FY8904 Assignment 3

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Abstract

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Introduction

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[2]

Theory

The periodic surface Rayleigh equation

We will solve numerically the *periodic surface Rayleigh equation*

$$\sum_{\boldsymbol{K}'_\parallel} \hat{I}\Big(-\alpha_0(K'_\parallel,\omega)\big|\boldsymbol{K}_\parallel - \boldsymbol{K}'_\parallel\Big) M\big(\boldsymbol{K}_\parallel\big|\boldsymbol{K}'_\parallel\big) r\big(\boldsymbol{K}'_\parallel\big|\boldsymbol{k}_\parallel\big) = -\hat{I}\Big(\alpha_0(k_\parallel,\omega)\big|\boldsymbol{K}_\parallel - \boldsymbol{k}_\parallel\Big) N\big(\boldsymbol{K}_\parallel\big|\boldsymbol{k}_\parallel\big), \tag{1}$$

or

$$\sum_{\boldsymbol{K}'_\parallel} \hat{I}\Big(-\alpha_0(K'_\parallel,\omega)\big|\boldsymbol{G}_\parallel - \boldsymbol{G}'_\parallel\Big) M\big(\boldsymbol{K}_\parallel\big|\boldsymbol{K}'_\parallel\big) r\big(\boldsymbol{K}'_\parallel\big|\boldsymbol{k}_\parallel\big) = -\hat{I}\Big(\alpha_0(k_\parallel,\omega)\big|\boldsymbol{G}_\parallel\Big) N\big(\boldsymbol{K}_\parallel\big|\boldsymbol{k}_\parallel\big), \tag{2}$$

where the lateral wave vectors $\boldsymbol{K}_\parallel$ and $\boldsymbol{K}_\parallel$ are defined as

$$\boldsymbol{K}_\parallel = \boldsymbol{k}_\parallel + \boldsymbol{G}_\parallel \qquad\qquad \boldsymbol{K}'_\parallel = \boldsymbol{k}_\parallel + \boldsymbol{G}'_\parallel, \tag{3}$$

and $\boldsymbol{G}_\parallel$ are the lattice sites of the reciprocal lattice of the doubly periodic surface profile $\xi(\boldsymbol{x})$, given by

$$\boldsymbol{G}_\parallel(\boldsymbol{h}) = h_1\boldsymbol{b}_1 + h_2\boldsymbol{b}_2, \qquad h_i \in \mathbb{Z}. \tag{4}$$

We will use a square lattice with translation vectors $\boldsymbol{a}_1 = a\hat{\boldsymbol{x}}_1$ and $\boldsymbol{a}_2 = a\hat{\boldsymbol{x}}_2$ which means that the reciprocal lattice vectors are $\boldsymbol{b}_1 = (2\pi/a)\hat{\boldsymbol{x}}_1$ and $\boldsymbol{b} = (2\pi/a)\hat{\boldsymbol{x}}_2$, and

$$\boldsymbol{G}_\parallel(\boldsymbol{h}) = h_1\frac{2\pi}{a}\hat{\boldsymbol{x}}_1 + h_2\frac{2\pi}{a}\hat{\boldsymbol{x}}_2, \qquad h_i \in \mathbb{Z}. \tag{5}$$

The wave vector $\boldsymbol{k}$ represents the incident wave, and is written in the form

$$\boldsymbol{k} = \boldsymbol{k}_\parallel \pm \alpha_0(k_\parallel,\omega)\hat{\boldsymbol{x}}_3 \tag{6}$$

with

$$\alpha_0(k_\parallel,\omega) = \begin{cases} \sqrt{\frac{\omega^2}{c^2} - k_\parallel^2} & k_\parallel^2 < \frac{\omega^2}{c^2} \\ i\sqrt{k_\parallel^2 - \frac{\omega^2}{c^2}} & k_\parallel^2 \geq \frac{\omega^2}{c^2} \end{cases}. \tag{7}$$

The wavelength of the incident beam is denoted by λ, and is related to the angular frequency ω via $\omega/c = 2\pi/\lambda$. From geometry considerations it can be shown that

$$\boldsymbol{k}_\parallel = \frac{\omega}{c}\sin\theta_0\big(\cos\phi_0, \sin\phi_0, 0\big). \tag{8}$$

The set of solutions $\big\{r\big(\boldsymbol{K}'_\parallel\big|\boldsymbol{k}_\parallel\big)\big\}$ of Eq. (1) describes the reflection of an incident scalar wave of lateral wave vector $_\parallel$ that is scattered by a periodic surface $\xi(\boldsymbol{x}_\parallel)$ into reflected waves characterized by the wave vector $\boldsymbol{K}'_\parallel$.

