Assignment 3: Wave scattering and diffraction

I. Simonsen

Department of Physics, NTNU – Norwegian University of Science and Technology
NO-7491 Trondheim, Norway

Surface du Verre et Interfaces, UMR 125 CNRS/Saint-Gobain, F-93303 Aubervilliers, France

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The wave equation and the plane wave solution

- The wave equation reads

$$\left[\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right]\Psi(\boldsymbol{x}, t) = 0$$

- This equation has a *plane wave solution* of the form

$$\Psi(\boldsymbol{x}, t) = \Psi_0 \exp\left(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x} - \mathrm{i}\omega t\right), \tag{1}$$

under certain conditions. Which conditions?

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  under certain conditions. Which conditions?
- The relation

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

  has to be satisfied, for Eq. (1) being a solution of the wave equation. This relation is known as the dispersion relation and it always needs to be satisfied.

- Let us write the wave vector, $\boldsymbol{k}$, in the following manner

$$\begin{aligned}\boldsymbol{k} &= k_1\widehat{\mathbf{x}}_1 + k_2\widehat{\mathbf{x}}_2 + k_3\widehat{\mathbf{x}}_3 \\ &= \boldsymbol{k}_\parallel \pm \alpha_0(k_\parallel, \omega)\widehat{\mathbf{x}}_3\end{aligned}$$

where

$$\boldsymbol{k}_\parallel = k_1\widehat{\mathbf{x}}_1 + k_2\widehat{\mathbf{x}}_2 \qquad\qquad k_3 = \pm\alpha_0(k_\parallel, \omega)$$

- The function $\alpha_0(k_\parallel, \omega)$ is determined by the dispersion relation $\boldsymbol{k}\cdot\boldsymbol{k} = \omega^2/c^2$ to be

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

- By the introduction of this function

$$\begin{aligned}\Psi(\boldsymbol{x}, t) &= \psi(\boldsymbol{x}|\omega)\exp\left(-\mathrm{i}\omega t\right) \\ &= \Psi_0 \exp\left[\mathrm{i}\boldsymbol{k}_\parallel\cdot\boldsymbol{x}_\parallel \pm \mathrm{i}\alpha_0(k_\parallel, \omega)x_3\right]\exp\left(-\mathrm{i}\omega t\right)\end{aligned}$$

will be a plane wave by *construction*.

Propagating and evanecent waves

The plane-wave

$$\psi(\boldsymbol{x}|\omega) = \exp\left[\mathrm{i}\boldsymbol{k}_{\parallel}\cdot\boldsymbol{x}_{\parallel} \pm \mathrm{i}\alpha_0(k_{\parallel},\omega)x_3\right]$$

can be both propagating and evanecent.

When

- $k_{\parallel} < \omega/c$, the wave $\psi(\boldsymbol{x}|\omega)$ is propagating since the function $\alpha_0(k_{\parallel},\omega)$ is real and we have

$$k_{\parallel} = \frac{\omega}{c}\sin\theta_0 \qquad\qquad \alpha_0(k_{\parallel},\omega) = -\frac{\omega}{c}\cos\theta_0$$

- $k_{\parallel} > \omega/c$, the wave is exponentially damped (in the positive x_3-direction), called an evanecent wave, since

$$\alpha_0(k_{\parallel},\omega) = \mathrm{i}\beta_0(k_{\parallel},\omega)$$

is a *purely imaginary* function (with β_0 real) so that the wave becomes

$$\psi(\boldsymbol{x}|\omega) = \exp\left(\mathrm{i}\boldsymbol{k}_{\parallel}\cdot\boldsymbol{x}_{\parallel}\right)\exp\left(-\beta_0(k_{\parallel},\omega)x_3\right).$$

Boundary conditions (BCs)

There are two important boundary conditions for the Helmholtz equation

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

the Fourier transform of the wave equation.

For the surface $x_3 = \zeta(\boldsymbol{x}_\parallel)$ they are

- Dirichlet BC

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

- Neumann BC

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

  where $\partial_n = \widehat{\mathbf{n}} \cdot \boldsymbol{\nabla}$ denotes the normal derivative of the surface at point $\boldsymbol{x}_\parallel$.

