

and the unit vector $\hat{\sigma}$ represents the same state of polarization of the incident and reflected fields. The electric field given in Eq. (1.1.4) represents a plane wave propagating along the z axis away from the interface set at $z = 0$. In addition, t is the complex-valued transmission coefficient, which can be estimated by $t = E(0)/E_0 = 1 + r$. Finally, the complex Poynting vector has its real part, as evaluated at the boundary $z = 0$, which is given by $\mathrm{Re}[\vec{S}(0)] = \hat{z}S_0|t|^2\mathrm{Re}(n_2)$. Therefore, $T = |t|^2\,\mathrm{Re}(n_2)/n_1$ gives the wave transmittance. Note that $T + R = 1$ by conservation of energy.

1. Show that the electric field in the half-space $z < 0$ satisfies the Robin-type boundary condition

$$\left[ik_1 E(z) + \frac{\partial E(z)}{\partial z}\right]_{z=z_1} = 2ik_1 E_0 \exp(ik_1 z_1), \tag{1.1.5}$$

   which is established at any transverse plane $z = z_1$, called *input port*, provided that $z_1 < 0$. In the half-space $z > 0$, the electric field satisfies the *Sommerfeld radiation condition*,

$$\left[ik_2 E(z) - \frac{\partial E(z)}{\partial z}\right]_{z=z_2} = 0, \quad \text{and} \quad z_2 > 0, \tag{1.1.6}$$

   which is established at the *output port*, $z = z_2$.

For numerical purposes, set the amplitude $E_0 = 1$ V/m, the vacuum wavelength $\lambda_0 = 500$ nm (where $k_0 = 2\pi/\lambda_0$), and $c = 3\ 10^8$m/s. Also set the input and output ports at $z_2 = -z_1 = 2\lambda_0$.

2. Find numerically the solution to the second-order linear homogeneous ODE,

$$\left[\frac{\partial^2}{\partial z^2} + k_0^2 n^2(z)\right]E(z) = 0, \quad \text{where} \quad z_1 \le z \le z_2, \tag{1.1.7}$$

   providing the z dependence of the electric field, $E(z)$, where $n(z) = n_1$ within $z_1 \le z < 0$, and $n(z) = n_2$ within $0 < z \le z_2$. Firstly use $n_1 = 1$ and $n_2 = 1.5$. Apply the Robin boundary condition (1.1.5) at the input port, and the radiation condition (1.1.6) at the output port.
   Hint: use the normalized coordinate $x = k_0 z$, and the functions $u(x) = E(z)$ and $a(x) = n^2(z)$, to transform Eq. (1.1.7) into $\partial_x^2 u(x) + a(x)u(x) = 0$, to be used with the built-in symbol `NDSolve[]`.
   Alternatively, one may take the following steps:

   - use the normalized coordinate $x = k_0 z$, and the functions $u(x) = E(z)$, $a(x) = n^2(z)$, and $c = -1$, in order to transform Eq. (1.1.7) into the *coefficient form* $\nabla\cdot(-c\nabla u) + au = 0$ of ODEs, as managed by Mathematica®, to be used with the built-in symbol `NDSolve[]`.
   - use the functions $q(x) = in(z)$ and $g(x) = 0$, both evaluated at the boundary $x_2 = k_0 z_2$, in order to transform Eq. (1.1.6) into the Robin boundary condition $\hat{n}\cdot(c\nabla u) = g - qu$ as treated by Mathematica®, and implement it by means of the built-in symbol `NeumannValue[]`.

- use the functions $q(x) = in(z)$ and $g(x) = 2in(x)E_0 \exp[in(x)x]$, both evaluated at the boundary $x_1 = k_0 z_1$, in order to transform Eq. (1.1.5) into the Robin boundary condition $\hat{n} \cdot (c\nabla u) = g - qu$ as treated by Mathematica®, to be implemented by `NeumannValue[]`.

3. Plot the real and imaginary part of the wave function $E(z)$ (or $u(x)$) which was found previously. Also plot $|E(z)|$ within the region of computation.
   Hint: use the built-in symbol `ReImPlot[]`.

4. Find numerically the reflection coefficient r given in Eq. (1.1.3), and compare with the analytical expression
$$r = \frac{n_1 - n_2}{n_1 + n_2}. \tag{1.1.8}$$
   Estimate the reflectance and transmittance by using your numerical results, and also compare it with the theoretical predictions.

5. Repeat 2–4 assuming now that $n_2 = 0.055 + i4.0$ (silver at $\lambda_0 = 600$ nm). For a better convergence of the numerical evaluation, set $z_2 = \lambda_0/2$ to shift the output port closer to the vacuum/silver interfase, and use the Dirichlet boundary condition $E(z) = 0$ at $z = z_2$.
   Hint: use the built-in symbol `DirichletCondition[]`.

1.1.3 The Fourier transform, the Fourier series expansion and the DFT

Let us consider an optical signal characterized by a 1-D function $f(t)$, where t may stand for the time coordinate. The Fourier transform (FT) of f can be represented by the symbol $\mathcal{F}(f)$ giving

$$\mathcal{F}(f)(\omega) = F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(t) \exp(i\omega t) \mathrm{d}t, \tag{1.1.9}$$

where ω is the spectral coordinate in the Fourier domain. Some useful properties of the FT are:

- If $f_a(t) = f(t/a)$ then $\mathcal{F}(f_a)(\omega) = |a| F(a\omega)$.
- If $f_0(t) = f(t - t_0)$ then $\mathcal{F}(f_0)(\omega) = F(\omega) \exp(i\omega t_0)$.
- If $f_e(t) = f(t) \exp(-i\omega_0 t)$ then $\mathcal{F}(f_e)(\omega) = F(\omega - \omega_0)$.
- If $f'(t) = df(t)/dt$ then $\mathcal{F}(f')(\omega) = -i\omega F(\omega)$.
- $\mathcal{F}(f \circledast g)(\omega) = \sqrt{2\pi} F(\omega) G(\omega)$, where $(f \circledast g)(t) = \int_{-\infty}^{+\infty} f(t') g(t - t') dt'$.
- $\mathcal{F}(\mathcal{F}(f))(t) = f(-t)$. As a consequence, $f(t) = \mathcal{F}(F)(-t) = \mathcal{F}^{-1}(F)(t)$, where $\mathcal{F}^{-1}$ is the inverse Fourier transform.
- *Plancherel theorem* (also called Parseval-Plancherel identity): $\int_{-\infty}^{+\infty} |f(t)|^2 \mathrm{d}t = \int_{-\infty}^{+\infty} |F(\omega)|^2 \mathrm{d}\omega$.

1. Find the FT of the following functions:
   * The rectangle function $f(t) = \mathrm{rect}(t) = 1$ if $|t| < 1/2$, otherwise vanishing.
   * The sinc (or *sinus cardinalis*) function $F(\omega) = \mathrm{sinc}(\omega) \equiv \sin(\omega)/\omega$.
   * The modulated time-harmonic signal $f(t) = \exp(-i\omega_0 t) \exp[-(t/\tau)^2]$, where $\tau > 0$ is the pulse length and $\omega_0 > 0$ is the so-called carrier frequency.
   * The time-limited Gaussian function $f(t) = \exp[-(t/\tau)^2] \, \mathrm{rect}(t/\Delta t)$, where $\tau, \Delta t > 0$.