The $\hat{I}$-integrals are defined in the next section.

To be able to solve Eq. (1) we limit the values of

$$\boldsymbol{K}'_{\parallel}(\boldsymbol{h}) = \boldsymbol{k} + \boldsymbol{G}'_{\parallel}(\boldsymbol{h}) \tag{9}$$

by limiting the components of $\boldsymbol{h} = (h_1, h_2)$ to

$$h_i \in [-H, H] \quad (h_i \in \mathbb{Z}), \tag{10}$$

where H is a positive integer. We then have a finite set of $N = n^2 = (2H+1)^2$ unknown scattering amplitudes $r(\boldsymbol{K}'_{\parallel}|\boldsymbol{k}_{\parallel})$. We then let $\boldsymbol{K}_{\parallel}$ take the same values as $\boldsymbol{K}'_{\parallel}$, which gives us N different variants of Eq. (1). We can then express Eq. (1) as a linear system of N equations and N unknowns, $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$, where

$$\boldsymbol{A} = \begin{pmatrix} A_{1,1} & A_{1,2} & \dots & A_{1,N} \\ A_{2,1} & A_{2,2} & \dots & A_{2,N} \\ \vdots & \vdots & \ddots & \vdots \\ A_{N,1} & A_{N,2} & \dots & A_{N,N} \end{pmatrix} \tag{11}$$

where $A_{i,j}$ is the pre-factor before r in the sum in Eq. (1),

$$A_{i,j} = \hat{I}\left(-\alpha_0\left(K'^{j}_{\parallel}, \omega\right)\middle|\boldsymbol{K}^{i}_{\parallel} - \boldsymbol{K}'^{j}_{\parallel}\right) M\left(\boldsymbol{K}^{i}_{\parallel}\middle|\boldsymbol{K}'^{j}_{\parallel}\right), \tag{12}$$

and

$$\boldsymbol{K}^{i}_{\parallel} = \boldsymbol{K}_{\parallel}(\boldsymbol{h}_i) \tag{13}$$

$$\boldsymbol{K}'^{j}_{\parallel} = \boldsymbol{K}'_{\parallel}(\boldsymbol{h}_j) \tag{14}$$

Further we have

$$\boldsymbol{x} = \begin{pmatrix} r\left(\boldsymbol{K}'^{1}_{\parallel}|\boldsymbol{k}_{\parallel}\right) \\ r\left(\boldsymbol{K}'^{2}_{\parallel}|\boldsymbol{k}_{\parallel}\right) \\ \dots \\ r\left(\boldsymbol{K}'^{N-1}_{\parallel}|\boldsymbol{k}_{\parallel}\right) \\ r\left(\boldsymbol{K}'^{N}_{\parallel}|\boldsymbol{k}_{\parallel}\right) \end{pmatrix} \tag{15}$$

and

$$\{\boldsymbol{h}_i\} = \boldsymbol{h}_1, \boldsymbol{h}_2, \dots, \boldsymbol{h}_n = \begin{matrix} (h_1, h_1), & (h_1, h_2), & \dots & (h_1, h_{n-1}), & (h_1, h_n), \\ (h_2, h_1), & (h_2, h_2), & \dots & (h_2, h_{n-1}), & (h_2, h_n), \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ (h_{n-1}, h_1), & (h_{n-1}, h_2), & \dots & (h_{n-1}, h_{n-1}), & (h_{n-1}, h_n), \\ (h_n, h_1), & (h_n, h_2), & \dots & (h_n, h_{n-1}), & (h_n, h_n). \end{matrix}$$

($\{\boldsymbol{h}_i\}$ is not not a matrix, but is represented in a matrix form above to more easily make the connection to the matrix in Eq. (11)). In practice this is implemented as

$$\boldsymbol{h}_i = (h_j, h_k) \quad \text{where} \quad j = i \mathbin{/\!/} n \quad \text{and} \quad k = i \bmod n, \tag{16}$$

where $/\!/$ is integer division and mod is the *modulo* operator. This allows us to loop over the linear index i in the code.

