**NTNU** **Institutt for fysikk**

Contact during the exam:
Professor Ingve Simonsen
Telephone: 9 34 17 or 470 76 416

# Exam in TFY4235/FY8904 Computational Physics

May 08, 2017
09:00

Allowed help: Alternativ **A**

This problem set consists of 19 pages.

This exam is published on Monday, May 8 at 09:00 hours. You can work on your solution till **Thr. May 11, 2017 at 23:00** ("the deadline"). Before the deadline you should submit your final report in the pdf-format and a zip-file containing the documented source code via the system "Inspera". For the filenames please use `<lastname>_TFY4235_report.pdf` and `<lastname>_TFY4235_code.zip`; for those of you taking the course using the the FY8904 code, replace the TFY code by this code. Since "Inspera" also is new to me, a detailed account of how the submission shall be done, and potential updates, will be given on the course homepage no later than a day before the deadline However, my understanding is that you shortly after the exam has started will receive an email on how and where to submit your report and computer code. Prior to the deadline you are *also* expected[1], to send the final report to me at email `Ingve.Simonsen@ntnu.no` with subject TFY4235 of FY8904.[2]

There are no constraints on the aids you may want to use in connection with this exam, including discussing it with anybody. However, *the report and the computer code you will have to write yourself*. Please attach your computer codes as appendices to the report. Give as a footnote the names of your collaborators during the exam. The report may be written in either Norwegian (either variants) or in English.

Should you run short on time, you are advised to spend the time to do properly what you do instead of following a strategy of doing a little bit here-and-there.

Information posted during the exam, like potential misprints, links to papers, extended deadline etc. will be posted on the web-page of the course at `http://web.phys.ntnu.no/~ingves/Teaching/TFY4235/#Exam` and/or `http://web.phys.ntnu.no/~ingves/Teaching/TFY4235/Exam/`. *It is your responsibility to check this information regularly!*

[1] Useful in the unlikely event that something should go wrong with the digital submission via "Inspera" (or you cannot get it to work properly).

[2] Warning: If your email is too large, the gmail system, to which I also forward my email, may notify you that the message was too large to by delivered to my gmail account. This means that your message was received successfully by the ntnu email system, if you were not informed otherwise.

There are no formal requirements for the format of the report in addition to what was said above. The report should explain what you have been doing, your results, and how you interpret these results. Details should be included to the extent that we as graders can follow your way of reasoning. General background theory that, for instance, can be found i textbooks, is not needed in the report. It is documentation of your work we are interested in! Remember that if you have written an original and clever code for solving the problem, but are not able to explain it well in the report, it is hard to give you full credit.

I plan to have office hours from 13:00-16:00 on Monday May 08 in case you have questions to the problems.

Good luck to all of you!

# Problem 1

Your suggested solution for *Assignment no 3* [1] should be handed in as part of the report. It will count 15% towards the final grade of the course.

# Problem 2

This takehome exam is motivated from the quantum mechanical scattering of atoms from surfaces. Atom scattering at thermal energies is one of the most sensitive experimental techniques for obtaining detailed information about the structure of surfaces. This is partly due to the wavelength of such atoms beams, such as Helium beams, being comparable to the interparticle spacings in solids, and the energies are of the order of the maximum crystal phonon energies [13, Ch. 8]. Thus the scattering of such atoms is ideally suited for studies of both surface structure and surface vibrations.

In general, the scattering of an atom beam from a surface is a complex many-body quantum mechanical problem due to the interaction between the atoms in the beam and the particles that constitute the surface. At low energies, this problem is often simplified by describing the presence of the surface by an associated potential, so that the original scattering problem reduces to finding solutions of the Schrödinger equation. The detailed nature of the potential, and how it can be constructed, is a topic by itself that we here will not go into: see for instance Ref. [13] for details.

It should be noted that even in the case of *elastic scattering* from a rigid ordered surface, that is a pure single-body problem, the extended nature of the potential and the lack of symmetry means that the solution method will not always be simple. In the case of *inelastic scattering* from a vibrating surface, we are faced with a many-body problem which must be treated with a variety of approximation methods. Disorder on the surface can contribute both to the *elastic* and *inelastic* scattering. Such scattering manifest itself as a diffuse background intensity as well as by reducing the intensity of the diffraction peaks.

Below we will first start by presenting some useful background theory. Thereafter, the actual tasks that you are asked to solve in this takehome exam are outlined using the concepts and notation introduced in the theory section.

## 2.1 Motivation from quantum mechanics

The objective of the scattering calculation for the elastic problem is to solve the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{x})\right]\psi(\boldsymbol{x}) = E\psi(\boldsymbol{x}), \tag{1}$$

where $V(\boldsymbol{x})$ denotes the potential at spatial position $\boldsymbol{x}$, $E$ denotes the energy of the atoms, and $\psi(\boldsymbol{x})$ represents the wave function of the atoms (or particles) of mass $m$.

The scattering geometry that we will consider is depicted in Fig. 1. The surface is placed in the vicinity of the horizontal plane $x_3 = 0$ and we will denote the surface profile function by $\zeta(\boldsymbol{x}_\parallel)$ where $\boldsymbol{x}_\parallel = (x_1, x_2, 0)$. Initially, the surface profile function will not be required to have any particular form, i.e. it can be ordered, disordered of anything in between. Only

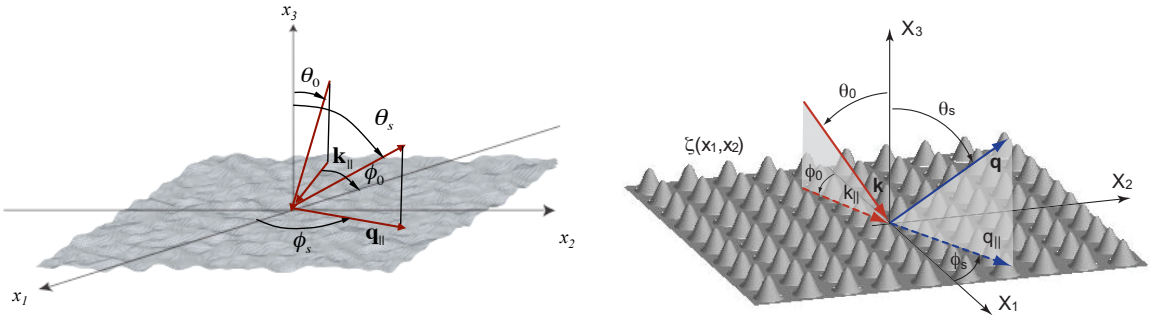


Figure 1: Schematics of the scattering geometry considered: (left) disordered and (right) periodic systems.

later will we specialize to the case for which the surface profile function is a periodic function (as illustrated in the right panel of Fig. 1).

For simplicity, it will be assumed that the medium below the surface is rigid, that is, it is a "hard wall", so that the quantum mechanical potential that appears in Eq. (1) reads

$$V(\boldsymbol{x}) = \begin{cases} 0 & x_3 > \zeta(\boldsymbol{x}_\parallel) \\ \infty & x_3 \leq \zeta(\boldsymbol{x}_\parallel) \end{cases}. \tag{2}$$

This has the consequence that the wave function will vanish when $x_3 \leq \zeta(\boldsymbol{x}_\parallel)$, so that, in particular, we at the surface have the *Dirichlet boundary condition*

$$\psi(\boldsymbol{x}|\omega)|_{x_3=\zeta(\boldsymbol{x}_\parallel)} = 0. \tag{3}$$

On the other hand, in the region far above the surface, $x_3 > \zeta(\boldsymbol{x}_\parallel)$, the wave function consists of a free incoming particle and a sum of scattered waves.

