Exact solution for square-wave grating covered with graphene: surface plasmon-polaritons in the terahertz range

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Abstract
We provide an analytical solution to the problem of scattering of electromagnetic radiation by a square-wave grating with a flat graphene sheet on top. We show that for deep grooves there is a strong plasmonic response, with light absorption in the graphene sheet reaching more than 45% due to the excitation of surface plasmon-polaritons. The case of a grating with a graphene sheet presenting an induced periodic modulation of the conductivity is also discussed.

1. Introduction
Plasmonic effects in graphene are currently an active research topic. The strong plasmonic response of graphene at room temperature is tied to its optical response, which can be controlled externally in different ways. The unique features of the optical conductivity of single-layer graphene stem from the Dirac-like nature of quasi-particles [1–3], and have been extensively studied in the past few years, both theoretically [4–11, 1, 2, 12–16] and experimentally [17–24], including in the terahertz (THz) spectral range [25–28].

Indeed, graphene holds many promises for cutting edge THz applications [29], which would be able to fill the so-called THz gap. More recently, the interest has been focused on how graphene interacts with electromagnetic radiation in the THz region [30–36]. One of the goals is to enhance the absorption of graphene for the development of more efficient photodetectors in that spectral region. This can be done in several different ways: by (i) producing micro-disks of graphene on a layered structure [30]; (ii) exploiting the physics of quantum dots and metallic arrays on graphene [37, 32]; (iii) using a graphene-based grating [38–44]; (iv) putting graphene inside an optical cavity [45, 46]; and (v) depositing graphene on a photonic crystal [15]. In cases (i)–(iii), the excitation of plasmons [47–50] is responsible for the enhancement of the absorption. In case (iv), photons undergo many round-trips inside the cavity, enhancing the chances of being absorbed by graphene. In case (v), the authors consider a photonic crystal made of SiO₂/Si. In the visible range of the spectrum, the dielectric constants of SiO₂ and Si differ by more than one order of magnitude and by choosing the width of the SiO₂/Si appropriately it is possible to induce a large photonic band gap in the visible range. By combining the presence of the band gap with an initial spacer layer the absorption can be enhanced by a factor of four. In the case studied in [15], the optical conductivity of graphene is controlled by interband transitions. Although that work [15] focused on the visible spectrum, there is a priori no reason why the same principle cannot be extended to the THz region.

The physics of surface plasmon-polaritons in graphene has also been explored for the development of devices for optoelectronic applications [51–53]. Such devices include optical switches [54] and polarizers [55]. It has been shown that metallic single-wall carbon nanotubes, which have a linear spectrum close to zero energy, can act as polarizers as well [27]. Theoretical studies of the optical response
that Maxwell’s equations can be put in a form equivalent to solids and for which an exact solution exists. We will show of the Kronig–Penney model appearing in the band theory of Fortunately, the geometry of the problem is equivalent to that the exact eigenfunctions in the region of the grooves [66].

In general, the conductivity of graphene is a sum of two contributions: (i) a Drude-type term, describing intraband processes and (ii) a term describing interband transitions. At zero temperature the optical conductivity has a simple analytical expression [4, 5, 62, 1, 2, 8]. In what concerns our study, the physics of the system is dominated by the intraband contribution [63], which reads

\[
\sigma_D = \sigma_0 \frac{4E_F}{\pi \hbar \Gamma - i \hbar \omega}, \tag{1}
\]

where \(\sigma_0 = \frac{\pi e^2}{2(2h)}\), \(\Gamma\) is the relaxation rate, \(E_F > 0\) is the Fermi level position with respect to the Dirac point, and \(\omega\) is the radiation frequency. It should be noted that \(\sigma_D\) has a strong frequency dependence and is responsible for the optical behavior of graphene in the THz spectral range.

The problem we consider in this work is the scattering of electromagnetic radiation by graphene deposited on a grating with a square-wave profile, as illustrated in figure 1. We further assume that the radiation is p-polarized (TM wave), that is, we take \(\mathbf{B} = (0, B_z, 0)\) and \(\mathbf{E} = (E_x, 0, E_z)\). The square-wave profile is rather pathologic due to the infinite derivative at the edges of the steps, therefore the usual methods fail [64, 65, 40, 42]. An alternative route is to obtain the exact eigenfunctions in the region of the grooves [66]. Fortunately, the geometry of the problem is equivalent to that of the Kronig–Penney model appearing in the band theory of solids and for which an exact solution exists. We will show that Maxwell’s equations can be put in a form equivalent to the Schrödinger equation for the Kronig–Penney model, and hence an exact solution for the fields in the region of the grooves is possible.