The $\hat{I}$-integral

For a *doubly periodic cosine profile* of period a and amplitude ξ_0 we can calculate the $\hat{I}$-integral in closed form as [1]

$$\hat{I}\left(\gamma|\boldsymbol{G}_{\parallel}(\boldsymbol{h})\right) = (-i)^{h_1} \mathrm{J}_{h_1}\left(\frac{\gamma\xi_0}{2}\right)(-i)^{h_2} \mathrm{J}_{h_2}\left(\frac{\gamma\xi_0}{2}\right), \tag{17}$$

where $\mathrm{J}_n(\cdot)$ is the Bessel function of first kind and order n. The Bessel functions are evaluated via the `SciPy` function `scipy.special.jv` with the argument `order=n`.

For a truncated cone surface profile it can be shown that [1]

$$\hat{I}\big(\gamma|\boldsymbol{G}_\parallel(\boldsymbol{h})\big) = \delta_{\boldsymbol{G}_\parallel,\boldsymbol{0}} + 2\pi\frac{\rho_t^2}{a^2}\Big[\exp\left(-i\gamma\xi_0\right)\Big]\frac{J_1(G_\parallel\rho_t)}{G_\parallel\rho_t} \tag{18}$$

$$+ 2\pi\frac{\rho_b-\rho_t}{a^2}\sum_{n=1}^{\infty}\frac{(-i\gamma\xi_0)^n}{n!}\int_0^1 \mathrm{d}u_\parallel\left[\rho_b-(\rho_b-\rho_t)u_\parallel\right]J_0\Big(G_\parallel\left[\rho_b-(\rho_b-\rho_t)u_\parallel\right]\Big)u_\parallel^n, \tag{19}$$

where δ is the Kronecker-delta, and a change of variable has been performed

$$u_\parallel = \frac{\rho_b - x_\parallel}{\rho_b-\rho_t}. \tag{20}$$

Finally, for a truncated cosine surface profile we have [1]

$$\hat{I}\big(\gamma|\boldsymbol{G}_\parallel(\boldsymbol{h})\big) = \delta_{\boldsymbol{G}_\parallel,\boldsymbol{0}} + \frac{2\pi}{a^2}\sum_{n=1}^{\infty}\frac{(-i\gamma)^n}{n!}\int_0^{\rho_0}\mathrm{d}x_\parallel x_\parallel J_0(G_\parallel x_\parallel)\xi^n(x_\parallel) \tag{21}$$

The integrals in Eqs. (19) and (21) were evaluated numerically, and enough terms were included in the sum for it to converge (typically 5-10 terms were needed).

Nondimensionalizing

We will be using the wavelength as the length scale $x_0 = \lambda$ when numerically solving the equations.