When the potential (2) is introduced into Eq. (1) one finds that in the region above the surface, the Schrödinger equation can be written in the form

$$\left[\nabla^2 + \frac{\omega^2}{c^2}\right] \psi(\boldsymbol{x}|\omega) = 0, \tag{4}$$

where we have defined

$$\frac{\omega^2}{c^2} = \frac{2mE}{\hbar^2}. \tag{5}$$

Equation (4) has the form of a *Helmholtz equation* where $\omega$ represents the anuglar frequency of the wave and $c$ its velocity. The Helmholtz equation is obtained by taking the Fourier transform over time of the scalar wave equation (or equivalently assuming a harmonic time dependence of the wave). The original quantum mechanical scattering problem is therefore equivalent to the scattering of classical scalar waves. Hence, if you feel more comfortable about thinking about the classical scattering problem, as we will do below, you are free to do so in the following.

## 2.2 Theory

In this section we outline some useful theoretical results. The discussion is somewhat detailed and the formulas may seem somewhat overwhelming at first. However, we stress that to numerically solve the problems to be presented later, it is not required that you can follow every individual step of the mathematical derivation. Therefore, when you read this section focus on getting an overview of the material presented and try to understand the physics of the scattering problem. Should you still struggle to understand the problem, please do not hesitate to ask!

### 2.2.1 Scattering theory

The incident wave we will take as a plane wave (the incident atom beam) and we write it as

$$\psi_{\text{inc}}(\boldsymbol{x}|\omega) = \exp\left[i\boldsymbol{k}\cdot\boldsymbol{x}\right]. \tag{6}$$

Here $\boldsymbol{k}$ represents the wave vector of the scalar wave. When the incident wave from Eq. (6) is substitute into the Helmholtz equation (4) one finds that it satisfies this latter equation only when the following condition is fulfilled

$$\boldsymbol{k}\cdot\boldsymbol{k} = \frac{\omega^2}{c^2}. \tag{7}$$

The expression in Eq. (7) is known as the *dispersion relation* of the scalar wave and it should always be satisfied. To make sure that this is the case, we write the wave vector $\boldsymbol{k}$ in the form

$$\boldsymbol{k} = \boldsymbol{k}_{\parallel} \pm \alpha_0(k_{\parallel},\omega)\hat{\boldsymbol{x}}_3 \tag{8}$$

with

$$\alpha_0(k_{\parallel},\omega) = \begin{cases} \sqrt{\frac{\omega^2}{c^2} - k_{\parallel}^2} & k_{\parallel}^2 < \frac{\omega^2}{c^2} \\ i\sqrt{k_{\parallel}^2 - \frac{\omega^2}{c^2}} & k_{\parallel}^2 \geq \frac{\omega^2}{c^2} \end{cases}. \tag{9}$$

Here the component of the wave vector that is parallel to the $x_3$-plane has been denoted $\boldsymbol{k}_{\parallel}$ while the vertical component of the same wave vector (that is perpendicular to the $x_3$-plane) we write $k_3 \equiv \pm\alpha_0(k_{\parallel},\omega)$. Moreover, the perpendicular component is treated as a function of the independent variables $\boldsymbol{k}_{\parallel}$ and $\omega$ and the functional form of $\alpha_0(k_{\parallel},\omega)$ is dictated by the dispersion relation (7). When $k_{\parallel} < \omega/c$, the associated wave is said to be *propagating*, while on the other hand when $k_{\parallel} > \omega/c$ we have an *evanescent wave* (that is decaying in the positive $x_3$-direction).

With Eqs. (8) and (9) it follows that the incident wave can be written in the form

$$\psi_{\text{inc}}(\boldsymbol{x}|\omega) = \exp\left[i\boldsymbol{k}_{\parallel}\cdot\boldsymbol{x}_{\parallel} - i\alpha_0(k_{\parallel},\omega)x_3\right]. \tag{10}$$

It should be noted that the form of the incident field automatically satisfies the dispersion relation and is therefore a solution of the Helmholtz equation (4). We have chosen a negative sign in front of the $\alpha_0$ term; physically this signifies that the incident wave is propagating in the negative $x_3$-direction (see Fig. 1), i.e. *downwards* towards the surface located at $x_3 = \zeta(\boldsymbol{x}_{\parallel})$, when $k_{\parallel}^2 < \omega^2/c^2$ (as we will assume here).

The scattered field we write in the form

$$\psi_{\mathrm{sc}}(\boldsymbol{x}|\omega) = \int_{\mathbb{R}^2} \frac{\mathrm{d}^2 q_\parallel}{(2\pi)^2}\, R(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) \exp\left[i\boldsymbol{q}_\parallel \cdot \boldsymbol{x}_\parallel + i\alpha_0(q_\parallel,\omega)x_3\right], \tag{11}$$

that is a superposition of *upward* plane waves. Here $R(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$ are the unknown (and to be determined) *scattering (or reflection) amplitudes* of the scalar wave from incident lateral wave vector $\boldsymbol{k}_\parallel$ into the scattered lateral wave vector $\boldsymbol{q}_\parallel$ (see Fig. 1). Note that the $q_\parallel$-integration is over the whole $\mathbb{R}^2$ plane, i.e. $q_1$ and $q_2$ can take on any real value in the interval $(-\infty, \infty)$.

The total field in the region $x_3 > \max\zeta(\boldsymbol{x}_\parallel)$ is the sum of the incident and scattered field from Eqs. (10) and (11) so that

$$\begin{aligned}\psi(\boldsymbol{x}|\omega) &= \psi_{\mathrm{inc}}(\boldsymbol{x}|\omega) + \psi_{\mathrm{sc}}(\boldsymbol{x}|\omega) \\ &= \exp\left[i\boldsymbol{k}_\parallel \cdot \boldsymbol{x}_\parallel - i\alpha_0(k_\parallel,\omega)x_3\right] + \int_{\mathbb{R}^2} \frac{\mathrm{d}^2 q_\parallel}{(2\pi)^2}\, R(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) \exp\left[i\boldsymbol{q}_\parallel \cdot \boldsymbol{x}_\parallel + i\alpha_0(q_\parallel,\omega)x_3\right].\end{aligned} \tag{12}$$

From Fig. 1 it is observed that the incident lateral wave vector $\boldsymbol{k}_\parallel$ is related to the polar and azimuthal angles of incidence $(\theta_0, \phi_0)$ by

$$\boldsymbol{k}_\parallel = \frac{\omega}{c}\sin\theta_0(\cos\phi_0, \sin\phi_0, 0); \tag{13a}$$

similarly, the lateral scattered wave vector is in the propagating regime ($q_\parallel < \omega/c$) related to the angles of scattering $(\theta_s, \phi_s)$ via

$$\boldsymbol{q}_\parallel = \frac{\omega}{c}\sin\theta_s(\cos\phi_s, \sin\phi_s, 0). \tag{13b}$$

It is straight forward to show from Eq. (9) that for propagating waves one has

$$\alpha_0(k_\parallel,\omega) = \frac{\omega}{c}\cos\theta_0 \tag{14a}$$

$$\alpha_0(q_\parallel,\omega) = \frac{\omega}{c}\cos\theta_s. \tag{14b}$$

On the other hand, if we are in the evanescent regime, the relations in Eqs. (13) and (14) no longer holds, at least not for real angles.

### 2.2.2 Rayleigh equation for rigid surfaces

In the expression for the total field, Eq. (12), the scattering amplitudes $R(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$ are unknown. In order to determine these amplitudes we impose the boundary conditions (3). To this end, we will use an approximation known as the Rayleigh hypothesis [14, Ch. 4] which amounts to assuming that the expression in Eq. (12) for the total field can be used all the way down to the surface. This approximation is expected to be good when the local slopes of the surface are not too large [14, Ch. 4] but the precise region of validity of this approximation is still not known for a general surface profile function.