* The normalized hyperbolic secant function $f(t) = \text{sech}(\sqrt{\pi/2}t)$.
* The Dirac delta function $f(t) = \delta(t - t_0)$.
* The Dirac comb function $f(t) = \text{comb}(t) = \sum_{n=-\infty}^{\infty} \delta(t - n)$.
* The periodic function $f(t) = \cos^2(t)$.

Hint: use the built-in symbol `FourierTransform[]` (also `Integrate[]`). In addition, the option `Assumptions -> τ>0` can be applied to the modulated time-harmonic signal, to mention an example.

2. Plot $f(t)$ and $F(\omega)$ for the functions previously analyzed in 1. Allocate numerical values to the parameters τ, Δt, and ω_0 freely. In cases involving Dirac delta functions, one may use that $\delta(x) \to \varepsilon/[\pi(x^2 + \varepsilon^2)]$ in the limit $\varepsilon \to 0^+$.
Hint: use the built-in symbol `ReImPlot[]` for complex-valued functions.

In particular, a periodic function, $f_p(t + \Delta t) = f_p(t)$, has a Fourier series expansion given by

$$f_p(t) = \sum_{s=-\infty}^{+\infty} c_s \exp(-is\Delta\omega t), \quad \text{where} \quad c_s = \frac{1}{\Delta t} \int_{-\Delta t/2}^{\Delta t/2} f_p(t) \exp(is\Delta\omega t)\, dt, \tag{1.1.10}$$

is the Fourier coefficient of the s-th harmonic, and $\Delta\omega = 2\pi/\Delta t$ is the fundamental frequency. Therefore, its FT $F_p(\omega) = \mathcal{F}(f_p)(\omega)$ is characterized by a discrete but generally infinite number of coefficients c_s, which can be expressed as a modulated *comb* function,

$$F_p(\omega) = \sqrt{2\pi} \sum_{s=-\infty}^{+\infty} c_s \delta(\omega - s\Delta\omega). \tag{1.1.11}$$

Some useful properties of the Fourier series expansion are:

- *Parseval's theorem*: If f_p belongs to $L^2([0, \Delta t])$, then

$$\frac{1}{\Delta t} \int_{-\Delta t/2}^{\Delta t/2} |f_p(t)|^2 dt = \sum_{s=-\infty}^{+\infty} |c_s|^2. \tag{1.1.12}$$

- The integral in Eq. (1.1.10) giving the Fourier coefficient c_s can be interpreted as the FT of the time-limited function $f(t) = f_p(t)\,\text{rect}(t/\Delta t)$, when evaluated at frequencies $s\Delta\omega$, namely $c_s = (\sqrt{2\pi}/\Delta t) F(s\Delta\omega)$. As a consequence,

  1. Equation (1.1.11) can be written as $F_p(\omega) = F(\omega)\,\text{comb}(\omega/\Delta\omega)$.
  2. The FT of the time-limited function $f(t)$, when evaluated at frequencies $s\Delta\omega$, is directly proportional to the Fourier coefficients of $f_p(t)$, namely $F(s\Delta\omega) = (\sqrt{2\pi}/\Delta\omega)c_s$. This property is useful when applied to sampled functions, as we will see below.

3. Find the Fourier series expansion of the following periodic functions given in the central *unit cell* $|t| < \Delta t/2$:

* The squared cosine function $f_p(t) = \cos^2(t)$, with period $\Delta t = \pi$.
* The rectangle function $f_p(t) = \text{rect}(t)$, with period $\Delta t \geq 1$.

- ∗ The truncated Gaussian function $f_p(t) = \exp[-(t/\tau)^2]\,\mathrm{rect}(t/\Delta t)$, with period Δt, including the limiting cases $\Delta t \ll \tau$ and $\Delta t \gg \tau$.
- ∗ The Dirac comb function $f_p(t) = \mathrm{comb}(t)$, with period $\Delta t = 1$.

Hint: use the built-in symbol `FourierCoefficient[]` and its option `FourierParameters ->` $\{1, -2\pi/\Delta t\}$ to indicate the period (also `FourierSeries[]` can be used).

4. Plot $f_p(t)$ and its Fourier expansion (1.1.10) by considering a finite but increasing number of Fourier coefficients c_s, for the functions previously analyzed in 3. In each case, plot the list of Fourier coefficients c_s in the range $|s| \leq 10$. Where required, allocate numerical values to the parameters Δt and τ freely.
Hint: use the built-in symbol `ReImPlot[]` for complex-valued functions and `DiscretePlot[]` for the Fourier coefficients.

We may take a step further by sampling the periodic signal $f_p(t)$ at a rate $N/\Delta t$, giving

$$f_p(t) \approx \tilde{f}_p(t) = \frac{\Delta t}{N}\sum_{r=1}^{N} f(t_r)\delta(t-t_r), \quad \text{and} \quad \tilde{f}_p(t) = \sum_{s=-\infty}^{+\infty} \tilde{c}_s \exp\left(-is\Delta\omega t\right), \tag{1.1.13}$$

in the range $0 \leq t < \Delta t$, where $t_r = (r-1)\Delta t/N$. The periodic function $\tilde{f}_p(t)$ is composed of N Dirac delta functions which are regularly distributed within one period, Δt. Such approach is useful provided that $f_p(t)$ is not itself a finite set of Dirac delta functions within one period, so such cases are disregarded from here on. Some observations can be highlighted:

- The periodic function $f_p(t)$ is approximated to

$$\tilde{f}_p(t) = f_p(t)\,\mathrm{comb}\left(\frac{t}{\Delta t/N}\right), \tag{1.1.14}$$

which is a comb function of period $\Delta t/N$ modulated by $f_p(t)$ itself.

- Due to the periodicity of $f_p(t)$, equations (1.1.13) and (1.1.14) can be transformed into

$$\tilde{f}_p(t) = \frac{1}{N}\sum_{r=1}^{N} f_p(t_r)\,\mathrm{comb}\left(\frac{t-t_r}{\Delta t}\right), \tag{1.1.15}$$

set as a combination of N comb functions of period Δt and mutually shifted by $\Delta t/N$. This can also be inferred by means of the identity $\mathrm{comb}(x/\Delta) = N^{-1}\sum_{s=1}^{N}\mathrm{comb}[(x-x_s)/N\Delta]$, with $x_s = (s-1)\Delta$, applied in Eq. (1.1.14).

- The Fourier coefficients of $\tilde{f}_p(t)$ satisfy the recursive relationship $\tilde{c}_{s+N} = \tilde{c}_s$. Consequently, one can find only N independent Fourier coefficients of $\tilde{f}_p(t)$. From here on we will use the set $\{\tilde{c}_0, \tilde{c}_1, \ldots, \tilde{c}_{N-1}\}$

- Following Eq. (1.1.11), the FT of $\tilde{f}_p(t)$ yields

$$\tilde{F}_p(\omega) = \frac{\sqrt{2\pi}}{N\Delta\omega}\sum_{s=1}^{N}\tilde{c}_{s-1}\,\mathrm{comb}\left(\frac{\omega-\omega_s}{N\Delta\omega}\right), \tag{1.1.16}$$

with $\omega_s = (s-1)\Delta\omega$, which is also a periodic function with period $N\Delta\omega$. Note that $\tilde{F}_p(\omega)$ is characterized by a finite number N of Fourier coefficients providing the modulation of the N delta functions found within one period.