Results and discussion

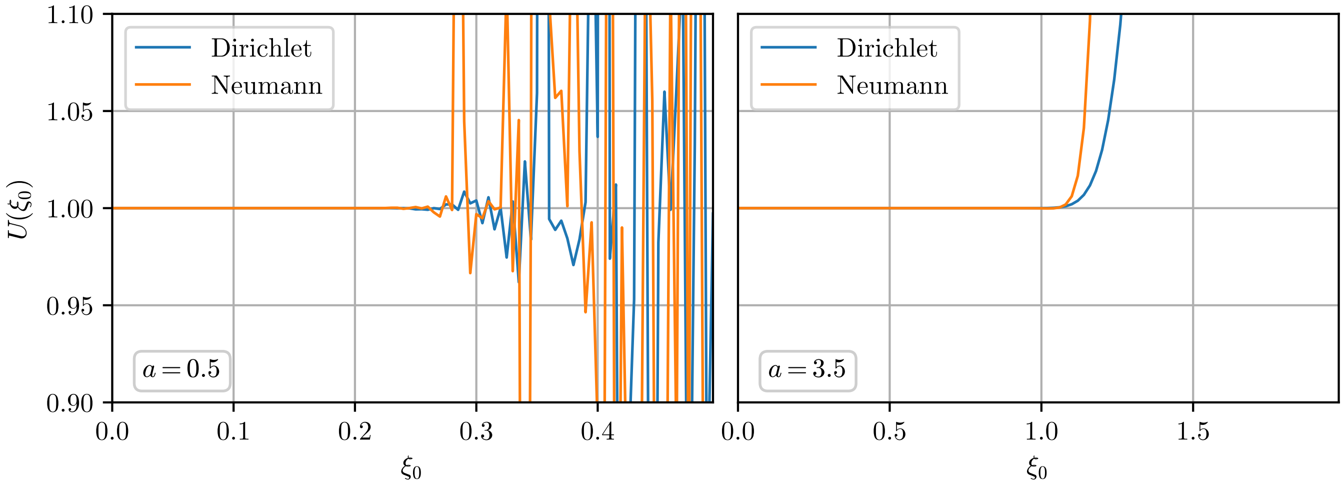


Figure 1: Plot of $\mathcal{U}$ as function of the surface profile amplitude ξ_0 for normal incidence, $\boldsymbol{k}_\parallel = 0$. In the left plot we have used $a/\lambda = 0.5$ and in the right $a/\lambda = 3.5$. The results for both Dirichlet and Neumann doubly periodic cosine surfaces are shown. A value of $H = 9$ was used in all computations.