Under the assumption of the Rayleigh hypothesis, imposing the boundary condition (3) on the total field from Eq. (12) gives the relation

$$\int_{\mathbb{R}^2} \frac{\mathrm{d}^2 q_\parallel}{(2\pi)^2}\, R(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) \exp\left[i\boldsymbol{q}_\parallel \cdot \boldsymbol{x}_\parallel + i\alpha_0(q_\parallel,\omega)\zeta(\boldsymbol{x}_\parallel)\right] = -\exp\left[i\boldsymbol{k}_\parallel \cdot \boldsymbol{x}_\parallel - i\alpha_0(k_\parallel,\omega)\zeta(\boldsymbol{x}_\parallel)\right]. \tag{15}$$

We now introduce the integral representation

$$I(\gamma|\boldsymbol{Q}_\parallel) = \int_{\mathbb{R}^2} \mathrm{d}^2 x_\parallel \, \exp\left[-i\gamma\zeta(\boldsymbol{x}_\parallel)\right] \exp\left[-i\boldsymbol{Q}_\parallel \cdot \boldsymbol{x}_\parallel\right] \tag{16a}$$

or equivalently

$$\exp\left[-i\gamma\zeta(\boldsymbol{x}_\parallel)\right] = \int_{\mathbb{R}^2} \frac{\mathrm{d}^2 Q_\parallel}{(2\pi)^2} \, I(\gamma|\boldsymbol{Q}_\parallel) \exp\left[i\boldsymbol{Q}_\parallel \cdot \boldsymbol{x}_\parallel\right]. \tag{16b}$$

The function $I(\gamma|\boldsymbol{Q}_\parallel)$ is a Fourier type integral of $\exp\left[-i\gamma\zeta(\boldsymbol{x}_\parallel)\right]$ and it encodes the surface profile function $\zeta(\boldsymbol{x}_\parallel)$.

If Eq. (15) is multiplied by the factor $\exp\left[-i\boldsymbol{p}_\parallel \cdot \boldsymbol{x}_\parallel\right]$ where $\boldsymbol{p}_\parallel$ is an arbitrary lateral wave vector, integrating the resulting expression over $\boldsymbol{x}_\parallel$, using the delta function representation

$$\delta(\boldsymbol{x}_\parallel) = \int \frac{\mathrm{d}^2 Q_\parallel}{(2\pi)^2} \exp\left(i\boldsymbol{Q}_\parallel \cdot \boldsymbol{x}_\parallel\right), \tag{17}$$

and using Eq. (16b), one is led to the following equation

$$\int_{\mathbb{R}^2} \frac{\mathrm{d}^2 q_\parallel}{(2\pi)^2} \, I\left(-\alpha_0(q_\parallel,\omega)\big|\boldsymbol{p}_\parallel - \boldsymbol{q}_\parallel\right) M(\boldsymbol{p}_\parallel|\boldsymbol{q}_\parallel) R(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) = -I\left(\alpha_0(k_\parallel,\omega)\big|\boldsymbol{p}_\parallel - \boldsymbol{k}_\parallel\right) N(\boldsymbol{p}_\parallel|\boldsymbol{k}_\parallel), \tag{18}$$

where $M(\boldsymbol{p}_\parallel|\boldsymbol{q}_\parallel)$ and $N(\boldsymbol{p}_\parallel|\boldsymbol{k}_\parallel)$ are known functions. Equation (18) is known as the *Rayleigh equation* and it is an inhomogenious integral equation for the scattering (or reflection) amplitude $R(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$. It is this type of equation that we will solve in this takehome exam. Note that the surface profile enters only via the integrals $I(\gamma|\boldsymbol{Q}_\parallel)$.

*Dirichlet and Neumann surfaces*: For a Dirichlet scattering problem, for which the total field on the surface vanishes, the functions $M(\boldsymbol{p}_\parallel|\boldsymbol{q}_\parallel)$ and $N(\boldsymbol{p}_\parallel|\boldsymbol{k}_\parallel)$ are particularly simple as they are both unity, i.e.

$$M(\boldsymbol{p}_\parallel|\boldsymbol{q}_\parallel) = 1 \qquad\qquad N(\boldsymbol{p}_\parallel|\boldsymbol{k}_\parallel) = 1. \tag{19}$$

A *Neumann surface*, on the other had, is defined by the boundary condition that the normal derivative of the total field vanishes on the surface, or in terms of mathematics,

$$\partial_n \psi(\boldsymbol{x}|\omega)\big|_{x_3=\zeta(\boldsymbol{x}_\parallel)} = 0, \tag{20}$$

where $\partial_n$ denotes the normal derivative of the surface at point $\boldsymbol{x}_\parallel$. In this case the corresponding Rayleigh equation can still be written in the form of Eq. (18) but with different forms for the following functions [11]

$$M(\boldsymbol{p}_\parallel|\boldsymbol{q}_\parallel) = \frac{\frac{\omega^2}{c^2} - \boldsymbol{p}_\parallel \cdot \boldsymbol{q}_\parallel}{\alpha_0(q_\parallel,\omega)} \tag{21a}$$

and

$$N(\boldsymbol{p}_\parallel|\boldsymbol{k}_\parallel) = -\frac{\frac{\omega^2}{c^2} - \boldsymbol{p}_\parallel \cdot \boldsymbol{k}_\parallel}{\alpha_0(k_\parallel,\omega).} \tag{21b}$$

### 2.2.3 Rayleigh equation for periodic rigid surfaces

In the discussion in the previous subsubsection, the surface profile function was in principle arbitrary. However, in this subsection our main concern will be surface profile $\zeta(\mathbf{x}_\parallel)$ that are doubly periodic functions of $\mathbf{x}_\parallel$. We express this by requiring that

$$\zeta\left(\mathbf{x}_\parallel + \mathbf{x}_\parallel(\boldsymbol{\ell})\right) = \zeta\left(\mathbf{x}_\parallel\right), \tag{22}$$

where $\{\boldsymbol{x}_\parallel(\boldsymbol{\ell})\}$ are the translation vectors of a two-dimensional Bravais lattice [9]. They are expressed by

$$\mathbf{x}_\parallel(\boldsymbol{\ell}) = \ell_1\mathbf{a}_1 + \ell_2\mathbf{a}_2, \tag{23}$$

where $\mathbf{a}_1$ and $\mathbf{a}_2$ are the two noncollinear primitive translation vectors of the lattice, while $\ell_1$ and $\ell_2$ are any positive or negative integers, or zero, which we denote collectively by $\boldsymbol{\ell} = (\ell_1, \ell_2)$. The area of a primitive unit cell of this lattice is $a_c = |\mathbf{a}_1 \times \mathbf{a}_2|$. In this work our main concern will be a square lattice for which $\mathbf{a}_1 = a\,\widehat{\mathbf{x}}_1$ and $\mathbf{a}_2 = a\,\widehat{\mathbf{x}}_2$ (and thus $a_c = a^2$).

It will be convenient for what follows to introduce the lattice that is reciprocal to the one defined by Eq. (23). Its lattice sites are given by

$$\mathbf{G}_\parallel(\boldsymbol{h}) = h_1\mathbf{b}_1 + h_2\mathbf{b}_2, \qquad h_i \in \mathbb{Z}, \tag{24}$$

where the primitive translation vectors of this lattice are defined by the equations

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij} \qquad i,j = 1,2, \tag{25}$$

with $\delta_{ij}$ denoting the Kronecker symbol. In Eq. (24), $h_1$ and $h_2$ are any positive or negative integers, or zero, which we denote collectively by $\boldsymbol{h}$. For a square lattice of parameter $a$ the primitive reciprocal lattice vectors are $\mathbf{b}_1 = (2\pi/a)\,\widehat{\mathbf{x}}_1$ and $\mathbf{b}_2 = (2\pi/a)\,\widehat{\mathbf{x}}_2$.