- Namely, the Fourier coefficients of $\tilde{f}_p(t)$ yield

$$\tilde{c}_{s-1} = \frac{1}{N}\sum_{r=1}^{N} f_{r-1} \exp\left[\frac{2\pi i(r-1)(s-1)}{N}\right], \quad \text{for} \quad s = \{1, 2, \ldots, N\}, \tag{1.1.17}$$

  where $f_{r-1} = f(t_r)$. Note that the zeroth-harmonic term appears at position 1 in the resulting list.

Finally, the list of N elements $\mathbf{c} = \{\tilde{c}_0, \tilde{c}_1, \ldots, \tilde{c}_{N-1}\}$ can be evaluated by applying the discrete Fourier transform (DFT) to the list $\mathbf{f} = \{f_0, f_1, \ldots, f_{N-1}\}$, such that[1] $\mathbf{c} = (1/\sqrt{N})\texttt{Fourier}[\mathbf{f}]$, where `Fourier[]` is a built-in symbol as defined by default in Mathematica®.

5. Use the DFT to evaluate the N Fourier coefficients $\tilde{c}_s$ of $\tilde{f}_p(t)$, derived by sampling the periodic functions $f_p(t)$ which were considered in 3. Where required, allocate numerical values to the parameters Δt and τ freely. Employ lists of $N = 2^5$ elements. In addition,

   - Compare these results with the Fourier coefficients c_s of $f_p(t)$, derived analytically in 3, where now $s = \{-\infty, \ldots, -2, -1, 0, 1, 2, \ldots, +\infty\}$.
   - Discuss if $\tilde{c}_{N-1}$ is closer to either c_{N-1} or c_{-1}. Do the same comparing $\tilde{c}_{N-2}$ with the Fourier coefficients c_{N-2} and c_{-2}. Can you find a more general rule?
   - Discuss the main differences when using $N = 2^6$ elements instead.

   Hint: use the built-in symbol `Table[]` to generate a list.

As previously mentioned, a sampled FT of a time-limited signal $f(t)$ of length τ_0 can be obtain by simply replicating such function at different instants in order to generate a periodic function $f_p(t)$ of period $\Delta t \geq \tau_0$, the latter used to subsequently calculate its Fourier coefficients c_s. These coefficients provide $F(\omega)$ at a discrete number of frequencies, which are multiples of the fundamental frequency $\Delta\omega = 2\pi/\Delta t$ (see 2). Namely, $F(s\Delta\omega) = (\sqrt{2\pi}/\Delta\omega)c_s$. Finally, the estimation of c_s is reduced to the (analytically or numerically) evaluation of the integral (1.1.10).

6. Analyze the validity of the approximation $F(\omega_s) \equiv F_{s-1} \approx \tilde{F}_{s-1}$, where $\tilde{F}_{s-1}$ are elements of the list $\mathbf{F} = (\sqrt{2\pi}/\Delta\omega)\mathbf{c}$ for $s = \{1, 2, \ldots, N\}$, and $\omega_s = (s-1)\Delta\omega$. Note that $\tilde{F}_{s+N} = \tilde{F}_s$. For that purpose:

   - Show that this problem is equivalent to comparing the Fourier transform of $f_p(t)$, which can be set as $F_p(\omega) = F(\omega)\,\text{comb}(\omega/\Delta\omega)$, and $\tilde{F}_p(\omega)$ given in Eq. (1.1.16).
     Hint: use the identity $\text{comb}(\omega/\Delta\omega) = N^{-1}\sum_{s=1}^{N}\text{comb}[(\omega-\omega_s)/N\Delta\omega]$.
   - Use the DFT to evaluate the N elements of $\mathbf{F}$, derived by sampling the functions $f(t)$ which were considered in 1 at a rate $N/\Delta t$. Where required, allocate numerical values to the parameters τ, Δt, and ω_0 freely. Disregard cases involving Dirac delta functions. Employ lists of $N = 2^5$ elements.
   - Compare these results with the Fourier transforms $F(\omega)$ derived analytically in 1, when evaluated at frequencies $\omega_s = (s-1)\Delta\omega$, where now $s = \{-\infty, \ldots, -2, -1, 0, 1, 2, \ldots, +\infty\}$. In particular, discuss if $\tilde{F}_{N-1}$ is closer to either F_{N-1} or F_{-1}. Do the same comparing $\tilde{F}_{N-2}$ with F_{N-2} and F_{-2}. Can you find a more general rule?

[1] Other definitions of the DFT are used in some scientific and technical fields.

- Using a given time-limited function $f(t)$ within the working range $|t| \leq \Delta t/2$, is there any improvement in the DFT-based estimation of the FT by using $N = 2^6$ elements? And using $N = 2^7$ elements? Note that the length Δt of the working range is kept fixed but the sampling rate is being doubled in each step.
- Compare the accuracy of the DFT obtained for a given time-limited function $f(t)$ within the working range $|t| \leq \Delta t/2$ when using $N = 2^5$ points, with the DFT of the same function but doubling the length of the working range to $2\Delta t$, by applying a zero padding in the range $\Delta t/2 < |t| \leq \Delta t$, and also doubling the number of points to $2N = 2^6$. Note that the sampling rate $N/\Delta t$ is conserved in both cases.
- Plot the lists $\mathbf{F}$ and $F(\omega_s)$ for all the functions previously analyzed.

Hint: consider using the built-in symbol `RotateLeft[`*list*`,`*len*`/2]`, where *len* `= Length[`*list*`]`, to swaps the left and right halves of *list*. The latter serves to transform $\mathbf{F}$ into the list $\left\{\tilde{F}_{-N/2}, \tilde{F}_{-N/2+1}, \ldots, \tilde{F}_{-1}, \tilde{F}_0, \tilde{F}_1, \ldots, \tilde{F}_{N/2-1}\right\}$, leaving $\tilde{F}_0$ in the center of the list.

1.2 Interference by division of wavefront

Introductory notes: rotation of plane waves

Consider a monochromatic plane wave of time frequency ω propagating in free space. The analytic representation of the electric field can be written as $\vec{E}(\vec{r},t) = \hat{\sigma} E_0 \exp(i\vec{k}\cdot\vec{r} - i\omega t)$, where $\hat{\sigma}$ is a unit vector ($\hat{\sigma}\cdot\hat{\sigma}^* = 1$) characterizing its state of polarization, E_0 is the complex-valued amplitude of the electric field measured in V/m, $\vec{k} = k\hat{q}$ is the wave vector, $\hat{q}\cdot\hat{q}^* = 1$, $k = \omega/c$ is the wavenumber, and $c = 1/\sqrt{\epsilon_0\mu_0}$ is the speed of light in vacuum. Note that:

1. The electric field is a transverse wave, i.e. $\hat{q}\cdot\hat{\sigma} = 0$. In other words, $\vec{E} \perp \vec{k}$.

2. The magnetic field of the plane wave can be set as $\vec{H}(\vec{r},t) = \hat{\pi} H_0 \exp(i\vec{k}\cdot\vec{r} - i\omega t)$, provided that the unit vector $\hat{\pi} = \hat{q}\times\hat{\sigma}$ and the amplitude of the magnetic field $H_0 = E_0/Z_0$, where $Z_0 = \sqrt{\mu_0/\epsilon_0}$ ($\approx 376.7\ \Omega$) is the intrinsic impedance of free space.