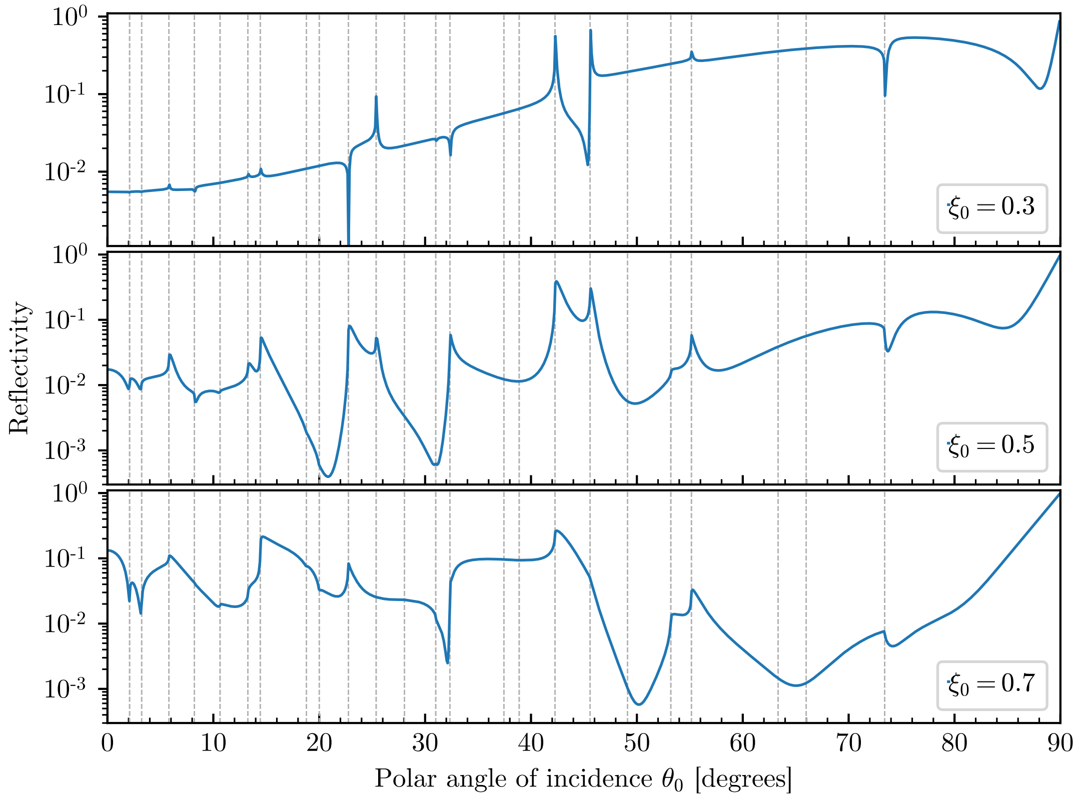


Figure 2: Fig1

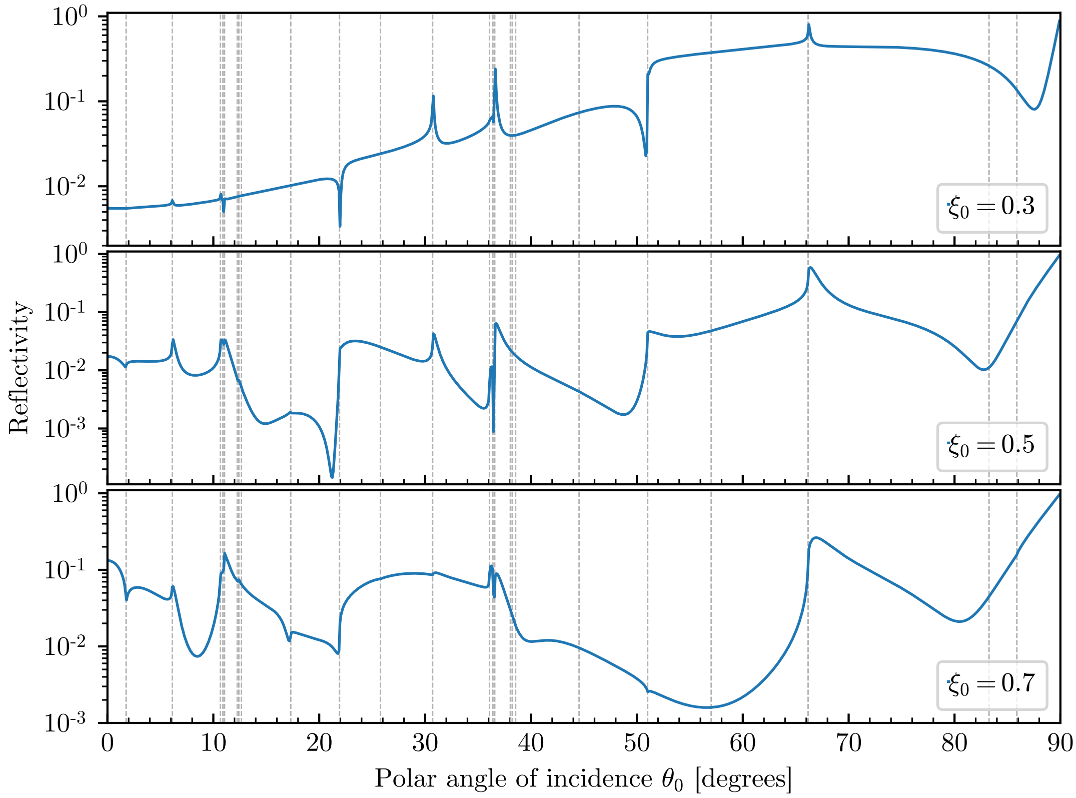


Figure 3: Fig2