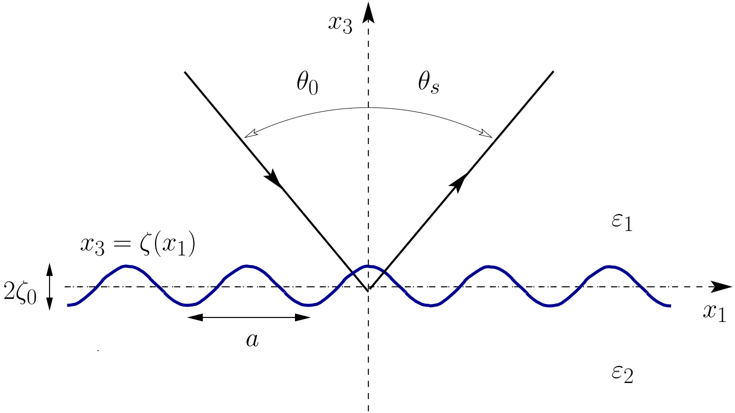
A primer on diffraction?

What is diffraction?

Here are a few youtube videos to remind you, if needed

1. Video 1 (short); `https://www.youtube.com/watch?v=SO7ZlMJv5ZM`
2. Video 2 (long); `https://www.youtube.com/watch?v=UFh7hkLeL10`

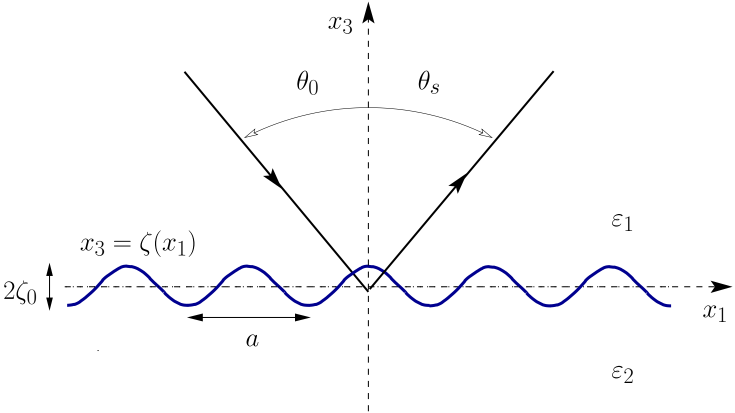
- Geometry



- Angle of incidence θ_0, wavelength λ and period *a*

Diffraction from a one-dimensional periodic surface

- Geometry



- Angle of incidence θ_0, wavelength λ and period *a*
- ...but what determines the angular positions of the diffractive modes?

The grating formula (one-dimension)

- The grating formula determines the angle of scattering $\theta_s = \theta_m$ of the m'th diffractive order

$$\boxed{\sin\theta_m = \sin\theta_0 + m\frac{\lambda}{a}} \qquad m \in \mathbb{Z}$$

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- Alternative formulation: Introducing the reciprocal lattice constant, $2\pi/a$, the 1D grating equation can be defined as

$$\boxed{q_{\parallel}(m) = k_{\parallel} + G_{\parallel}(m)}$$

where

$$q_{\parallel}(m) = \frac{\omega}{c}\sin\theta_m \qquad k_{\parallel} = \frac{\omega}{c}\sin\theta_0 \qquad G_{\parallel}(m) = m\frac{2\pi}{a}.$$

Here $k_{\parallel}$ denote the wave vector component parallel to the flat surface.

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- Rayleigh anomalies (in reflection) occur when

$$\boxed{q_{\|}(m) = \frac{\omega}{c}}$$

- Lattice vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ defines the structure in real space
  - they are two noncollinear primitive translation vectors of the lattice
  - Square lattice: $\boldsymbol{a}_i = a\widehat{\mathbf{x}}_i$
- Reciprocal space is defined by the primitive reciprocal lattice vectors $\boldsymbol{b}_i$ defined by

$$\boldsymbol{a} \cdot \boldsymbol{b}_j = 2\pi\,\delta_{ij} \qquad i, j = 1, 2$$

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Diffraction from a two-dimensional periodic surface

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$$\boxed{\boldsymbol{G}_{||}(h) = h_1\boldsymbol{b}_1 + h_2\boldsymbol{b}_2} \qquad h_i \in \mathbb{Z}$$

where h collectively denotes h_1 and h_2 [i.e. $h = \{h_1, h_2\}$]

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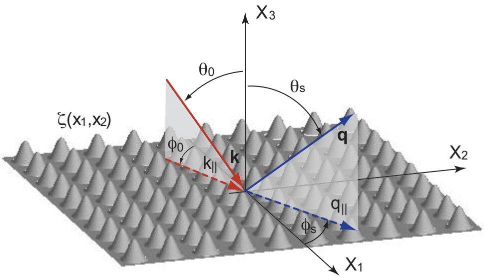
- The grating equation, valid for a two-dimensional period structure, reads

$$\boxed{\boldsymbol{q}_{\parallel}(h) = \boldsymbol{k}_{\parallel} + \boldsymbol{G}_{\parallel}(h)}$$