3. Using the fact that the rotation of a vector $\vec{x}$ by an angle θ around the axis characterized by the unit vector $\hat{u}$ can be written as[2]

$$R_u(\theta)\vec{x} = \hat{u}(\hat{u}\cdot\vec{x}) + \cos(\theta)(\hat{u}\times\vec{x})\times\hat{u} + \sin(\theta)(\hat{u}\times\vec{x}),$$

the electric field and magnetic field of the plane wave given above can satisfy Maxwell's equations under the rotational transformations $R_{\hat{u}}(\theta)\vec{k}$, $R_{\hat{u}}(\theta)\hat{\sigma}$, and $R_{\hat{u}}(\theta)\hat{\pi}$, applied simultaneously, and occurring independently of the orientation of the rotation unit vector $\hat{u}$.
Note: in Mathematica®, one may use `RotationMatrix[`θ`,{`u_x`,`u_y`,`u_z`}]` to generate a 3D rotation matrix equivalent to $R_u(\theta)$.

4. A generalization of 3 can be established when the rotation is described by the multiplication matrix $R = R_z(\alpha)\,R_y(\beta)\,R_x(\gamma)$, whose yaw, pitch, and roll angles are α, β and γ, respectively, which is applied to the vectors $\vec{k}$, $\hat{\sigma}$, and $\hat{\pi}$ characterizing an electromagnetic plane wave.

1.2.1 Interference of two plane waves

First, consider an optical plane wave whose electric field is $\mathbf{E}(\vec{r},t) = \mathrm{Re}[\vec{E}(\vec{r},t)]$, where $\vec{E}(\vec{r},t) = \hat{\sigma}E_0\exp(i\vec{k}\cdot\vec{r} - i\omega t)$, which propagates along the z-axis ($\hat{q} = \hat{z}$) in free space ($k = \omega/c$), having a wavenumber $k = 4\pi\ \mu\mathrm{m}^{-1}$ ($\lambda = 0.5\ \mu$m), an amplitude $E_0 = 1$ V/m, and a state of polarization characterized by the unit vector $\hat{\sigma} = \hat{y}$, i.e. the plane wave is linearly polarized.

1. Plot the time evolution of the electric field $\mathbf{E}(\vec{r},t)$ at different points of the 3-D domain Ω_3, given by $|x| \le \lambda$, $|y| \le \lambda$, and $0 \le z \le 2\lambda$. Show that the electric field vector executes a simple-harmonic oscillation of period $T = \lambda/c$ ($T = 1.67$ fs in our case) along the y axis.
Hint: use `VectorPlot3D[]` to show $\mathbf{E}(\vec{r},t)$ in a given instant t within Ω, and `Animate[]` in $0 \le t \le T$ to represent its time evolution.

2. Plot the time evolution of the energy density, $U(\vec{r},t) = U_e(\vec{r},t) + U_m(\vec{r},t)$, where

$$U_e(\vec{r},t) = \frac{1}{2}\epsilon_0\mathbf{E}\cdot\mathbf{E}, \quad \text{and} \quad U_m(\vec{r},t) = \frac{1}{2}\mu_0\mathbf{H}\cdot\mathbf{H},$$

where $\mathbf{H}(\vec{r},t) = \mathrm{Re}[\vec{H}(\vec{r},t)]$ (see introductory notes), and the Poynting vector,

$$\mathbf{S}(\vec{r},t) = \mathbf{E}\times\mathbf{H},$$

[2] https://en.wikipedia.org/wiki/Rotation_matrix

in points of Ω_3. Show that they exhibit a periodic oscillation of period $T/2$. Finally, show that one can set $\mathbf{S}(\vec{r},t) = S_z(z,t)\hat{z}$, and plot $S_z(z,t)$ in $0 \le z \le 2\lambda$.
Hint: use `ContourPlot[]` to represent scalar fields such as $U(\vec{r},t)$ in different planes ($y=0$, for instance) within Ω_3.

3. Show that the time-averaged energy density, defined as

$$w(\vec{r}) = \frac{1}{T}\int_0^T U(\vec{r},t)\mathrm{d}t = \frac{1}{4}\epsilon_0 \vec{E}\cdot\vec{E}^* + \frac{1}{4}\mu_0 \vec{H}\cdot\vec{H}^*,$$

leads to a uniform pattern, $w(\vec{r}) = w_0$, where $w_0 = \epsilon_0|E_0|^2/2$. Also show that the time-averaged Poynting vector, which is determined by the real part of the complex Poynting vector

$$\vec{S}(\vec{r}) = \frac{1}{2}\vec{E}\times\vec{H}^*,$$

yields the vector $S_0\hat{q}$ at every point of the space, where the intensity $S_0 = w_0 c = |E_0|^2/(2Z_0)$.

4. Next, consider that the plane wave of electric field $\vec{E}(\vec{r},t)$ is split into two identical plane waves of amplitude $E_0/2$ each one, giving $\vec{E}_1 = \vec{E}_2 = \vec{E}/2$. By optical means, the electric field $\vec{E}_1(\vec{r},t)$ is transformed into $\vec{E}_1'(\vec{r},t)$ by a rotation $R_y(\beta_0)$ in the terms given in the introductory notes (see 3), where the pitch angle $\beta_0 = \pi/4$. However the electric field $\vec{E}_2(\vec{r},t)$ is transformed into $\vec{E}_2'(\vec{r},t)$ by a rotation $R_y(-\beta_0)$. Finally, consider the interference of the rotated wave fields, $\vec{E}'(\vec{r},t) = \vec{E}_1'(\vec{r},t) + \vec{E}_2'(\vec{r},t)$, occurring in the region of interest.

   - Plot the time evolution of the electric field, $\mathbf{E}'(\vec{r},t) = \mathrm{Re}[\vec{E}'(\vec{r},t)]$, determined at points in Ω_3. Show that the wave field is periodic along the x axis with a spatial period $p_x = \lambda/\sin(\beta_0)$, however it is invariant under translations along the y axis. Analyze the state of polarization at the observed points in Ω_3. Finally, plot the time evolution of the y component of the electric field, $\hat{y}\cdot\mathbf{E}'(\vec{r},t)$, in the 2-D domain Ω_2 given by $|x| \le p_x$ and $0 \le z \le 2\lambda$.
   - Plot the time evolution of the energy density of the superposition of these two polarized plane waves at points of Ω_2. Plot the Poynting vector at points of Ω_3. Show that they exhibit a time-domain oscillation of period $T/2$. Show that one can set $\mathbf{S}(\vec{r},t) = S_x(x,z,t)\hat{x} + S_z(x,z,t)\hat{z}$, and plot $\mathbf{S}(\vec{r},t)$ in Ω_2. Is there any periodicity of the evaluated patterns along the x axis? And along the z axis?
   Hint: use `ContourPlot[]` to represent the scalar field $U(\vec{r},t)$ within Ω_2. Use `VectorPlot[]` to represent the vector field $\mathbf{S}(\vec{r},t)$ in Ω_2.
   - Plot the time-averaged energy density in Ω_2 and the time-averaged Poynting vector at points of either Ω_2 or Ω_3. Show that one can set $w(\vec{r}) = w_0[\cos^2(\beta_0)\cos^2(2\pi x/p_x) + \sin^2(\beta_0)/2]$ and $\mathrm{Re}(\vec{S}) = S_0\cos(\beta_0)\cos^2(2\pi x/p_x)\hat{z}$, the latter describing the *Young fringes* pattern.