In this work we assume that graphene is doped. In a practical implementation, this can be achieved via gating or by chemical means [67, 68]. Note that in a bottom gate structure the conductivity of graphene becomes position dependent along the x-direction [40]. In this case, the analysis presented below is incomplete (see, however, section 6, where a simplified model is analyzed). Nevertheless, the results of [40] show that a position-dependent conductivity alone already induces surface plasmon-polaritons on graphene. Therefore, a spatially modulated optical response, when combined with a grating, will enhance the excitation of surface plasmon-polaritons, as confirmed by the analysis given in section 6. For the top gate configuration and for chemical doping, the problem of a spatially dependent conductivity does not arise [69].

It can be argued that in the geometry we are considering (see figure 1) the portion of graphene over the grooves will be strained. Clearly, experimental setups can be designed so as to overcome (at least partially) such effects, e.g., by filling the grooves with a different dielectric and using a top gate or a chemically doped graphene. However, in the bottom gate configuration, even with filled grooves, graphene will have a position-dependent conductivity. A complete description should thus include all contributions: the grating effect itself, inhomogeneous doping, and the strain fields in graphene. In this work we assume that the graphene sheet remains flat. First, the optical conductivity will be taken as homogeneous in order to study solely the effect of a dielectric grating in the presence of uniform graphene. The additional effect of periodic modulation of the graphene conductivity, with the same period as the grating, will be considered in section 6. We believe that our calculations are accurate for the cases of either electrostatic doping by a top gate [69], or doping by chemical means [67, 68].

2. Exact eigenmodes in the grating region

For TM polarized light with angular frequency \(\omega\) (see figure 1) the Helmholtz equation assumes the simple form

\[
(\Delta || + \mu_0 \varepsilon_0 \omega^2) B_\gamma(x, z) = 0, \tag{2}
\]

where \(\mu_0\) is the vacuum permeability and \(\Delta || = \partial_x^2 + \partial_z^2\). Since the boundary between the vacuum and the dielectric is piecewise, the Helmholtz equation holds true in the regions of width \(rd\) and \((1 - r)d\) with the appropriate change of the dielectric constant, \(\varepsilon\) in the former and \(\varepsilon_0\) in the latter. For \(z > h\) the dielectric constant is homogeneous and equal to \(\varepsilon_0\), whereas for \(z < 0\) it is \(\varepsilon = \varepsilon_0 \varepsilon_r\), and \(\varepsilon_r\) is the relative permittivity.

We search for solutions of equation (2) in the form

\[
B_\gamma = B_\gamma(x, z) = X(x)e^{\pm i \Lambda z}, \tag{3}
\]

where \(\Lambda\) is a constant. With this ansatz, the Helmholtz equation reduces to

\[
\partial_x^2 X(x) = (\Lambda^2 - \mu_0 \varepsilon_0 \omega^2) X(x), \tag{4}
\]

whose solution is

\[
X(x) = A_0 e^{ik_x x} + B_0 e^{-ik_x x}, \tag{5}
\]

and where \(k_j^2\) is given by

\[
k_j^2 = \mu_0 \varepsilon_0 \omega^2 - \Lambda^2, \tag{6}
\]

with the subscript \(j = 1\) \([j = 2]\) referring to the region \((1 - r)d\) \([rd]\). Putting all the pieces together, the field component
follows

It is convenient to write these two equations in matrix form as

\[
\begin{bmatrix}
A_1 & B_1 \\
A_2 & B_2
\end{bmatrix}
\begin{bmatrix}
k_1 \\
k_2
\end{bmatrix}
= \begin{bmatrix}
e_1 e_{\theta r} \\
e_2 e_{\theta r}
\end{bmatrix}
\]

where \(e_1 = \cos \theta\) and \(e_2 = \sin \theta\).

Figure 2. Effective stratified medium along the x-direction in the region \(0 < z < h\).

The determination of \(\Lambda\) in equation (7) leads to an eigenvalue problem that will be considered in section 3. We note that \(\Lambda\) can be either real or pure imaginary: real values correspond to propagating diffracted orders, whereas imaginary ones correspond to evanescent waves. From Maxwell’s equations it follows that the electric field components in the region \(0 < z < h\) read:

\[
E_x^{(i)} = \frac{\pm \Lambda}{\mu_0 \epsilon_0} [A_1 e^{ik y} + B_1 e^{-ik y}] e^{\pm i \Lambda z},
\]

(8)

\[
E_x^{(f)} = \frac{-k_i}{\mu_0 \epsilon_0} [A_1 e^{ik y} - B_1 e^{-ik y}] e^{\pm i \Lambda z}.
\]

(9)

As shown in what follows, there is a relation between the coefficients \(A_j\) and \(B_j\), which is obtained from the solution of the eigenvalue problem.