Due to the periodicity of the surface profile function [Fig. 1], $\zeta(\boldsymbol{x}_\parallel)$ the field in the vacuum must satisfy the Floquet-Bloch condition [16], *i.e.*

$$\psi\big(\mathbf{x}_\parallel + \mathbf{x}_\parallel(\boldsymbol{\ell}), x_3|\omega\big) = \exp\left[i\mathbf{k}_\parallel \cdot \mathbf{x}_\parallel(\boldsymbol{\ell})\right]\psi\big(\mathbf{x}_\parallel, x_3|\omega\big)\,. \tag{26}$$

Consequently, we rewrite the amplitudes $R(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$ of the scattered scalar field in the form

$$R(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) = \sum_{\mathbf{G}_\parallel} (2\pi)^2\,\delta\left(\mathbf{q}_\parallel - \mathbf{k}_\parallel - \mathbf{G}_\parallel\right) r(\mathbf{k}_\parallel + \mathbf{G}_\parallel|\boldsymbol{k}_\parallel). \tag{27}$$

In writing Eq. (27) we have replaced summation over $\boldsymbol{h}$ by summation over $\mathbf{G}_\parallel$. For a periodic surface, we write Eq. (16a) in the form

$$I\left(\gamma|\mathbf{Q}_\parallel\right) = \sum_{\boldsymbol{\ell}} \int\limits_{a_c(\boldsymbol{\ell})} d^2x_\parallel\, \exp\Big(-i\boldsymbol{Q}_\parallel \cdot \boldsymbol{x}_\parallel\Big) \exp\left[-i\gamma\zeta(\boldsymbol{x}_\parallel)\right], \tag{28}$$

make the change of variable $\boldsymbol{x}_\parallel = \boldsymbol{x}_\parallel(\boldsymbol{\ell}) + \boldsymbol{u}_\parallel$ and use the the periodicity property (22) of the surface to obtain

$$\begin{aligned} I\left(\gamma|\mathbf{Q}_\parallel\right) &= \sum_{\boldsymbol{\ell}} \int\limits_{a_c} d^2u_\parallel\, \exp\Big[-i\boldsymbol{Q}_\parallel \cdot \big(\boldsymbol{x}_\parallel(\boldsymbol{\ell}) + \boldsymbol{u}_\parallel\big)\Big] \exp\left[-i\gamma\zeta(\boldsymbol{u}_\parallel + \boldsymbol{x}_\parallel(\boldsymbol{\ell}))\right] \\ &= \sum_{\boldsymbol{\ell}} \exp\Big[-i\boldsymbol{Q}_\parallel \cdot \boldsymbol{x}_\parallel(\boldsymbol{\ell})\Big] \int\limits_{a_c} d^2u_\parallel\, \exp\Big(-i\boldsymbol{Q}_\parallel \cdot \boldsymbol{u}_\parallel\Big) \exp\left[-i\gamma\zeta(\boldsymbol{u}_\parallel)\right]. \end{aligned} \tag{29}$$

Now, taking advantage of the relation

$$\sum_{\boldsymbol{\ell}} \exp\left[-i\boldsymbol{Q}_{\parallel}\cdot\boldsymbol{x}_{\parallel}(\boldsymbol{\ell})\right] = \sum_{\boldsymbol{G}_{\parallel}} \frac{(2\pi)^2}{a_c}\delta\left(\boldsymbol{Q}_{\parallel}-\boldsymbol{G}_{\parallel}\right), \tag{30}$$

enables us to write Eq. (29) in the form

$$I\left(\gamma|\mathbf{Q}_{\parallel}\right) = \sum_{\mathbf{G}_{\parallel}} (2\pi)^2\,\delta\big(\mathbf{Q}_{\parallel}-\mathbf{G}_{\parallel}\big)\,\widehat{I}\left(\gamma|\mathbf{G}_{\parallel}\right), \tag{31}$$

with

$$\widehat{I}\left(\gamma\mid\mathbf{G}_{\parallel}\right) = \frac{1}{a_c}\int_{a_c} d^2x_{\parallel}\ \exp\left(-i\mathbf{G}_{\parallel}\cdot\mathbf{x}_{\parallel}\right)\exp\left[-i\gamma\zeta(\mathbf{x}_{\parallel})\right]. \tag{32}$$

When the expansions (27) and (31) are substituted into the Rayleigh equation (18), the equation satisfied by the amplitudes $\left\{r(\mathbf{k}_{\parallel}+\mathbf{G}_{\parallel}|\boldsymbol{k}_{\parallel})\right\}$ is obtained in the form

$$\begin{aligned}\sum_{\mathbf{K}_{\parallel}}(2\pi)^2\delta\left(\boldsymbol{p}_{\parallel}-\boldsymbol{K}_{\parallel}\right)\ \sum_{\mathbf{K}'_{\parallel}}\widehat{I}\left(-\alpha_0(K'_{\parallel})\big|\boldsymbol{K}_{\parallel}-\boldsymbol{K}'_{\parallel}\right)M\left(\boldsymbol{K}_{\parallel}|\boldsymbol{K}'_{\parallel}\right)r(\boldsymbol{K}'_{\parallel}|\boldsymbol{k}_{\parallel})\\ = -\sum_{\mathbf{K}_{\parallel}}(2\pi)^2\,\delta\left(\boldsymbol{p}_{\parallel}-\boldsymbol{K}_{\parallel}\right)\widehat{I}\left(+\alpha_0(k_{\parallel})\big|\boldsymbol{K}_{\parallel}-\boldsymbol{k}_{\parallel}\right)N\left(\boldsymbol{K}_{\parallel}|\boldsymbol{k}_{\parallel}\right).\end{aligned} \tag{33}$$

In writing this equation, we have defined the two lateral wave vectors

$$\boldsymbol{K}_{\parallel} = \boldsymbol{k}_{\parallel}+\boldsymbol{G}_{\parallel} \qquad\qquad \boldsymbol{K}'_{\parallel} = \boldsymbol{k}_{\parallel}+\boldsymbol{G}'_{\parallel}, \tag{34}$$

and summations over $\boldsymbol{G}_{\parallel}$ and $\boldsymbol{G}'_{\parallel}$ have been replaced by summations over $\boldsymbol{K}_{\parallel}$ and $\boldsymbol{K}'_{\parallel}$, respectively. Equating coefficients of delta functions on both sides of Eq. (33) gives

$$\sum_{\mathbf{K}'_{\parallel}}\widehat{I}\left(-\alpha_0(K'_{\parallel})\big|\boldsymbol{K}_{\parallel}-\boldsymbol{K}'_{\parallel}\right)M(\boldsymbol{K}_{\parallel}|\boldsymbol{K}'_{\parallel})\,r(\boldsymbol{K}'_{\parallel}|\boldsymbol{k}_{\parallel}) \quad = -\widehat{I}\left(\alpha_0(k_{\parallel})\big|\boldsymbol{K}_{\parallel}-\boldsymbol{k}_{\parallel}\right)N(\boldsymbol{K}_{\parallel}|\boldsymbol{k}_{\parallel}). \tag{35}$$

Equation (35) is the final form of the *periodic surface Rayleigh equation*. The set of solutions of this equation $\{r(\boldsymbol{K}'_{\parallel}|\boldsymbol{k}_{\parallel})\}$ describes the reflection of an incident scalar wave of lateral wave vector $\boldsymbol{k}_{\parallel}$ that is scattered by the periodic surface $\zeta(\boldsymbol{x}_{\parallel})$ into reflected waves characterized by the lateral wave vector $\boldsymbol{K}'_{\parallel} = \boldsymbol{k}_{\parallel}+\boldsymbol{G}'_{\parallel}$.