5. Repeat 4 but considering the interference of two plane waves with initial (prior to the application of rotation) state of polarization given by the unit vector $\hat{\sigma} = \hat{x}$. In addition, consider wave rotations of pitch angle: (a) $\beta_0 = \pi/4$, and (b) $\beta_0 = \pi/2$. Here, one may plot the time evolution of the x and z components of the electric field in Ω_2, simultaneously.

6. Repeat 4 but considering the interference of two plane waves with original state of polarization given by the unit vector $\hat{\sigma} = (\hat{x} + i\hat{y})/\sqrt{2}$. In addition, consider a pitch angle $\beta_0 = \pi/4$.

1.2.2 Periodic interference patterns (optional)

First, consider an optical plane wave whose electric field is $\vec{E}(\vec{r},t) = \hat{\sigma} E_0 \exp(i\vec{k}\cdot\vec{r} - i\omega t)$, which propagates along the z-axis ($\hat{q} = \hat{z}$) in free space ($k = \omega/c$), having a wavenumber $k = 4\pi\ \mu\text{m}^{-1}$ ($\lambda = 0.5\ \mu$m), an amplitude $E_0 = 1$ V/m, and a state of polarization characterized by the unit vector $\hat{\sigma} = \hat{y}$, i.e. the plane wave is linearly polarized.

Next, consider that the plane wave of electric field $\vec{E}(\vec{r},t)$ is split into an odd number $M = 3$ of identical plane waves with amplitude E_0/M each one, giving wavelets of electric field $\vec{E}_m = \vec{E}/M$, with $m = 0, \pm 1, \ldots, (M-1)/2$. By optical means, the electric field $\vec{E}_1(\vec{r},t)$ of one wavelet is transformed into $\vec{E}'_1(\vec{r},t)$ by a rotation $R_y(\beta_0)$ in the terms given in the introductory notes (see 3), where the pitch angle $\beta_0 = \pi/18$. The electric field $\vec{E}_{-1}(\vec{r},t)$ is transformed into $\vec{E}'_{-1}(\vec{r},t)$ by a mirror-symmetric transformation $R_y(-\beta_0)$. In general, the electric field $\vec{E}_m(\vec{r},t)$ of the m-th wavelet is transformed into $\vec{E}'_m(\vec{r},t)$ by the rotation $R_y(\beta_m)$, provided that

$$\sin(\beta_m) = m \sin(\beta_0), \tag{1.2.1}$$

and $|\beta_m| \leq \pi/2$. Finally, consider the interference of the rotated wave fields, $\vec{E}'(\vec{r},t) = \sum_m \vec{E}'_m(\vec{r},t)$, occurring in the region of interest.

1. Show that the electric field satisfies the following periodicity property:

   $$\vec{E}'(x + p_x, y, z, t) = \vec{E}'(x, y, z, t),$$

   where $p_x = \lambda/\sin\beta_0$ is the period along the x axis. Show that the electric field is invariant under translations in the spatial coordinate y.
   Note: Equation 1.2.1 becomes $\sin(\beta_m) = m\lambda/p_x$, which is formally equivalent to the *grating equation* when light is normally incident on the grating.

2. Plot the time evolution of the electric field, $\text{Re}[\vec{E}'(\vec{r},t)]$, determined at different points of the plane $z = 0$, provided that $|x| \leq 2p_x$. Furthermore, analyze the state of polarization at the observed points of the xy plane.

3. Plot the time-averaged energy density and the time-averaged Poynting vector at different points of the plane $z = 0$.

4. Repeat 2–3 but considering the interference of: (a) $M = 5$, and (b) $M = 7$ plane waves with initial state of polarization given by the unit vector $\hat{\sigma} = \hat{y}$.

5. Find the maximum number (M_{max}) of plane waves to interfere under the restriction $|m| \leq 1/\sin(\beta_0)$, which can be derived from $|\sin(\beta_m)| \leq 1$. Furthermore, repeat 2–3 but considering the interference of M_{max} plane waves with initial state of polarization given by the unit vector $\hat{\sigma} = \hat{y}$.

6. Repeat 2–4 but considering the interference of plane waves with initial state of polarization given by the unit vector $\hat{\sigma} = (\hat{x} + \hat{y})/\sqrt{2}$.

1.3 Interference by division of amplitude

Introductory notes: Scattered fields in 1-D domains under normal incidence

Consider a semi-space $z < 0$ filled with an isotropic homogeneous material of index of refraction n_1, which is real valued and positive for convenience. In $z > L$ (with $L > 0$) the medium is isotropic and homogeneous with index of refraction n_2, which is not necessarily real valued ($\mathrm{Im}(n_2) \geq 0$ is always imposed). In the intermediate space, $0 < z < L$, the medium is inhomogeneous with index of refraction $n(z)$. Finally, the photonic systems is free of charges and currents.

1. In $z < 0$, a 1-D time-harmonic electric field $\vec{E}(z) = \hat{\sigma} E(z) \exp(-i\omega t)$ satisfies the Helmholtz equation, $\left[\partial_z^2 + k_0^2 n_1^2\right] E(z) = 0$, where $k_0 = \omega/c$ is the wavenumber in a vacuum, and $\hat{\sigma}$ is a complex, unitary ($\hat{\sigma} \cdot \hat{\sigma}^* = 1$), transverse ($\hat{\sigma} \cdot \hat{z} = 0$) vector denoting the state of polarization of the wave field. In addition, its magnetic field $\vec{H}(z) = \hat{\pi} H(z) \exp(-i\omega t)$ can be determined by means of $H(z) = (ik_0 Z_0)^{-1} \partial_z E(z)$, where $Z_0 = (\mu_0/\epsilon_0)^{1/2}$ is the intrinsic impedance in free space, and $\hat{\pi} = \hat{z} \times \hat{\sigma}$.

   (a) Furthermore, $E(z) = E_0 \left[\exp(ik_1 z) + r \exp(-ik_1 z)\right]$ is a solution of the 1-D Helmholtz equation in $z < 0$, E_0 and r are complex-valued constants, and $k_1 = k_0 n_1$ is the wave number in the medium. In fact, r is the reflection coefficient, which can be estimated by means of $r = \frac{E(0)}{E_0} - 1$, and $R = |r|^2$ gives its reflectance. Finally, the magnetic field is set as $H(z) = n_1 H_0 \left[\exp(ik_1 z) - r \exp(-ik_1 z)\right]$, where $H_0 = E_0/Z_0$ is its amplitude.

   (b) The complex Poynting vector, $\vec{S}(z) = \frac{1}{2} \vec{E}(z) \times \vec{H}^*(z) = \hat{z} S_z(z)$, has its real part at the boundary $z = 0$ given by $\mathrm{Re}[S_z(0)] = n_1 S_0 (1 - |r|^2)$, where the intensity $S_0 = \frac{1}{2} |E_0|^2 / Z_0$.

   (c) The electric field in $z \leq 0$ satisfies the boundary condition $\left[ik_1 E(z) + \partial_z E(z)\right]_{z=z_1} = 2ik_1 E_0 \exp(ik_1 z_1)$, which can be applied at a transverse plane $z = z_1$ with $z_1 \leq 0$.

2. In $z > L$, the 1-D electric field satisfies the Helmholtz equation, $\left[\partial_z^2 + k_2^2\right] \vec{E}(z) = 0$, where $k_2 = k_0 n_2$. Note that, in general, k_2 is complex valued, and $\mathrm{Im}(k_2) \geq 0$ always occurs.