3. Transfer matrix and the eigenvalue equation

Along the x-direction, and for \(0 < z < h\), we have a stratified medium with alternating dielectric constants. Then we can relate the amplitudes \(A_j\) and \(B_j\) with \(A_{j+1}\) and \(B_{j+1}\) using the boundary conditions at the interfaces of the two dielectrics. Furthermore, using the Bloch theorem we can find an eigenvalue equation for the parameter \(\Lambda\). The amplitudes in the different regions of the stratified medium are represented in figure 2. The continuity of the z-component of the electric field at the boundary \(x = r d\) imposes a relation between the amplitudes \(A\) and \(B\) in regions \(j = 2, 3\) (refer to figure 2 for the definition of the different regions), i.e.,

\[
k_2 \frac{A_2 e^{ik y} - B_2 e^{-ik y}}{\epsilon_r} = k_1 [A_3 e^{ik y} - B_3 e^{-ik y}].
\]

(10)

Note that according to the definition in equation (6), we must have \(k_3 = k_1\) and \(k_4 = k_2\). At the same boundary, the continuity of the magnetic field yields

\[
A_2 e^{ik y} + B_2 e^{-ik y} = A_3 e^{ik y} + B_3 e^{-ik y}.
\]

(11)

It is convenient to write these two equations in matrix form as follows

\[
\begin{bmatrix}
A_2 \\
B_2
\end{bmatrix}
= \Phi(k_2 r d)\begin{bmatrix}
A_3 \\
B_3
\end{bmatrix},
\]

(12)

where

\[
\Phi(x) = \begin{bmatrix}
e^{-i x} & 0 \\
0 & e^{i x}
\end{bmatrix}.
\]

(13)

Combining equations (12) and (18), we arrive at the following result

\[
T = \Phi(k_2 r d)\begin{bmatrix}
A_4 \\
B_4
\end{bmatrix} = \begin{bmatrix}
A_2 \\
B_2
\end{bmatrix}.
\]

(19)

where a global phase was absorbed in the coefficients \(A_4\) and \(B_4\). The transfer matrix,

\[
T = \Phi(k_2 r d)\begin{bmatrix}
A_4 \\
B_4
\end{bmatrix} = \begin{bmatrix}
A_2 \\
B_2
\end{bmatrix}.
\]

(20)

Combining equations (10) and (17), we arrive at the following constraints

\[
k_1 [A_3 e^{ik y} - B_3 e^{-ik y}] = \frac{k_2}{\epsilon_r} [A_4 e^{ik y} - B_4 e^{-ik y}].
\]

(16)

\[
A_3 e^{ik y} + B_3 e^{-ik y} = A_4 e^{ik y} + B_4 e^{-ik y}.
\]

(17)

Similar continuity conditions apply to the boundary at \(x = d\), resulting in the following constraints

\[
k_1 [A_3 e^{ik y} - B_3 e^{-ik y}] = \frac{k_2}{\epsilon_r} [A_4 e^{ik y} - B_4 e^{-ik y}].
\]

(16)

\[
A_3 e^{ik y} + B_3 e^{-ik y} = A_4 e^{ik y} + B_4 e^{-ik y}.
\]

(17)

As before, these equations can be written in matrix form as

\[
\begin{bmatrix}
A_2 \\
B_2
\end{bmatrix} = \Phi(k_2 r d)\begin{bmatrix}
A_4 \\
B_4
\end{bmatrix}.
\]

(19)

where a global phase was absorbed in the coefficients \(A_4\) and \(B_4\). The transfer matrix,

\[
T = \Phi(k_2 r d)\begin{bmatrix}
A_4 \\
B_4
\end{bmatrix} = \begin{bmatrix}
A_2 \\
B_2
\end{bmatrix}.
\]

(20)

Combining equations (12) and (18), we arrive at the following result

\[
\begin{bmatrix}
A_3 \\
B_3
\end{bmatrix} = \Phi(k_2 r d)\begin{bmatrix}
A_4 \\
B_4
\end{bmatrix} = \begin{bmatrix}
A_2 \\
B_2
\end{bmatrix}.
\]

(20)