### 2.3 The I-integral

In order to completely define the Rayleigh equation for a periodic surface, Eq. (35), the $\widehat{I}$-integrals that appear in this equation have to be calculated. From the definitions of these integrals, Eq. (32), it should be apparent that to do so one is required to assume a specific form for the periodic surface profile function that we write as

$$\zeta(\mathbf{x}_{\parallel}) = \sum_{\boldsymbol{\ell}} S\left(\mathbf{x}_{\parallel}-\mathbf{x}_{\parallel}(\boldsymbol{\ell})\right). \tag{36}$$

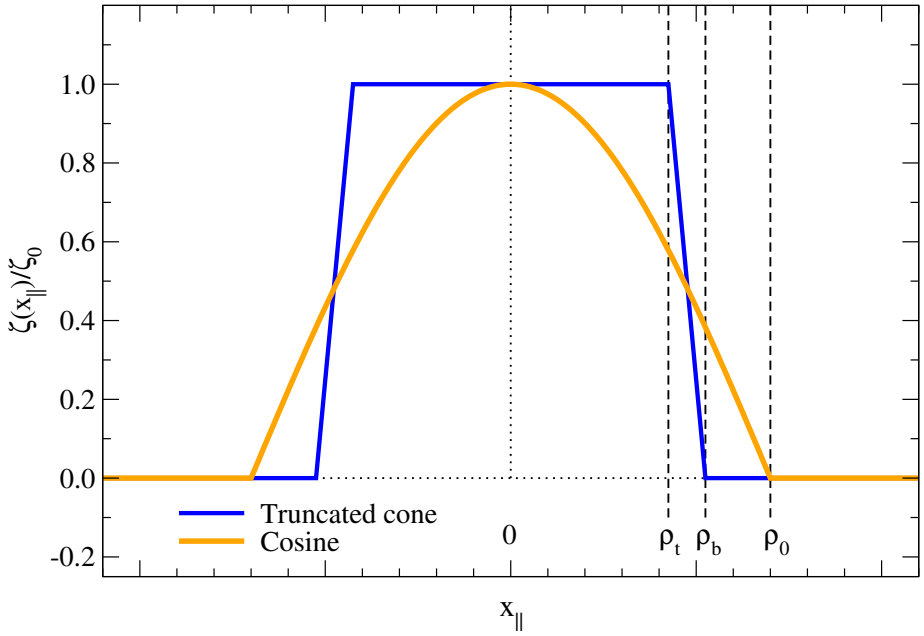


Figure 2: The truncated cone and cosine forms assumed for the surface profile in the modeling.

Here $S(\mathbf{x}_\parallel)$ represents the part of the surface profile that is repeated inside each unit cell. In this work we will carry out numerical calculations assuming several forms of this function, some of which are rotational symmetric about the $x_3$-axis, and the forms having this symmetry are depicted in Fig. 2.

The first form of $S(\mathbf{x}_\parallel)$ that we will consider is a *double period sinusoidal* profile of period $a$ defied by

$$S(\boldsymbol{x}_\parallel) = \frac{\zeta_0}{2}\left[\cos\left(\frac{2\pi x_1}{a}\right) + \cos\left(\frac{2\pi x_2}{a}\right)\right], \tag{37}$$

where $\zeta_0 \geq 0$ is an amplitude. This surface profile function is obviously not rotational symmetric. However, the advantage of this profile function is that the $\widehat{I}$-integral (32) that is associated with it can be calculated in closed analytic form. With $\boldsymbol{G}_\parallel(\boldsymbol{h})$ defined by Eq. (24) with $\boldsymbol{h} = (h_1, h_2)$, a direct calculation gives

$$\widehat{I}\left(\gamma|\boldsymbol{G}_\parallel(\boldsymbol{h})\right) = (-i)^{h_1}\,\mathrm{J}_{h_1}\left(\frac{\gamma\zeta_0}{2}\right)(-i)^{h_2}\,\mathrm{J}_{h_2}\left(\frac{\gamma\zeta_0}{2}\right), \tag{38}$$

where $J_n(\cdot)$ represents the Bessel function of first kind and order $n$.

The second form of $S(\mathbf{x}_\parallel)$ that we will consider is the *truncated cone* of in-plane circular cross-section characterized by top and base radii $\rho_t$ and $\rho_b$ (see Fig. 2), respectively. Mathematically this function can be defined as

$$S(\boldsymbol{x}_\parallel) = \begin{cases} \zeta_0 & 0 \leq x_\parallel < \rho_t \\ \zeta_0 \frac{\rho_b - x_\parallel}{\rho_b - \rho_t} & \rho_t \leq x_\parallel < \rho_b \\ 0 & \rho_b \leq x_\parallel \end{cases}, \tag{39}$$

where $0 \leq \rho_t \leq \rho_b$, the amplitude $\zeta_0 \geq 0$ and $x_\parallel = |\boldsymbol{x}_\parallel|$. This profile is rotational symmetric.

Instead of calculating directly the $\widehat{I}$-integral associated with the truncated cone, we will start with a simpler calculation for which the surface profile function is a the circular pillar of height $\zeta_0$ and radius $\rho_0$. The corresponding profile function is defined as a special case of a Eq. (39) obtained when $\rho_t = \rho_b = \rho_0$. In this case and with Eq. (32), a direct calculation leads to

$$\begin{aligned}
\widehat{I}\left(\gamma|\mathbf{G}_\parallel\right) &= \frac{1}{a_c}\int\limits_{a_c} d^2x_\parallel \ \left\{1+\exp\left[-i\gamma\zeta(\mathbf{x}_\parallel)\right]-1\right\}\exp\left(-i\mathbf{G}_\parallel\cdot\mathbf{x}_\parallel\right) \\
&= \delta_{\mathbf{G}_\parallel,\mathbf{0}} + \frac{1}{a_c}\int\limits_0^{\rho_0} dx_\parallel \ x_\parallel \int\limits_{-\pi}^{\pi} d\phi \ \left[\exp\left(-i\gamma\zeta_0\right)-1\right]\exp\left(-iG_\parallel x_\parallel\cos\phi\right) \\
&= \delta_{\mathbf{G}_\parallel,\mathbf{0}} + \frac{2\pi}{a_c}\left[\exp\left(-i\gamma\zeta_0\right)-1\right]\int\limits_0^{\rho_0} dx_\parallel \ x_\parallel J_0(G_\parallel x_\parallel)
\end{aligned} \tag{40}$$

where $\delta_{\mathbf{G}_\parallel,\mathbf{0}}$ denotes a Kronecker delta function. In obtaining this result, a factor of one has been added and subtracted from the exponential function containing the surface profile function so that the function $\exp\left[-i\gamma\zeta(\boldsymbol{x}_\parallel)\right]-1$ vanishes whenever the surface profile function $\zeta(\boldsymbol{x}_\parallel)$ vanishes. Moreover, in arriving at Eq. (40) polar coordinates have been introduced and we have used that the Bessel function of the first kind and order zero has the integral representation [15]

$$J_0(z) = \frac{1}{2\pi}\int\limits_{-\pi}^{\pi} d\theta \ \exp\left(iz\cos\theta\right). \tag{41}$$

This function enters into the expressions for $\widehat{I}\left(\gamma|\mathbf{G}_\parallel\right)$ due to the rotational symmetry of the profile function $S(\boldsymbol{x}_\parallel) = S(x_\parallel)$. The integral that appears in Eq. (40) can be evaluated analytically with the results that [12]

$$\widehat{I}\left(\gamma|\mathbf{G}_\parallel\right) = \delta_{\mathbf{G}_\parallel,\mathbf{0}} + 2\pi\frac{\rho_0^2}{a^2}\left[\exp\left(-i\gamma\zeta_0\right)-1\right]\frac{J_1(G_\parallel\rho_0)}{G_\parallel\rho_0}, \tag{42}$$

where $J_1(\cdot)$ denotes the Bessel function of the first kind and order one and we have used that $a_c = a^2$ for a square lattice. We note that when $G_\parallel\rho_0 = 0$ in Eq. (42) then $J_1(G_\parallel\rho_0)/(G_\parallel\rho_0) = 1/2$.