   (a) One find the solution $E(z) = E_0 t \exp\left[ik_2(z - L)\right]$ to the Helmholtz equation in $z > L$, where $\vec{E}(z) = \hat{\sigma} E(z)$, and $\hat{\sigma}$ represents the same state of polarization of the incident and reflected fields. Here, t is the transmission coefficient, which can be estimated by $t = \frac{E(L)}{E_0}$. Also, the magnetic field $\vec{H}(z) = \hat{\pi} H(z)$, where $H(z) = n_2 H_0 t \left[ik_2(z - L)\right]$.

   (b) The complex Poynting vector yields $\mathrm{Re}[\vec{S}(z)] = \mathrm{Re}[\vec{S}(L)] \exp[-2\,\mathrm{Im}(k_2)(z - L))]$, if $z > L$, where $\mathrm{Re}[\vec{S}(L)] = \hat{z} S_0 |t|^2 \,\mathrm{Re}(n_2)$. Thus, $T = |t|^2 \,\mathrm{Re}(n_2)/n_1$ gives the optical transmittance.

   (c) In $z \geq L$, the electric field satisfies the *radiation condition*, $\left[ik_2 E(z) - \partial_z E(z)\right]_{z=z_2} = 0$, which is established at any transverse plane $z = z_2$ provided that $z_2 \geq L$.

3. In the stratified medium, $0 < z < L$, the electric field $\vec{E}(z) = \hat{\sigma} E(z)$ satisfies the equation,

$$\left[\frac{\partial^2}{\partial z^2} + k_0^2 n^2(z)\right] E(z) = 0, \tag{1.3.1}$$

   for an arbitrary state of polarization $\hat{\sigma}$ of the incident wave field. In addition:

   (a) The magnetic field can be evaluated as $\vec{H}(z) = \hat{\pi} H(z)$, where $H(z) = (i\omega\mu_0)^{-1} \partial_z E(z)$.

(b) Continuity of $E(z)$ and $\partial_z E(z)$ can be used as boundary conditions under the presence of discontinuities of the index of refraction $n(z)$.

(c) For instance, assuming a homogeneous scattering layer, where $n(z) = n_L$:

- One finds the solution to the Helmholtz equation (1.3.1) as follows,

$$E(z) = E_0 \left[t_L \exp\left(ik_L z \right) + r_L \exp\left(ik_L z \right) \right], \quad 0 < z < L. \tag{1.3.2}$$

Here, $k_L = k_0 n_L$, and t_L and r_L are complex-valued constants.

- One may show the validity of the *Airy's formulae* given as [2, section 4.2]

$$r = \frac{r_{1L} + r_{L2}\exp(2ik_L L)}{1 - r_{L1}r_{L2}\exp(2ik_L L)}. \tag{1.3.3}$$

$$t = \frac{t_{1L}t_{L2}\exp(ik_L L)}{1 - r_{L1}r_{L2}\exp(2ik_L L)}, \tag{1.3.4}$$

$$t_L = \frac{t_{1L}}{1 - r_{L1}r_{L2}\exp(2ik_L L)}, \tag{1.3.5}$$

$$r_L = \frac{t_{1L}r_{L2}\exp(2ik_L L)}{1 - r_{L1}r_{L2}\exp(2ik_L L)}, \tag{1.3.6}$$

where the *Fresnel transmission* and *reflection coefficients* are given by

$$r_{\alpha\beta} = \frac{n_\alpha - n_\beta}{n_\alpha + n_\beta} = -r_{\beta\alpha}, \tag{1.3.7}$$

$$t_{\alpha\beta} = \frac{2n_\alpha}{n_\alpha + n_\beta} = 1 + r_{\alpha\beta}. \tag{1.3.8}$$

(d) By applying Poynting's theorem in the stratified medium, $\mathrm{Re}[S_z(0)] - \mathrm{Re}[S_z(L)] = n_1 S_0 A$, one finds the optical absorbance $A = 1 - T - R$.

1.3.1 Antireflection coatings

An *antireflection coating* can be used to completely eliminate the reflection of light appearing at a flat interface between two media of distinct indices of refraction, $n_1 \neq n_2$ [2, sections 4.4.1 and 7.3]. It consists of a quarter-wave layer ($k_L L = \pi/2$) set in $0 < z < L$, with $n(z) = n_L$ satisfying $n_L^2 = n_1 n_2$.

1. Show that $r_{1L} = r_{L2}$ in an antireflection coating and, therefore, the reflection coefficient r given in Eq. (1.3.3) vanishes.

For numerical purposes, set the amplitude $E_0 = 1$ V/m, and the vacuum wavelength $\lambda_0 = 500$ nm which the antireflection coating is designed for. Here, $n(z) = n_1$ within $z_1 \leq z < 0$, and $n(z) = n_2$ within $L < z \leq z_2$. Firstly use $n_1 = 1$ and $n_2 = 1.5$. Also set the input and output ports at $z_2 = -z_1 = 2\lambda_0$.

2. Evaluate the index of refraction n_L and the layer width L of our antireflection coating.

3. Find numerically the solution to the Helmholtz equation (1.3.1) within the whole interval $z_1 \leq z \leq z_2$, providing the z dependence of the electric field, $E(z)$. Apply the Robin boundary condition (1.1.5) at the input port, and the radiation condition (1.1.6) at the output port.

4. Plot the real and imaginary part of the wave function $E(z)$ (or $u(x)$, see 2) which was found previously. Also plot $|E(z)|$ within the region of computation.

5. Repeat 3–4 for the boundary wavelengths in the visible, $\lambda_0 = 390$ nm and $\lambda_0 = 780$ nm, but keeping the layer width L (and n_L) as evaluated in 2 for $\lambda_0 = 500$ nm. In addition, calculate the optical reflectance $R = |r|^2$, both numerically and using Eq. (1.3.3), at both boundary wavelengths.

6. Repeat 3–4 for an antireflection coating of width: (a) $L + \lambda_0/(2n_L)$, and (b) $L + \lambda_0/n_L$, where $L = \lambda_0/(4n_L)$ and $\lambda_0 = 500$ nm. Discuss these results.

7. Repeat 3–4 considering an antireflection coating made of magnesium fluoride ($n_L = 1.38$), which is a frequently-used low-index film. Also, calculate the optical reflectance R, both numerically and using Eq. (1.3.3).

1.3.2 Optical tunneling in ultrathin metal films

It is known that thin films of noble metals have a maximum optical transmittance in the shorter part of spectrum. This can be in practice used to observe the *optical tunneling effect* under normal incidence. It occurs setting in $0 < z < L$ a layer of index of refraction $n(z) = n_L$, provided that $\mathrm{Re}(n_L^2) < 0$ and $k_0 L \ll 1$. In all cases, transmittance of thin metal films decreases with increasing film thickness L.

For numerical purposes, consider a silver layer of index of refraction $n_L = 0.055 + i4.0$ at $\lambda_0 = 600$ nm, deposited on a glass substrate of index $n_2 = 1.5$ and immersed in air ($n_1 = 1$). Again, set the amplitude $E_0 = 1$ V/m, and the input and output ports are located at $z_2 = -z_1 = 2\lambda_0$.

1. Find numerically the solution to the Helmholtz equation (1.3.1) within the whole interval $z_1 \le z \le z_2$, providing the z dependence of the electric field, $E(z)$. Consider a metal layer of thickness $L = 20$ nm. Apply the Robin boundary condition (1.1.5) at the input port, and the radiation condition (1.1.6) at the output port.