Diffraction from a two-dimensional periodic surface

$$\boxed{\boldsymbol{q}_{\|}(h) = \boldsymbol{k}_{\|} + \boldsymbol{G}_{\|}(h)}$$



The symbols mean

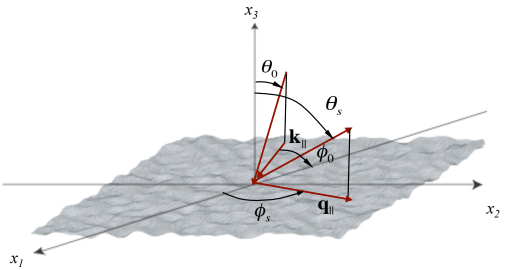
- $\boldsymbol{k}_{\|}$: the lateral wave vector of the incident wave
- $\boldsymbol{q}_{\|}$: the lateral wave vector of the diffracted wave characterized by $h = \{h_1, h_2\}$ (i.e. one of the scattered waves)
- $\boldsymbol{G}_{\|}(h)$: the reciprocal lattice vector characterized by h.

For *propagating waves* the lateral wave vectors are related to angles of incidence (θ_0, ϕ_0) and scattering $(\theta_s, \phi_s$ via

$$\boldsymbol{k}_{\|} = \frac{\omega}{c} \sin\theta_0 \,(\cos\phi_0, \sin\phi_0, 0) \qquad \boldsymbol{q}_{\|} = \frac{\omega}{c} \sin\theta_s \,(\cos\phi_s, \sin\phi_s, 0)$$

The random surface

$$\boxed{x_3 = \zeta(\boldsymbol{x}_\parallel)}$$



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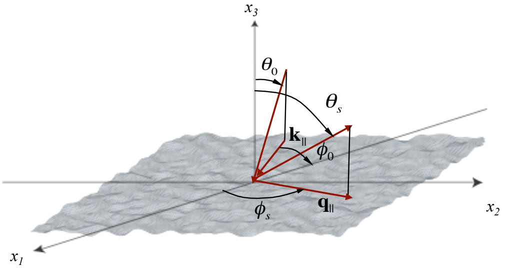

- The *total* field in the region $x_3 > \max \zeta(\boldsymbol{x}_\parallel)$ can be written as a sum of an incident and a scattered field as

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

- Here $R(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$ is the reflection amplitude from incident lateral wave vector $\boldsymbol{k}_\parallel$ to scattered lateral wave vector $\boldsymbol{q}_\parallel$.

The Rayleigh equation for a random surface is an integral equation of the form

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

where

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

and the matrix elements are

- Dirichlet surfaces

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

- Neumann surfaces

$$M(\boldsymbol{p}_\parallel|\boldsymbol{q}_\parallel) = \frac{\frac{\omega^2}{c^2} - \boldsymbol{p}_\parallel \cdot \boldsymbol{q}_\parallel}{\alpha_0(q_\parallel,\omega)} \qquad\qquad N(\boldsymbol{p}_\parallel|\boldsymbol{k}_\parallel) = -\frac{\frac{\omega^2}{c^2} - \boldsymbol{p}_\parallel \cdot \boldsymbol{k}_\parallel}{\alpha_0(k_\parallel,\omega)}$$

If the surface is periodic, i.e. if

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

where $\mathbf{x}_{\parallel}(\boldsymbol{\ell}) = \ell_1\mathbf{a}_1 + \ell_2\mathbf{a}_2$ are the translation vectors of a two-dimensional Bravais lattice, the reflection amplitude is non-zero in a finite number of directions.

One can show that

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

This is a consequence of the so-called Floquet-Bloch condition

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

The Rayleigh equation for the scattering amplitude $r(\mathbf{k}_\parallel + \mathbf{G}'_\parallel | \boldsymbol{k}_\parallel)$ of the periodic surface is

$$\sum_{\mathbf{K}'_\parallel} \hat{I}\left(-\alpha_0(K'_\parallel) \middle| \boldsymbol{K}_\parallel - \boldsymbol{K}'_\parallel\right) M(\boldsymbol{K}_\parallel | \boldsymbol{K}'_\parallel)\, r(\boldsymbol{K}'_\parallel | \boldsymbol{k}_\parallel) = -\hat{I}\left(\alpha_0(k_\parallel) \middle| \boldsymbol{K}_\parallel - \boldsymbol{k}_\parallel\right) N(\boldsymbol{K}_\parallel | \boldsymbol{k}_\parallel)$$

where

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

with a_c denoting the area of the unit cell, and

$$\boldsymbol{K}_\parallel = \boldsymbol{k}_\parallel + \boldsymbol{G}_\parallel \qquad\qquad \boldsymbol{K}'_\parallel = \boldsymbol{k}_\parallel + \boldsymbol{G}'_\parallel.$$

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Note

- $r(\boldsymbol{K}'_\parallel|\boldsymbol{k}_\parallel)$ is essentially a matrix
- The Rayleigh equation is an infinitely dimensional matrix equation
- How can we solve it?