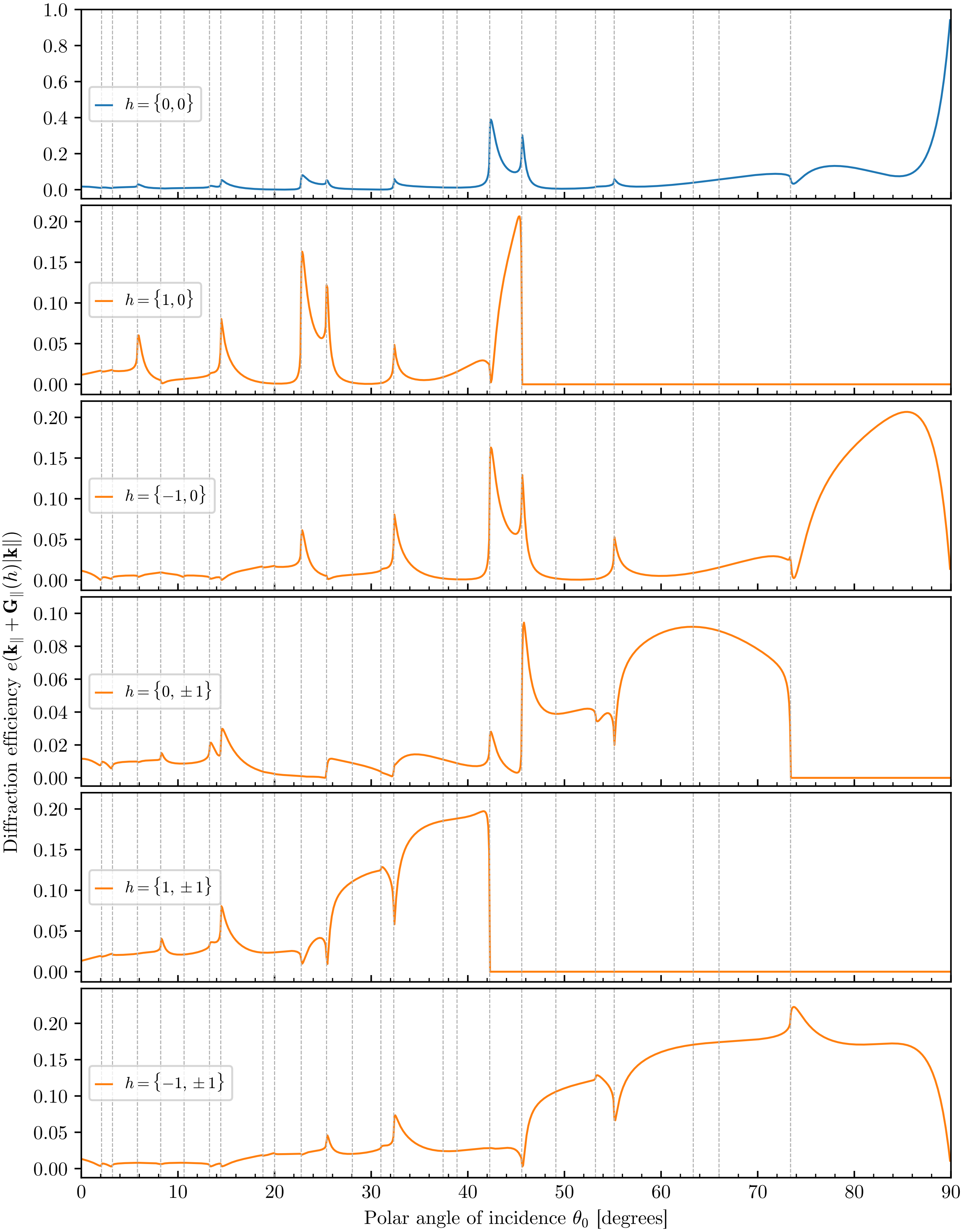
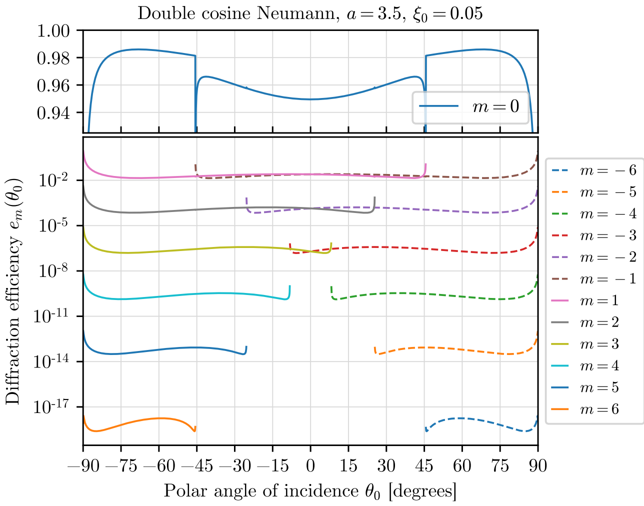
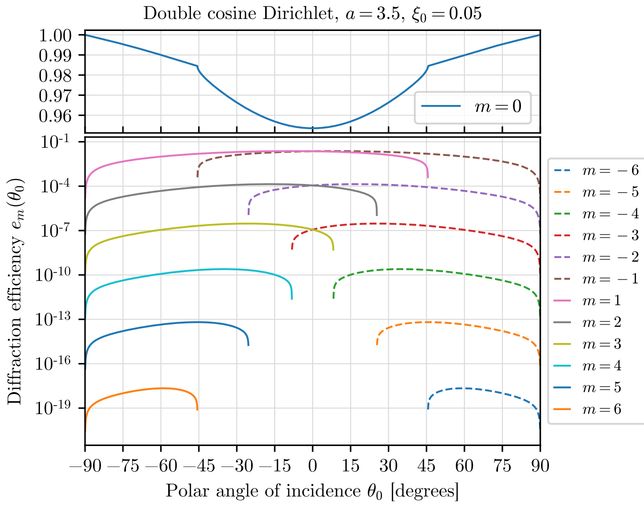