2. Plot the real and imaginary part of the wave function $E(z)$ (or $u(x)$, see 2) which was found previously. Also plot $|E(z)|$ within the region of computation. In addition, calculate the optical reflectance R, transmittance T, and absorbance A, both numerically and using Eq. (1.3.3).

3. Repeat 1–2 for a silver layer of thickness: (a) $L = 50$ nm, (b) $L = 100$ nm, (c) $L = 200$ nm, and (d) $L = \lambda_0$.
   Hint: higher accuracy and precision goals may give a different result for long lengths L, and increasing the goals extends the correct solution further; thus include the following options in `NDSolve[]`: `AccuracyGoal -> 20`, `PrecisionGoal -> 20`, `WorkingPrecision -> 35`.

4. Plot R, T, and A as a function of L, derived from Eq. (1.3.3).

1.4 Diffraction

Introductory notes: diffraction in the paraxial regime

Electromagnetic fields in an isotropic homogeneous medium of index of refraction $n > 0$ are governed in general by the scalar Helmholtz equation $(\nabla^2 + k^2)E(x, y, z) = 0$, where $E(x, y, z)$ is the analytic representation of a (scalar) field distribution that is harmonic in time as $\exp(-i\omega t)$, and $k = n\omega/c \equiv 2\pi/\lambda$.

In the paraxial regime around the z axis, it is convenient to extract the primary $\exp(ikz)$ propagation factor out of E, by writing $E(x, y, z) \equiv u(x, y, z)\exp(ikz)$. The slowly varying dependence of $u(x, y, z)$ on z, considered under the so-called *slowly varying envelope approximation*, can be expressed mathematically by the paraxial Helmholtz equation [3, chapter 16],

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + i2k\frac{\partial u}{\partial z} = 0, \tag{1.4.1}$$

which is valid provided that $|\partial_z^2 u| \ll |2k\partial_z u|$.

A solution to Eq. (1.4.1) can be set by means of Huygens' integral equation in the Fresnel approximation,

$$u(x, y, z) = \frac{1}{i\lambda z}\iint_{-\infty}^{+\infty} u_0(x_0, y_0)\exp\left\{\frac{ik}{2z}\left[(x - x_0)^2 + (y - y_0)^2\right]\right\}\mathrm{d}x_0\mathrm{d}y_0, \tag{1.4.2}$$

where $u_0(x, y) = u(x, y, 0)$ represents the wave field u evaluated at the reference plane $z = 0$. Equation (1.4.2) is also known as the *Huygens-Fresnel diffraction integral*, and is useful for the evaluation of diffracted fields by an aperture placed at $z = 0$. If the aperture has an amplitude transmittance $t(x, y)$ and is illuminated by a normally-incident plane wave of amplitude E_0 at $z = 0$, one can set $u_0(x, y) = E_0 t(x, y)$ when applying the *Kirchhoff boundary conditions*.

Note that Huygens-Fresnel diffraction integral given in (1.4.2) can be set as a 2-D convolution, $u(x, y, z) = (u_0 \circledast h_z)(x, y)$, where the impulse response $h_z(x, y) = h_z(x)h_z(y)$ and

$$h_z(x) = (i\lambda z)^{-1/2}\exp\left[ikx^2/(2z)\right].$$

As a consequence, one can use the properties of the Fourier transform, taking into account that $\mathcal{F}(h_z)(q_x, q_y) = H_z(q_x, q_y) = H_z(q_x)H_z(q_y)$, where $H_z(q_x) = (2\pi)^{-1/2}\exp\left[-izq_x^2/(2k)\right]$ (see 1.1.3).

Assuming that the wave function u_0 is invariant under translations along the y axis leading to $u_0(x, y) \equiv u_0(x)$, as we will do from here on, the diffracted fields in a plane $z \neq 0$ are also invariant under translations along the y axis, and therefore we may write $u(x, y, z) \equiv u(x, z)$. In this case, the paraxial Helmholtz equation (1.4.1) yields $(\partial_x^2 + i2k\partial_z)u(x, z) = 0$. Furthermore, Huygens' diffraction integral (1.4.2) is reduced to $u(x, z) = (u_0 \circledast h_z)(x)$. As mentioned before, the properties of the Fourier transform allow us to evaluate the diffracted wave fields as

$$u(x, z) = \mathcal{F}\left\{U_0(q_x)\exp\left[-izq_x^2/(2k)\right]\right\}(-x), \tag{1.4.3}$$

where $U_0(q_x) = \mathcal{F}(u_0)(q_x)$. This method is efficient when applied sufficiently near the reference plane, that is, for the evaluation of the so-called *near field* within $0 \leq z \leq z_1$, where $z_1 = 2k/q_{\max}^2$ provided that $|U_0(q_x)|$ reaches significant values in the spectral band $|q_x| \leq q_{\max}$.

On another note, using the definition of the Fourier transform given in Eq. (1.1.9), Huygens' diffraction integral can also be set as

$$u(x, z) = \sqrt{2\pi}h_z(x)F_z(q_x), \tag{1.4.4}$$

where $F_z(q_x) = \mathcal{F}(f_z)(q_x)$ is the 1-D Fourier transform of the wave function

$$f_z(x) = u_0(x)\exp[ikx^2/(2z)],$$

provided that the spatial frequency $q_x = -kx/z$. This method is efficient when applied sufficiently far from the reference plane, $z \geq z_2$, with $z_2 = kx_{\max}^2/2$ provided that $|u_0(x)|$ reaches significant values in the range $|x| \leq x_{\max}$. In the *far field* ($z \gg z_2$) one can observe the *Fraunhofer diffraction pattern*, which is evaluated by using the approximation $f_z(x) \to u_0(x)$.

Typically, one may find that $q_{\max}$ is of the order of $2/x_{\max}$, yielding $z_1 \approx z_2$ that is a distance sometimes called *Rayleigh range*. In this context, diffraction equations can be conveniently rewritten in terms of normalized spatial coordinates $\xi = x/x_{\max}$ and $\zeta = z/z_R$, where $z_R = kx_{\max}^2/2$ is the Rayleigh range. For instance, the 1-D paraxial wave equation yields

$$\left(\partial_\xi^2 + 4i\partial_\zeta\right)\tilde{u}(\xi,\zeta) = 0, \tag{1.4.5}$$

where $u(x,z) = E_0\tilde{u}(\xi,\zeta)$. Similarly, equation (1.4.3) becomes

$$\tilde{u}(\xi,\zeta) = \mathcal{F}\{\tilde{U}(q_\xi,0)\exp(-i\zeta q_\xi^2/4)\}(-\xi), \tag{1.4.6}$$

where $q_\xi = x_{\max}q_x$. Finally, equation (1.4.4) becomes

$$\tilde{u}(\xi,\zeta) = (i\zeta/2)^{-1/2}\exp(i\xi^2/\zeta)\mathcal{F}(\tilde{f}_\zeta)(q_\xi), \quad \text{with} \quad \tilde{f}_\zeta(\xi) = \tilde{u}(\xi,0)\exp(i\xi^2/\zeta), \tag{1.4.7}$$

and $q_\xi = -2\xi/\zeta$.