(Note that \(\det(T) = 1\). On the other hand, by virtue of the Bloch theorem we have:

\[
\begin{bmatrix}
A_4 \\
B_4
\end{bmatrix} = e^{ik_0 d \sin \theta} \begin{bmatrix}
A_2 \\
B_2
\end{bmatrix},
\]

(22)

where \(k_0 \sin \theta\) is the x-component of the wavevector of the incoming electromagnetic radiation (figure 1). We thus arrive at the important intermediate result

\[
e^{ik_0 d \sin \theta} \begin{bmatrix}
A_2 \\
B_2
\end{bmatrix} = T \begin{bmatrix}
A_2 \\
B_2
\end{bmatrix}.
\]

(23)

The compatibility condition of equation (23) provides the eigenvalue equation

\[
2 \cos(k_0 d \sin \theta) = \text{Tr}(T),
\]

(24)

or explicitly,

\[
2 \cos(k_0 d \sin \theta) = 2 \cos(k_1 d(1 - r)) \cos(k_2 dr)
\]

(25)

Equation (25) allows the determination of the permitted values of \(\Lambda^2\) and is very similar to the eigenvalue equation of the Kronig–Penney model of electron bands.
The relation (12) allows us to express the coefficients $A_3$ and $B_3$ in terms of $A_2$ and $B_2$. Thus, the function $X(x)$ over the whole unit cell can be written in terms of $A_2$ and $B_2$ only. Furthermore, equation (23) gives a relation between the coefficient $A_2$ and $B_2$, 

$$B_2 = -\frac{T_{12}}{T_{11}} + \frac{e^{id\sin\theta}}{T_{12}} A_2,$$  

(26)

where $T_{12}$ and $T_{22}$ are two matrix elements of the transfer matrix $T$. Therefore, the function $X(x)$ over the unit cell is proportional to the only coefficient, $A_2$. Note that the matrix elements contain $\Lambda^2$, therefore we shall label the possible functions $X(x)$ by index $\ell$ running over all possible eigenvalues ($\pm \Lambda_\ell$). The function $X_\ell(x)$ in a unit cell has the form

$$X_\ell(x) = \begin{cases} A_2 e^{ik_1 x} + B_2 e^{-ik_1 x}, & 0 < x < rd, \\ A_3 e^{ik_1 x} + B_3 e^{-ik_1 x}, & rd < x < d. \end{cases}$$  

(27)

Equation (12) can be written explicitly as

$$A_3 = aA_2 + bB_2, \quad B_3 = cA_2 + fB_2,$$

where

$$a = \frac{1}{2k_1 \epsilon_x} e^{-ik_1 h},$$

$$f = \frac{1}{2k_1 \epsilon_x} e^{ik_1 h},$$

$$b = \frac{1}{2k_1 \epsilon_x} e^{-ik_1 h},$$

$$c = \frac{1}{2k_1 \epsilon_x} e^{ik_1 h}.$$

Since the wavenumbers $k_1$ can be complex, $f$ is not necessarily the complex conjugate of $a$; the same applies to $b$ and $c$. In terms of these coefficients, $X_\ell(x)$ reads:

$$X_\ell(x) = \begin{cases} A_2 e^{ik_1 x} + B_2 e^{-ik_1 x}, & 0 < x < rd, \\ (aA_2 + bB_2) e^{ik_1 x} + (cA_2 + fB_2) e^{-ik_1 x}, & rd < x < d. \end{cases}$$  

(28)

We also note that equation (26) allows us to replace $B_2$ in equation (28). Finally, the magnetic field in the region $0 < z < h$ (hereafter denoted as region II) has the form

$$B^{\text{II}}_x = \sum_\ell X_\ell(x)(C_\ell e^{i\Lambda_\ell z} + D_\ell e^{-i\Lambda_\ell z}),$$  

(29)

where the summation is over all the eigenvalues determined from the solution of equation (25) and $C_\ell$ and $D_\ell$ are some coefficients that will be determined in section 4. With this we conclude the exact solution for the eigenmodes in the grating region.