We are now prepared to calculate the $\widehat{I}$-integral for the truncated cone; the procedure that we will follow mimics how the result in Eq. (42) was obtained. By introducing Eq. (39)

into Eq. (32) and using Eq. (41) one obtains

$$\begin{aligned}\widehat{I}\left(\gamma|\mathbf{G}_\parallel\right) &= \delta_{\mathbf{G}_\parallel,\mathbf{0}} + \frac{2\pi}{a_c}\int_0^{\rho_b} dx_\parallel\ x_\parallel J_0(G_\parallel x_\parallel)\left[\exp\left\{-i\gamma\zeta(x_\parallel)\right\}-1\right] \\ &= \delta_{\mathbf{G}_\parallel,\mathbf{0}} + \frac{2\pi}{a^2}\left[\exp\left(-i\gamma\zeta_0\right)-1\right]\int_0^{\rho_t} dx_\parallel\ x_\parallel J_0(G_\parallel x_\parallel) \\ &\quad + \frac{2\pi}{a^2}\int_{\rho_t}^{\rho_b} dx_\parallel\ x_\parallel J_0(G_\parallel x_\parallel)\left[\exp\left(-i\gamma\zeta_0\frac{\rho_b-x_\parallel}{\rho_b-\rho_t}\right)-1\right]. \end{aligned} \tag{43}$$

The two first terms on the right-hand-side of Eq. (43) are given by the right-hand-side of Eq. (42) if $\rho_0$ is replaced in this expression by $\rho_t$. To calculate the last integral of Eq. (43), we Taylor expand the exponential function that appears in the integrand and integrate the resulting expression term-by-term to obtain

$$\begin{aligned}\widehat{I}\left(\gamma|\mathbf{G}_\parallel\right) &= \delta_{\mathbf{G}_\parallel,\mathbf{0}} + 2\pi\frac{\rho_t^2}{a^2}\left[\exp\left(-i\gamma\zeta_0\right)-1\right]\frac{J_1(G_\parallel\rho_t)}{G_\parallel\rho_t} \\ &\quad + \frac{2\pi}{a^2}\sum_{n=1}^{\infty}\frac{(-i\gamma\zeta_0)^n}{n!}\int_{\rho_t}^{\rho_b} dx_\parallel\ x_\parallel J_0(G_\parallel x_\parallel)\left(\frac{\rho_b-x_\parallel}{\rho_b-\rho_t}\right)^n. \end{aligned} \tag{44}$$

If now the change of variable

$$u_\parallel = \frac{\rho_b - x_\parallel}{\rho_b-\rho_t} \tag{45}$$

is made in the last term in Eq. (44) one obtains after some rewriting

$$\begin{aligned}\widehat{I}\left(\gamma|\mathbf{G}_\parallel\right) &= \delta_{\mathbf{G}_\parallel,\mathbf{0}} + 2\pi\frac{\rho_t^2}{a^2}\left[\exp\left(-i\gamma\zeta_0\right)-1\right]\frac{J_1(G_\parallel\rho_t)}{G_\parallel\rho_t} \\ &\quad + 2\pi\frac{\rho_b-\rho_t}{a^2}\sum_{n=1}^{\infty}\frac{(-i\gamma\zeta_0)^n}{n!}\int_0^1 du_\parallel\ \left[\rho_b-(\rho_b-\rho_t)u_\parallel\right]\ J_0\left(G_\parallel\left[\rho_b-(\rho_b-\rho_t)u_\parallel\right]\right)u_\parallel^n. \end{aligned} \tag{46}$$

The integrals that appear in this equation have to be evaluated numerically, and in most cases, only a few terms are needed in the sum to obtain convergent results. It is readily checked that the expression in Eq. (46) in the limit $\rho_t \to \rho_b$ reduces to that of Eq. (42), as it should.

The final form of the surface profile function for which we will perform calculations is the *(truncated) cosine* surface profile (see Fig. 2) defined as

$$S(\mathbf{x}_\parallel) = \begin{cases}\zeta_0\cos\left(\dfrac{\pi x_\parallel}{2\rho_0}\right) & 0 < x_\parallel < \rho_0 \\ 0 & x_\parallel > \rho_0\end{cases}. \tag{47}$$

We now use this expression in Eq. (32) in order to obtain the corresponding expression for the integral $\widehat{I}$. The result is

$$\begin{aligned}\widehat{I}\left(\gamma|\mathbf{G}_\parallel\right) &= \delta_{\mathbf{G}_\parallel,\mathbf{0}} + \frac{1}{a_c}\int_0^{\rho_0} dx_\parallel\ x_\parallel \int_{-\pi}^{\pi} d\phi\ \left\{\exp\left[-i\gamma\zeta(x_\parallel)\right]-1\right\}\exp\left(-iG_\parallel x_\parallel\cos\phi\right)\\ &= \delta_{\mathbf{G}_\parallel,\mathbf{0}} + \frac{2\pi}{a^2}\int_0^{\rho_0} dx_\parallel\ x_\parallel J_0(G_\parallel x_\parallel)\left\{\exp\left[-i\gamma\zeta(x_\parallel)\right]-1\right\}\\ &= \delta_{\mathbf{G}_\parallel,\mathbf{0}} + \frac{2\pi}{a^2}\sum_{n=1}^{\infty}\frac{(-i\gamma)^n}{n!}\int_0^{\rho_0} dx_\parallel\ x_\parallel J_0(G_\parallel x_\parallel)\,\zeta^n(x_\parallel),\end{aligned} \tag{48}$$

where Eq. (41) and a Taylor series expansion of $\exp\left[-i\gamma\zeta(x_\parallel)\right]$ have been used in the first and last transmission, respectively. The integrals present in Eq. (48) have to be calculated numerically, and sufficiently many terms were included to reach convergence.

### 2.3.1 Efficiencies of the diffracted Bragg beams

From the knowledge of the reflection amplitudes the diffraction efficiencies of the scattered beam can be calculated. They are measurable quantities and in this section we will derive expressions for them.

To this end, we start by calculating the total, time-averages power flux that is incident and scattered by the surface. The magnitude of the total, time-averaged power flux incident on the surface (by a particle of mass $m$) is defined as

$$P_{\rm inc} = -\frac{\hbar}{m}{\rm Im}\int d^2x_\parallel\ \left[\psi^*_{\rm inc}(\boldsymbol{x}|\omega)\frac{\partial\psi_{\rm inc}(\boldsymbol{x}|\omega)}{\partial x_3}\right]_{x_3>\max\zeta(\boldsymbol{x}_\parallel)} \tag{49}$$

Here (and in later equations) the superscript asterisk denotes complex conjugation. The minus sign that appears on the right-hand side of Eq. (49) compensates for the fact that the incident flux is negative. With the form of the incident field from Eq. (6) it follows readily that

$$P_{inc} = \frac{\hbar}{m}L_1L_2\alpha_0(k_\parallel,\omega), \tag{50}$$

where $L_1$ and $L_2$ are the lengths of the mean scattering surface along the $x_1$- and $x_2$-axis, respectively.

Similarly, the magnitude of the total, time-averaged scattered power flux is with the use of Eq. (11) found to be [11]

$$\begin{aligned}P_{\rm sc} &= \frac{\hbar}{m}{\rm Im}\int d^2x_\parallel\ \left[\psi^*_{\rm sc}(\boldsymbol{x}|\omega)\frac{\partial\psi_{\rm sc}(\boldsymbol{x}|\omega)}{\partial x_3}\right]_{x_3>\max\zeta(\boldsymbol{x}_\parallel)}\\ &= \frac{\hbar}{m}{\rm Im}\int\frac{d^2q_\parallel}{(2\pi)^2}\ i\alpha_0(q_\parallel,\omega)\left|R(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\right|^2\exp\left[-2{\rm Im}\alpha_0(q_\parallel,\omega)x_3\right]\\ &= \frac{\hbar}{m}\int_{q_\parallel<\omega/c}\frac{d^2q_\parallel}{(2\pi)^2}\ \alpha_0(q_\parallel,\omega)\left|R(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\right|^2.\end{aligned} \tag{51}$$

The reason that the $q_\parallel$-integration that appears in this expression is limited to the domain $q_\parallel < \omega/c$ is a direct consequence of the imaginary value that appears in the first line of Eq. (51). When $q_\parallel > \omega/c$, we are evanescent in vacuum and $\alpha_0(q_\parallel)$ is purely imaginary. When this happens, the integrands in Eq. (51) are real and will therefore not contribute to $P_{\rm sc}$.