1.4.1 Diffraction gratings: Talbot effect

Consider a 1-D diffraction grating characterized by an amplitude transmittance $t(x)$, which is illuminated by a normally-incident plane wave of amplitude E_0 at $z = 0$. The transmittance function has a period Δx, i.e. $t(x + \Delta x) = t(x)$, and can be set in Fourier series expansion [see Eq. (1.1.10)], where c_s is the Fourier coefficient of its s-th harmonic. Typically, the fundamental spatial frequency $\Delta q_x = 2\pi/\Delta x$ of a diffraction grating is conveniently given in lines per centimeter.

1. Show that the field $u(x,z)$, evaluated by means of Eqs. (1.4.3) and (1.1.11), can be set as

   $$u(x,z) = E_0\sum_{s=-\infty}^{+\infty} c_s\exp\left[-i2\pi s(x/\Delta x)\right]\exp\left[-i2\pi s^2(z/z_T)\right], \tag{1.4.8}$$

   where $z_T = 2(\Delta x)^2/\lambda$ is the *Talbot length*. In addition:

   - Show that $u(x,z_T) = u(x,0) = E_0t(x)$. Therefore, the wave field of a light diffracting through a grating is periodically reproduced, with a period given by the Talbot length.[3]
   - Show that $u(x,z_T/2) = E_0t(x+\Delta x/2)$. At half the Talbot length, a self-image also occurs, but laterally shifted by half the width of the grating period.

2. Calculate the Fourier coefficients c_s of the transmittance function $t(x)$ given in $|x| < \Delta/2$, characterizing the following 1-D diffraction gratings of period Δx:

   - The *square-wave amplitude grating* composed of evenly spaced parallel slits, giving $t(x) = \mathrm{rect}(x/w)$, where $w \leq \Delta x$ is the slit width.

[3] https://en.wikipedia.org/wiki/Talbot_effect

- The *sinusoidal phase grating* with $t(x) = \exp[i\varphi_0 \sin(\Delta q_x x)]$, where φ_0 represents the peak excursion of the sinusoidal phase variation.
- The *square-wave phase grating* with transmittance function $t(x) = 1-[1-\exp(i\varphi_0)]\,\mathrm{rect}(x/w)$.
- The *blazed grating* with 'saw tooth' phase profile, giving $t(x) = \exp(i\varphi_0 x/\Delta x)$.

Hint: When analytical expressions of c_s cannot be found, use the DFT to find them numerically, namely $\tilde{c}_s$, as analyzed in 5.

3. Plot the normalized diffraction pattern $|u(x, z)|^2$ of the transmission gratings analyzed above, using Eq. (1.4.8) within the range $|x| \leq \Delta x/2$ and $0 \leq z \leq z_T$. For numerical purposes, use: (1) $E_0 = 1$, (2) $w = \Delta/2$, (3) $\varphi_0 = 1.84$ rads for the sinusoidal phase grating, $\varphi_0 = \pi$ for the square-wave phase grating, and $\varphi_0 = \{\pm\pi, \pm 2\pi\}$ for the blazed grating. Also plot the field $\mathrm{Re}[u(x, z)]$ for phase gratings. Take an even number N of Fourier harmonics, ranging from the $(-N/2)$-th to the $(+N/2 - 1)$-th order, and show that accuracy of the estimated wave fields increases as long as the parameter

$$\eta = \frac{\sum_{s=-N/2}^{+N/2-1} |c_s|^2}{\frac{1}{\Delta x}\int_{-\Delta x/2}^{\Delta x/2} |t(x)|^2 dx} \tag{1.4.9}$$

approaches to unity, as inferred from Parseval's theorem (1.1.12).
Hint: use normalized spatial coordinates $\xi = x/\Delta x$ and $\zeta = z/z_T$. Note that using $N > 32$ in the proposed method may result in a time-comsuming computation.

1.4.2 Diffraction by a slit

Consider a slit characterized by a transmittance function $t(x) = \mathrm{rect}(x/w)$, where w is the slit width. Consider a monochromatic plane wave propagating in free space, which electric field $\vec{E}(z, t) = \hat{x}E_0 \exp(ikz - i\omega t)$, where the wavenumber $k = 2\pi/\lambda$ and E_0 denotes a field amplitude. By setting the slit at $z = 0$, the diffracted field within the paraxial approximation $u(x, z) = E_0\tilde{u}(\xi, \zeta)$, where [3, chapter 18]

$$\tilde{u}(\xi, \zeta) = \frac{1}{2}\left[\mathrm{erf}\left(\frac{\xi + \frac{1}{2}}{\sqrt{i\zeta}}\right) - \mathrm{erf}\left(\frac{\xi - \frac{1}{2}}{\sqrt{i\zeta}}\right)\right], \quad \zeta > 0. \tag{1.4.10}$$

Here, $\xi = x/w$ and $\zeta = z/z_R$ are normalized spatial coordinates, $z_R = kw^2/2$ is the *Rayleigh range*, and $\mathrm{erf}(\tau) = 2\pi^{-1/2}\int_0^\tau \exp(-t^2)\mathrm{d}t$ is the error function.

1. Show the validity of Eq. (1.4.10) by means of Eq. (1.4.6).
Hint: use $\tilde{u}(\xi, 0) = \mathrm{rect}(\xi)$ and $\tilde{U}(q_\xi, 0) = (2\pi)^{-1/2}\,\mathrm{sinc}(q_\xi/2)$.

2. Plot the normalized intensity patterns $|\tilde{u}(\xi, \zeta)|^2$ at planes $\zeta = 1/(4\pi N_F)$ within the range $|\xi| \leq 1$, where the *Fresnel number* (a) $N_F = 2$, (b) $N_F = 5$, (c) $N_F = 10$, and (d) $N_F = 20$. Inspection will show that the diffraction patterns have essentially N_F large-scale ripples across the aperture width. Compare the intensity patterns obtained above with that observed at the slit plane $\zeta = 0$.

3. Repeat 2 by evaluating the DFT of $\tilde{U}(q_\xi, 0)\exp(-i\zeta q_\xi^2/4)$ in Eq. (1.4.6). Use $N = 2^5$ points, and analyze the accuracy of these results.
Hint: use a sampling rate $\Delta q_\xi = \pi$ in order to obtain a DFT in the range $|\xi| \leq 1$.

4. Show that the Fraunhofer diffraction pattern of a slit can be set as:

$$\tilde{u}_F(\xi,\zeta) = \frac{\exp(i\xi^2/\zeta)}{\sqrt{i\pi\zeta}}\,\mathrm{sinc}(\xi/\zeta), \quad \zeta \gg 1. \tag{1.4.11}$$

   Hint: use Eq. (1.4.7) with $\tilde{f}_\zeta(\xi) = \mathrm{rect}(\xi)$. Alternatively you may use the asymptotic expansion $\mathrm{erf}(t) = (2t/\sqrt{\pi})\exp(-t^2)$, as $t \to 0$, in Eq. (1.4.10).

5. Plot the normalized intensity patterns $|\tilde{u}(\xi,\zeta)|^2$, given in Eq. (1.4.10), at planes $\zeta = 1/(4\pi N_F)$ within the range $|\xi| \leq \max(1, 2\pi\zeta)$, where (a) $N_F = 1/20$, (b) $N_F = 1/10$, (c) $N_F = 1/5$, and (d) $N_F = 1/2$. Compare the intensity patterns evaluated above with $|\tilde{u}_F(\xi,\zeta)|^2$ obtained in the far field (1.4.11).

References

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[3] A. E. Siegman, *Lasers.* Mill Valley: University Science Books, 1986.