4. Solution of the scattering problem

We now derive the equations for the scattering problem represented in figure 1. For $z > h$ (region I) the magnetic field is written as

$$B^{\text{I}}_x = e^{i(\alpha x - \beta^{(1)}_n z)} + \sum_{n=-\infty}^{\infty} Re e^{i(\alpha x + \beta^{(1)}_n z)},$$  

(30)

and for $z < 0$ (region III) we have

$$B^{\text{III}}_x = \sum_{n=-\infty}^{\infty} T_n e^{i(\alpha x - \beta^{(2)}_n z)},$$  

(31)

where

$$\alpha_n = k_0 \sin\theta_i - 2\pi n / d,$$  

(32)

$$\beta^{(2)}_n = \sqrt{q^2 - \alpha_n^2}; \quad q_p \geq \alpha_n,$$  

(33)

with $q_p = \sqrt{E_p^\omega/c}$ and the definition $q_1 = k_0$; $n$ is an integer, $n \in [-\infty, \infty]$. Since we have four sets of unknown amplitudes, $C_\ell$, $D_\ell$, $E_\ell$, and $T_n$, and four boundary conditions, two at $z = h$ and other two at $z = 0$, we have a linear system of equations that can be solved in closed form if truncated to some finite order, $N_\ell$, which is the number of the eigenvalues needed in equation (29) for an accurate description of $B^{\text{III}}_x$ (we typically used $N_\ell \sim 20$).

The boundary conditions at $z = 0$ are

$$F^{\text{III}}_x(x, z = 0) = F^{\text{II}}_x(x, z = 0),$$  

(34)

$$B^{\text{III}}_x(x, z = 0) = B^{\text{II}}_x(x, z = 0),$$  

(35)

whereas those at $z = h$ read

$$E^{\text{III}}_x(x, z = h) = E^{\text{II}}_x(x, z = h),$$  

(36)

$$B^{\text{III}}_x(x, z = h) = B^{\text{II}}_x(x, z = h),$$  

(37)

The latter represents the magnetic field discontinuity across the graphene sheet [54].

These boundary conditions are $x$ dependent. Since the system has period $d$, we can eliminate this dependence by multiplying the boundary conditions by $e^{-i\omega_0 x}$ and integrating over the unit cell. After some algebra, we arrive at

$$\sum_{\ell=1}^{N_\ell} (\ell^{(1)}_m C_\ell + \ell^{(2)}_m D_\ell) = 0,$$  

(38)

$$\sum_{\ell=1}^{N_\ell} (\ell^{(1)}_m C_\ell + \ell^{(2)}_m D_\ell) = 2e^{-i\theta_0 h} b_{m,0},$$  

(39)

where

$$\ell^{(1)}_m = \frac{\beta^{(2)}_m}{\epsilon} \chi_{\ell m} \mp \Omega_{\ell m} \Lambda_\ell,$$

$$\ell^{(2)}_m = \left( \chi_{\ell m} \mp \frac{\sigma_0}{\omega} \Omega_{\ell m} \Lambda_\ell \mp e_0 \Omega_{\ell m} \Lambda_\ell^{(1)} \right) \frac{\beta^{(1)}_m}{\beta^{(2)}_m},$$

with

$$\chi_{\ell m} = \int_0^d dx X_\ell(x) e^{-i\omega_0 x},$$  

(40)

$$\Omega_{\ell m} = \int_0^d dx \frac{X_\ell(x)}{\epsilon(x)} e^{-i\omega_0 x}.$$  

(41)

Here $\epsilon(x)$ is defined as $\epsilon [\epsilon_0]$ for $x = rd [d(1 - r)]$. Equations (38) and (39) form a linear system of equations for the amplitudes $C_\ell$ and $D_\ell$, from which the reflectance and
Figure 3. Absorbance (a), reflectance (b), and transmittance (c) at normal incidence. The parameters are $E_F = 0.2$ eV, $d = 10$ µm, $r = 0.25$, $\theta_i = 0$, $\epsilon_i = 4$ (corresponding to SiO$_2$), and $\Gamma = 1$ meV. The thin dashed line is the case $r = 1$. For reference, we note that 1 THz corresponds to an energy of 4.1 meV.

transmittance can be computed. Taking $N_r$ odd, the integer $m$ belongs to the interval $m \in \left(-(N_r - 1)/2, (N_r - 1)/2\right]$. The transmittance and the reflectance amplitudes are given by:

$$T_m = \sum_{\ell=1}^{N_r} \chi^{\ell}_{m}(C_{\ell} + D_{\ell}),$$

$$R_m = \delta_{0,m}e^{-2j_{0}h_{\ell}} + e^{-j_{0}h_{\ell}} \sum_{\ell=1}^{N_r} \epsilon_{0}\Omega_{\ell} m A_{\ell} \frac{\Lambda_{\ell}}{\beta_m} \times (C_{\ell}e^{i\Lambda_{\ell}h} - D_{\ell}e^{-i\Lambda_{\ell}h}).$$

Since $X_{\ell}(x)$ is a sum of exponentials, the functions $\chi_{\ell m}$ and $\Omega_{\ell m}$ can be determined in closed form, which saves computational power. Explicit equations for $\chi_{\ell m}$ and $\Omega_{\ell m}$ are given in the appendix A.