The periodicity of the surface profile function $\zeta(\boldsymbol{x}_\parallel)$ is taken into account via the relations in Eq. (27). From these expressions one obtains the relation

$$\begin{aligned}\left|R(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\right|^2 &= \sum_{\boldsymbol{G}_\parallel}(2\pi)^2\delta\left(\boldsymbol{q}_\parallel-\boldsymbol{k}_\parallel-\boldsymbol{G}_\parallel\right)r^*(\boldsymbol{k}_\parallel+\boldsymbol{G}_\parallel|\boldsymbol{k}_\parallel)\\ &\quad\times\sum_{\boldsymbol{G}'_\parallel}(2\pi)^2\delta\left(\boldsymbol{q}_\parallel-\boldsymbol{k}_\parallel-\boldsymbol{G}'_\parallel\right)r(\boldsymbol{k}_\parallel+\boldsymbol{G}'_\parallel|\boldsymbol{k}_\parallel)\\ &= \sum_{\boldsymbol{G}_\parallel}\left[(2\pi)^2\delta\left(\boldsymbol{q}_\parallel-\boldsymbol{k}_\parallel-\boldsymbol{G}_\parallel\right)\right]^2\left|r(\boldsymbol{k}_\parallel+\boldsymbol{G}_\parallel|\boldsymbol{k}_\parallel)\right|^2\\ &= \sum_{\boldsymbol{G}_\parallel}(2\pi)^2\delta\left(\boldsymbol{0}\right)(2\pi)^2\delta\left(\boldsymbol{q}_\parallel-\boldsymbol{k}_\parallel-\boldsymbol{G}_\parallel\right)\left|r(\boldsymbol{k}_\parallel+\boldsymbol{G}_\parallel|\boldsymbol{k}_\parallel)\right|^2,\end{aligned}\tag{52}$$

which when combined with Eq. (51), gives

$$P_{\rm sc}=\frac{\hbar}{m}L_1L_2{\sum_{\boldsymbol{G}_\parallel}}'\alpha_0(|\boldsymbol{k}_\parallel+\boldsymbol{G}_\parallel|)\left|r(\boldsymbol{k}_\parallel+\boldsymbol{G}_\parallel|\boldsymbol{k}_\parallel)\right|^2.\tag{53}$$

Here we have used a prime on the summation symbol to indicate that the sum over $\boldsymbol{G}_\parallel$ only runs over values for which $|\boldsymbol{k}_\parallel+\boldsymbol{G}_\parallel|<\omega/c$. Equation (53) demonstrates that each diffracted beam contributes independently to the scattered flux.

When the scattered power flux is normalized by the power flux of the incident beam, $P_{\rm inc}$, one gets

$$\frac{P_{\rm sc}}{P_{\rm inc}}={\sum_{\boldsymbol{G}_\parallel}}'e\left(\boldsymbol{k}_\parallel+\boldsymbol{G}_\parallel|\boldsymbol{k}_\parallel\right),\tag{54}$$

where

$$e\left(\boldsymbol{k}_\parallel+\boldsymbol{G}_\parallel|\boldsymbol{k}_\parallel\right)=\frac{\alpha_0(|\boldsymbol{k}_\parallel+\boldsymbol{G}_\parallel|)}{\alpha_0(k_\parallel)}\left|r(\boldsymbol{k}_\parallel+\boldsymbol{G}_\parallel|\boldsymbol{k}_\parallel)\right|^2.\tag{55}$$

The quantity $e\left(\boldsymbol{k}_\parallel+\boldsymbol{G}_\parallel|\boldsymbol{k}_\parallel\right)$ is known as the *diffraction efficiency* of incident beam of lateral wave vector $\boldsymbol{k}_\parallel$ into the Bragg beam characterized by $\boldsymbol{k}_\parallel+\boldsymbol{G}_\parallel$. This quantity only has a physical meaning for those values of $\mathbf{G}_\parallel$ for which $|\boldsymbol{k}_\parallel+\boldsymbol{G}_\parallel|<\omega/c$; this situation is often referred to as *open diffraction channels*.

Since there is no absorption in the scattering from a rigid surface (or hard wall), all power incident on it must be scattered. Hence, the conservation of energy dictates that

$$\mathcal{U}={\sum_{\boldsymbol{G}_\parallel}}'e\left(\boldsymbol{k}_\parallel+\boldsymbol{G}_\parallel|\boldsymbol{k}_\parallel\right)\equiv 1.\tag{56}$$

This *energy conservation condition* is useful for testing, for instance, the quality of numerical simulations results. It is a necessary but not sufficient condition for the correctness of the simulation results.

The *reflectivity* of the periodic surface is obtained from the diffraction efficiency when $\boldsymbol{G}_\parallel = \boldsymbol{0}$;

$$\mathcal{R}(\boldsymbol{k}_\parallel) = e(\boldsymbol{k}_\parallel|\boldsymbol{k}_\parallel). \tag{57}$$

### 2.4 Grating equation

When an incident wave of lateral wave vector $\boldsymbol{k}_\parallel$ is scattered from a periodic surface, the possible scattered lateral wave vectors are given by

$$\boldsymbol{q}_\parallel(\boldsymbol{h}) = \boldsymbol{k}_\parallel + \boldsymbol{G}_\parallel(\boldsymbol{h}), \tag{58}$$

with $\boldsymbol{h} = (h_1, h_2, 0)$, $h_i \in \mathbb{Z}$, and for a square lattice of period $a$ [see Eq. (24)]

$$\boldsymbol{G}_\parallel(\boldsymbol{h}) = h_1 \frac{2\pi}{a}\widehat{\mathbf{x}}_1 + h_2 \frac{2\pi}{a}\widehat{\mathbf{x}}_2. \tag{59}$$

The result expressed by Eq. (58) is know as the *grating equation*, and from the preceding discussion, it should be apparent that it holds. This equation predicts for which directions the different diffraction orders (Bragg beams) will appear. Note that the this equation only gives the positions, that only depends on the period, and not the intensity of the diffractive orders.

Alternatively, when the grating equation (58) is combined with Eq. (13b) the angles of scatterings $(\theta_s, \phi_s)$ for the various diffractive orders can be derived.

### 2.5 Numerical solution of the Rayleigh equation for periodic surfaces

The purpose of this section is to present some ideas and comments on how to solve numerically the Rayleigh equation for a periodic surface, Eq. (35). You may chose to follow, or not follow the advises given here.

In order to obtain a numerical solution of the Rayleigh equation for a periodic surface profile function, Eq. (35), we start by restricting the indices $h_1$ and $h_2$ that appear in the wave vector $\boldsymbol{G}'_\parallel$ [see Eq. (24)] to the intervals $-H \leq h_i \leq H$, $(i = 1, 2)$, where $H$ is a positive integer.[3] This implies that the number of terms in the summation in Eq. (35) is reduced from an infinite number to a finite number. Therefore, we only have a finite set of unknown scattering amplitudes $r(\mathbf{k}_\parallel + \mathbf{G}'_\parallel|\mathbf{k}_\parallel)$ to solve for. To numerically calculate these scattering amplitudes, the Rayleigh equation (35) is converted into a linear system of equations. To this end, $r(\mathbf{k}_\parallel + \mathbf{G}'_\parallel|\mathbf{k}_\parallel)$ is mapped into a vector by adapting a certain storage convention for its elements that depends on both components of the lateral scattered wave vector $\mathbf{k}_\parallel + \mathbf{G}'_\parallel$. With the storage convention assumed, the elements $M(\boldsymbol{K}_\parallel|\boldsymbol{K}'_\parallel)$ times the prefactor appearing in the Rayleigh equation are mapped onto a matrix that forms the left-hand-side of the linear

[3] If you are concerned that using a rectangular cut-off in reciprocal $\boldsymbol{G}_\parallel$-space can introduce an anisotropy, you may restrict the sum over $\boldsymbol{G}'_\parallel$ (or $\boldsymbol{K}'_\parallel$) for which $G'_\parallel < H$. This is somewhat more complex to implement than using a rectangular domain but the implementation is more efficient since in total a lower number of modes are included in the calculation.

system. The linear system obtained in this way is then solved by standard routines from Lapack [8, 10]. The solution vector is then mapped back onto $r(\mathbf{k}_\parallel + \mathbf{G}'_\parallel|\mathbf{k}_\parallel)$, which is the quantity that we search, and from which physically observables like diffracted efficiencies can be calculated.