Steps to solve the Rayleigh equation (for the periodic surface)

1. Start by restricting $\boldsymbol{K}'_{\parallel}$ to a finite number of modes, e.g.
   - $K_{\parallel} \leq 5\omega/c <$
   - $|K_i| \leq 5\omega/c$ $(i = 1, 2)$
   - restrict $\boldsymbol{K}'_{\parallel} = \boldsymbol{K}'_{\parallel}(h)$ to $-H \leq h_i \leq H$ (i=1,2)

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3. Determine a storage convention to use of $r(\boldsymbol{K}'_{\parallel}|\boldsymbol{k}_{\parallel})$
   - If $r(\boldsymbol{K}'_{\parallel}(h)|\boldsymbol{k}_{\parallel})$ is represented by a matrix $r(h_1, h_2)$, a vector can be obtained by storing it column-by-column (or row-by-row). [Hint: reshape may be useful here!]
   - Note that the form of the matrix of the linear system depends on the storage convention that you choose.

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5. Use a linear solver to obtain $r(\boldsymbol{K}'_{\parallel}|\boldsymbol{k}_{\parallel})$

Physical observable — Diffraction efficiencies

The ratio of the total, time-averages power flux that is incident and scattered by the surface is

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

where the diffraction efficiency from $\boldsymbol{k}_\parallel$ into a mode characterized by $\boldsymbol{k}_\parallel + \boldsymbol{G}_\parallel$ is

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

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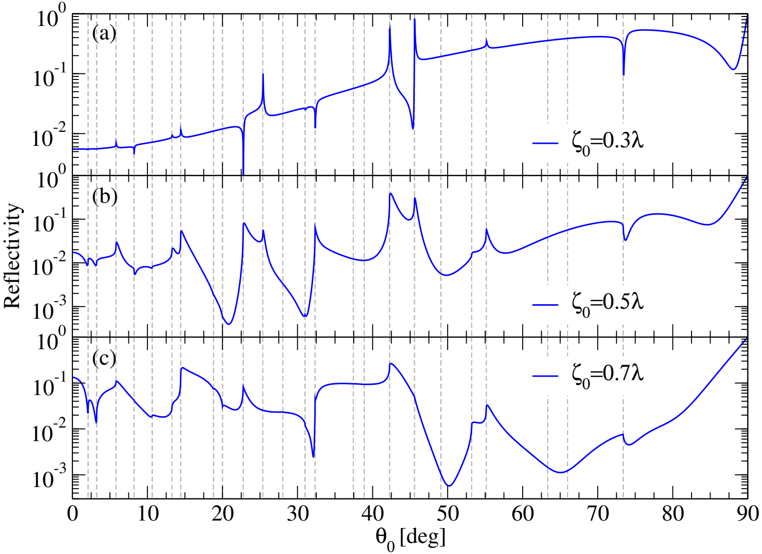
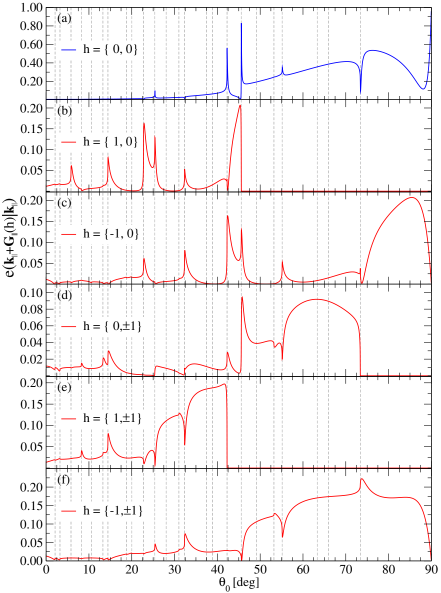
Energy conservation :
Since there is no absorption in the scattering from a rigid surface

$$\boxed{\mathcal{U} = \frac{P_{\mathrm{sc}}}{P_{\mathrm{inc}}} = \sum_{\boldsymbol{G}_\parallel}{}' e\left(\boldsymbol{k}_\parallel + \boldsymbol{G}_\parallel | \boldsymbol{k}_\parallel\right) \equiv 1}.$$

This condition can be used to check the quality of the simulation results.



Ref: Figure 1 from Low. Temp. Phys. **44**, 733 (2018)



Ref: Figure 4 from Low. Temp. Phys. **44**, 733 (2018)

Questions