5. Results for homogeneous graphene

We now provide a number of results obtained from the solution of equations (38) and (39). In figure 3 we depict the absorbance (a), reflectance (b), and transmittance (c) at normal incidence. For the parameters considered only the specular order exists; all the other diffraction orders are evanescent. Then, the absorbance is defined as

$$A = 1 - |R_0|^2 = \frac{R_0(0)}{\epsilon_i |R_0(0)|} |T_0|^2.$$  

A resonance is clearly seen in the absorbance curves at a frequency of about 16 meV, corresponding to the excitation of a surface plasmon-polariton. The position of the resonance depends on several parameters, given in the caption of figure 3 and chosen as typical values appropriate for THz physics. The thin dashed curve corresponds to graphene on a homogeneous dielectric (no grating, $r = 1$). The effect of increasing the depth of the grooves, from $h = d/10$ up to $d$ is to produce an enhancement of the absorption, which for $h = d$ is almost of 25% (in this case we are considering $r = 0.25$).

The dispersion of a surface plasmon-polaritons in graphene, when the sheet is sandwiched between two semi-infinite dielectrics, is, in the electrostatic limit, given by

$$\bar{\hbar} = \sqrt{2} \frac{\alpha c}{\bar{\epsilon}} f E_F c \bar{h} q,$$

$$\bar{\epsilon} = \epsilon_0(1 + \epsilon_i)/2.$$ 

Taking $q = 2\pi/d$, the smallest lattice wavevector, equation (45) predicts, for the parameters used in our calculation, a plasmon-polariton energy of

$$\hbar \omega = 12.1 \text{ meV},$$

which is in the ballpark of the numeric result. We should however note that the position of the resonance depends also on the parameter $r$, which is not captured by the above formula for the dispersion. We can include the effect of the parameter $r$ using an interpolative formula. We define a new $\bar{\epsilon}$ as

$$\bar{\epsilon} = \frac{\epsilon_0}{2}(2 - r + \epsilon_i r).$$

Using this formula we obtain

$$\hbar \omega = 16.3 \text{ meV},$$

which we can include in the numeric result.
Figure 4. Absorbance (a), reflectance (b), and transmittance (c) at normal incidence. The parameters are \(E_F = 0.2 \text{ eV}, d = 10 \mu \text{m}, h = d, \theta_i = 0, \epsilon_r = 4, \) and \(\Gamma = 1 \text{ meV}.\) The thin dashed line is the case \(r = 1.\)

When dealing with plasmonic effects an important quantity is the enhancement of the electromagnetic field close to the interface of the metal (in this case graphene) and the dielectric (the square-wave grating). It is this enhancement of the electromagnetic field due to the excitation of surface plasmon-polaritons in the vicinity of a metallic interface that is at the heart of sensing devices. The spatial intensity of the diffracted electromagnetic field from graphene is depicted in figure 5. For the case off-resonance (figure 5(a)) the magnetic field has a relatively small amplitude and is almost homogeneous along the \(x\)-axis, while along the \(z\)-axis it exhibits a discontinuity at the plane \(z = 0\) occupied by the graphene layer, in accordance with the boundary conditions.

The situation changes dramatically when the incident wave frequency coincides with that of a surface plasmon-polariton resonance (figures 5(b)–(d)). In this case the amplitude of the electromagnetic field in the vicinity of the graphene layer drastically increases. The electromagnetic field amplitude is maximal when the surface plasmon-polariton resonance occurs for the first harmonic (figure 5(b)), that is for \(q = 2\pi/d,\) while it gradually decreases as the harmonic’s order increases (compare with figure 5(c) for the second and figure 5(d) for the third harmonics, respectively). These harmonics correspond to the intersections of the light line with the subsequent polaritonic bands (see figure B.1).

6. Modulated doping: a simple model

As discussed in section 1, doping graphene using a bottom gate when the material lies on a grating leads to a position-dependent conductivity, which is periodic along the \(x\)-direction. In this section we consider a simple model where, in addition to the grating itself, the conductivity is position

a much better approximation to the numerical value (15.9 meV). To obtain the exact frequency of the resonance we have to compute the plasmonic band structure due to the periodic dielectric, that is, the band structure of a polaritonic crystal [41]. In the appendix B we give the polaritonic band structure of graphene on a square-wave grating.