In order to obtain accurate simulation results, the value of $H$ used in the calculations has to be sufficiently high so that the maximum wave number resolved in the simulations is well into the evanescent regime. One has to increase the value of $H$ until the diffraction efficiencies of the propagating modes do no longer depend on the value of $H$ being used, i.e. the cut-off in reciprocal space.

A better way of evaluating the quality of the obtained numerical results is to check that the simulations respect energy conservation when applied to a scattering system where none of the media involved have absorption. In our case there is no absorption so this means we have to show that Eq. (56). This equation is expected to be satisfied within an error that is no more than a fraction of a percent. It is up to you to chose the numerical parameters to make sure that this is the case.

To evaluate the $\hat{I}$-integrals, one will need to calculate the Bessel functions $J_n(z)$ for complex values of the argument $z$ [7, 17]. Routines for evaluating these functions can be found in Netlib [2] and the Fortran routines that provide them are called `cbesj` and `zbesj` for the single and double precision version, respectively. These functions are part of the general purpose (Fortran) library SLATEC Common Mathematical Library [3]. They are also provided by the TBCI templated C++ numerical library [4] (as wrappers to the Fortran routines).

It might be useful to note the following properties of the Bessel functions of the first kind and integer order $n$ [5]

$$J_{-n}(z) = (-1)^n J_n(z), \tag{60}$$

and that for purely complex arguments $z = ix$, where $x$ is real, one has [5]

$$J_n(ix) = (i)^n I_n(x). \tag{61}$$

Here $I_n(x)$ denotes the *modified Bessel function* of the first kind and order $n$ (for the real argument $x$). For real arguments $x$ the functions $J_n(x)$ and $I_n(x)$ are provided by the GNU Scientific Library [6] which is written in C and has wrappers to several programming languages.

## 2.6 Exam questions

This exam is devoted to the numerical solution of the Rayleigh equation for the scattering of a scalar beam from a periodic surface, Eq. (35). We will here concentrate on the Dirichlet problem if nothing is said to indicate otherwise.

We will denote the *wavelength* of the incident beam by $\lambda$; it is related to the angular frequency via $\omega/c = 2\pi/\lambda$. Since there is no absorption in our scattering problem, the dependence on the period $a$ and profile height $\zeta_0$ are only via the ratios $a/\lambda$ and $\zeta_0/\lambda$.

You are asked to address the following tasks:

1. Write a code that solves the Rayleigh equation for a periodic Dirichlet surface, Eqs. (35) and (19), given an incident lateral wave vector $\boldsymbol{k}_\parallel$ defined by the angles of incidence $(\theta_0, \phi_0)$. Assume in your implementation that the surface profile function is the double periodic sinusoidal function (37). You are free to make assumptions for the parameters of the problem that you find convenient.

   Do several consistency checks to motivate that your implementation is likely to be correct. For instance, such test could include the flat surface limit $\zeta_0 \to 0$, the test of energy conservation, and symmetry of the scattering problem when $\boldsymbol{k}_\parallel \to -\boldsymbol{k}_\parallel$.

   It is expected that the most challenging part of the implementation will be to consistently set up the linear system of equations that needs to be solved in order to calculate the scattering amplitudes $r(\boldsymbol{k}_\parallel + \boldsymbol{G}'_\parallel | \boldsymbol{k}_\parallel)$. Therefore, pay particular attention to this part of the implementation.

   When you in the report present numerical results here and for later tasks, *always* specify explicitly *all* the numerical parameters used in the simulations. In this case, this in particular applies to the value of $H$ being used (or equivalently the value of $\max_i G_i$).

2. Calculate the quantity $\mathcal{U}$ defined in Eq. (56), as a function of increasing values of the surface profile amplitude $\zeta_0$ assuming normal incidence [$\boldsymbol{k}_\parallel = \boldsymbol{0}$]. For what value of $\zeta_0/\lambda$ do you start seeing $\mathcal{U}$ departure from unity? This signals that the Rayleigh hypothesis may no longer be satisfied.

   In your calculations assume (a) $a/\lambda = 0.5$; and (b) $a/\lambda = 3.5$. The surface profile function is still assumed to have the double periodic sinusoidal form.

3. Under the assumption

$$\boldsymbol{k}_\parallel = \frac{\omega}{c} \sin\theta_0 \, \widehat{\mathbf{x}}_1, \qquad\qquad \boldsymbol{G}_\parallel(m) = m\frac{2\pi}{a} \, \widehat{\mathbf{x}}_1, \qquad m \in \mathbb{Z}$$

   calculate the diffraction efficiencies

$$e_m(\theta_0) \equiv e(\boldsymbol{k}_\parallel + \boldsymbol{G}_\parallel(m) | \boldsymbol{k}_\parallel)$$

   as functions of the the polar angle of incidence $\theta_0 \in [-90°, 90°]$ for all open (or propagating) diffractive channels[4] when (a) $a/\lambda = 0.5$; and (b) $a/\lambda = 3.5$. For the parameters under (b) also present the the "angular dependence" of the energy conservation condition $\mathcal{U}(\theta_0)$. Note that $\boldsymbol{G}_\parallel(m)$ is always in the plane of incidence (the $x_1x_3$-plane).

   For the height of the profile $\zeta_0/\lambda$ assume a value for which you found $\mathcal{U} \approx 1$. The profile $\zeta(\boldsymbol{x}_\parallel)$ is still of the double periodic sinusoidal form.

4. Repeat the calculations from Task 3 but now for the truncated cone (39). Choose some reasonable value of $\rho_b$ and $\rho_t$ (with $a/2 > \rho_b > \rho_t$). You may have to adjust the value for $\zeta_0/\lambda$ in order to get convergent results. Comment your findings.

5. Redo the calculations from Task 4 but now for the (truncated) cosine profile (47). Choose suitable values for the constants $a/2 > \rho_0 > 0$ and $\zeta_0 > 0$

[4] This means for all values of $m \in \mathbb{Z}$ for which $|\boldsymbol{K}_\parallel(m)| < \omega/c$.

6. Discuss how you would have solved the scattering problem if the surface profile $S(\boldsymbol{x}_{\parallel})$ inside a unit cell only was available numerically and not analytically as has been the case in the calculations done above. For this task no calculations are asked for, only a discussion.

7. (*Optional but for extra credit*) For the Neumann scattering problem, repeat the calculations from Tasks 3–5. Comment your results by comparing them to the corresponding findings for the Dirichlet problem.

## References


[1] Assignment no. 3 can be found here.

[2] Netlib homepage: `www.netlib.org`.

[3] Information on SLATEC Common Mathematical Library can be found at `https://en.wikipedia.org/wiki/SLATEC` and `http://people.sc.fsu.edu/~jburkardt/f_src/slatec/slatec.html`.

[4] The TBCI templated C++ numerical library homepage: `https://plasimo.phys.tue.nl/TBCI/online-docu/html/`.

[5] NIST Digital Library of Mathematical Functions: Bessel function page `http://dlmf.nist.gov/10`.

[6] GNU Scientific Library, `https://www.gnu.org/software/gsl/`.

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