In figure 4 we depict the absorbance (a), reflectance (b), and transmittance (c), as function of frequency, for different values of \(r,\) from \(r = 0.1\) up to 0.6, and keeping \(d = h,\) that is the limit of deep grooves. As \(r\) increases the position of the resonance shifts to the left. This happens because the width of the dielectric underneath graphene is increasing with \(r.\) Then, according to equation (48), the effective dielectric constant of the system increases, following from equation (45) that the resonance shifts toward lower energies. In the case of \(r = 0.6\) two resonances are seen in the frequency window considered. They correspond to the excitation of surface plasmon-polaritons of wavenumbers \(2\pi/d\) and \(4\pi/d.\) Then, according to equation (45), the position of the second resonance should be \(\sqrt{2}\) times the first resonance frequency. From the figure, the energy of the first resonance is \(\hbar \omega = 13.6 \text{ meV},\) while that of the second one is \(\hbar \omega = 19.3 \text{ meV};\) now we note that \(\sqrt{2} \times 13.6 = 19.2 \text{ meV},\) in agreement with the numerical result. We also note that the absorption of graphene is largest when \(r = 0.5,\) the symmetric case \((1 - d = 0.5),\) reaching a value higher than 30%. Although we do not show it here, we have found that the absorption grows monotonically with increasing \(h\) and attains a maximum at a value larger than 45% for \(h = 2d.\)

Finally, we note that the reflectance curves have a Fano-type shape [41]. This is due to the coupling of the external radiation field with the excitation of Bragg modes of surface plasmon-polaritons in periodically modulated structures.
where conductivity is then expanded in a Fourier series as

\[ \sigma(x) = \sigma_D\left(1 - \kappa \sin \frac{2\pi x}{d}\right), \]

(50)

where \( \kappa \) is a parameter controlling the degree of inhomogeneity. We also take \( r = 0.5 \) in our figures. This particular choice of \( r \) and \( \sigma(x) \) makes the latter commensurate with the profile of the grating. From the point of view of the calculation we have to replace \( \sigma_D \) by \( \sigma(x) \) in the formulas given above. The conductivity is then expanded in a Fourier series as

\[ \sigma(x) = \sum_{p=-\infty}^{\infty} \sigma_p e^{i2\pi p x / d}, \]

(51)

where

\[ \sigma_p = \frac{1}{d} \int_0^d \! dx \sigma(x) e^{-i2\pi px / d}. \]

(52)

For the case of the profile defined in equation (50), the Fourier series reduces to three terms only, those referring to \( p = 0, \pm 1 \). A non-sinusoidal profile for \( \sigma(x) \) will have more harmonics than just these three. Therefore, our model can also be considered the first term in the Fourier expansion of a more complex profile for \( \sigma(x) \).

Relative to the previous case of homogeneous conductivity, what changes in the equations is the form of the function \( g^{(\pm)}_{lm} \), which now reads

\[ g^{(\pm)}_{lm} = \left(\chi_{lm} + \frac{\sigma_D}{\omega} h_{lm} \Lambda_{\ell} \mp \epsilon_0 \Omega_{lm} \frac{\Lambda_{\ell}}{\beta_{lm}}\right) e^{\pm i\Lambda_{\ell} h}, \]

(53)

where

\[ h_{lm} = \Omega_{lm} - \frac{\kappa}{2i} \Omega_{l m+1} + \frac{\kappa}{2i} \Omega_{l m-1}. \]

(54)

The results for the absorbance, reflectance, and transmittance are given in figure 6, considering the case where \( \kappa = 0.5 \), a fairly large value, corresponding to deep grooves. The dashed line is the case where graphene has an inhomogeneous conductivity on top of a homogeneous dielectric (i.e., no grating). (This situation is artificial and is only included for the sake of comparison.) Two resonant peaks can be seen, with the second peak being much smaller than the one at lower energies. The dashed–dotted line is the case where we have homogeneous graphene on the grating, and the solid line corresponds to the case where we have graphene with an inhomogeneous conductivity on the grating. The main effect is a shift of the position of the resonant peaks toward lower energies and an enhancement of the absorption, which has its origin in the combined effect of the grating and of the periodic modulation of the conductivity. In the absorbance panel the energy of the resonance labeled (2) is \( \sqrt{2} \) larger than that of the resonance (1). Thus, the first resonance corresponds to an excitation of a surface plasmon-polariton of wavenumber \( q = 2\pi / d \), whereas the second peak corresponds to the excitation of a surface plasmon-polariton of wavenumber \( q = 4\pi / d \). When we compare the dashed curve to the solid one we also note the prominence of the second plasmonic peak in the latter case, which is almost as intense as the low-energy one. This is a consequence of the square profile and the dielectric nature of the grating. In metallic gratings the permittivity has a strong frequency dependence favoring the occurrence of the most intense plasmonic resonances at lower energies [42].

7. Conclusions and future work

We have shown that a flat sheet of graphene on top of a square-wave grating exhibits strong plasmonic behavior. With the help of the grating one can create a surface plasmon-polariton resonance. The effect is more pronounced in the case of deep grooves, where absorbances higher than 45% are attainable. We note that the parameter \( d \) is easy to control experimentally, providing a convenient way of tuning the position of the plasmonic resonance. The reflectance curves show a Fano-type line shape, which manifests the coupling of the external electromagnetic field (with a continuum of modes) to the surface plasmons in graphene (occupying a relatively narrow spectral band). The calculations we have performed assume that graphene is homogeneously doped (excluding section 6), which is a crude approximation for the case of a bottom gate configuration of graphene doping. Therefore, our results are only directly applicable to the cases of either chemical doping or doping by a top gate. This type of gating is within the state-of-the-art [69]. In the particular case of bottom gate, we have to consider both the effect of inhomogeneous doping and the effect of strain (if the grooves are not filled with another dielectric). Both effects result in a position-dependent conductivity. Then, the calculation of the properties of surface plasmon-polaritons requires the evaluation of the doping profile and the strain field. Once these are determined, one can use a Fourier expansion of the graphene conductivity, as we have considered in our phenomenological model. As
these preliminary results show, the coupling of the external wave to the surface plasmon-polaritons can be significantly enhanced in the presence of both the dielectric grating and periodic modulation of the conductivity. Detailed calculations for realistic graphene conductivity profiles are the goal of a future work.

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Appendix A. Explicit form of $\chi_{lm}$

The calculation of the integral in equation (40) has to be divided into two pieces. The function $\chi_{lm}$ can be written as

$$\chi_{lm} = \chi_{lm}^{(1)} + \chi_{lm}^{(2)},$$

where

$$\chi_{lm}^{(1)} = -i \frac{A_2 a}{d(k_1 - \alpha_m)} (e^{i(k_1 - \alpha_m)d} - e^{i(k_1 - \alpha_m)rd})$$

$$+ i \frac{A_2 c}{d(k_1 + \alpha_m)} (e^{-i(k_1 + \alpha_m)d} - e^{-i(k_1 + \alpha_m)rd}),$$

and

$$\chi_{lm}^{(2)} = -i \frac{B_2 b}{d(k_1 - \alpha_m)} (e^{i(k_1 - \alpha_m)dr} - 1)$$

$$+ i \frac{B_2 f}{d(k_1 + \alpha_m)} (e^{-i(k_1 + \alpha_m)dr} - 1).$$

Since the square profile has a piecewise structure, the function $\Omega_{lm}$ is obtained directly from the function $\chi_{lm}$ as

$$\Omega_{lm} = \frac{\chi_{lm}^{(1)}}{\epsilon_0} + \frac{\chi_{lm}^{(2)}}{\epsilon_f \epsilon_0}.$$ 

Appendix B. Polaritonic spectrum

The polaritonic spectrum, $h\omega(q)$, of the surface plasmon-polaritons (SPP) in graphene on a square-wave grating is represented in figure B.1, where $q = k_0 \sin \theta_i$ is the Bloch wavenumber. Here, and in order to avoid the appearance of an imaginary part of the eigenvalues, corresponding to surface plasmon-polariton damping, we considered graphene without disorder ($\Gamma = 0$). As expected, the periodicity of the grating induces a band structure in the SPP spectrum of graphene, showing energy gaps. At the same time, for normal incidence ($q = 0$) the frequency of the second band ($h\omega \approx 15.85$ meV) almost coincides with the numerically obtained resonant frequency $h\omega \approx 15.9$ meV. A similar good
agreement happens for the frequency of the fifth band and that of the second resonance ($\hbar\omega_0 \approx 23.1$ meV and $\hbar\omega_0 \approx 23$ meV, respectively), as well as for frequency of the sixth band and that of the third resonance ($\hbar\omega_0 \approx 28.3$ meV and $\hbar\omega_0 \approx 28.4$ meV, respectively).

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