Figure 4: Fig4


Double cosine Neumann, $a = 3.5$, $\xi_0 = 0.05$
$m = 0$
Diffraction efficiency $e_m(\theta_0)$
$m = -6$, $m = -5$, $m = -4$, $m = -3$, $m = -2$, $m = -1$, $m = 1$, $m = 2$, $m = 3$, $m = 4$, $m = 5$, $m = 6$
Polar angle of incidence θ_0 [degrees]


Double cosine Dirichlet, $a = 3.5$, $\xi_0 = 0.05$
$m = 0$
Diffraction efficiency $e_m(\theta_0)$
$m = -6$, $m = -5$, $m = -4$, $m = -3$, $m = -2$, $m = -1$, $m = 1$, $m = 2$, $m = 3$, $m = 4$, $m = 5$, $m = 6$
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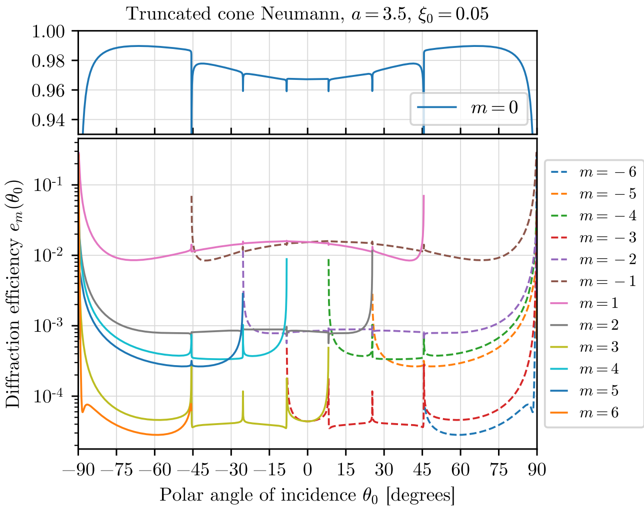
Truncated cone Neumann, $a = 3.5$, $\xi_0 = 0.05$
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Diffraction efficiency $e_m(\theta_0)$
$m = -6$, $m = -5$, $m = -4$, $m = -3$, $m = -2$, $m = -1$, $m = 1$, $m = 2$, $m = 3$, $m = 4$, $m = 5$, $m = 6$
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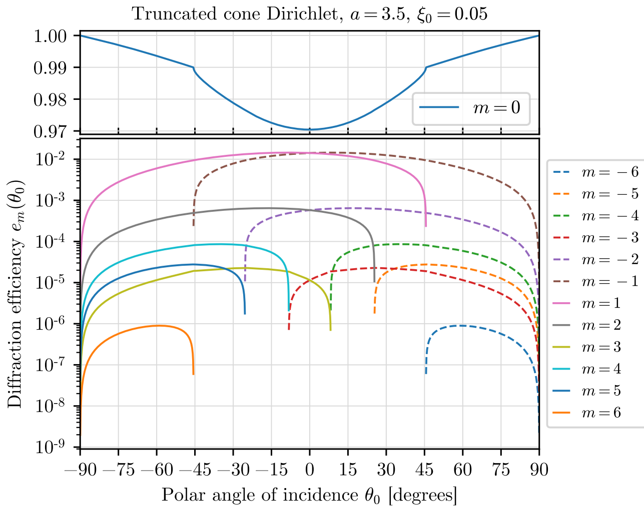
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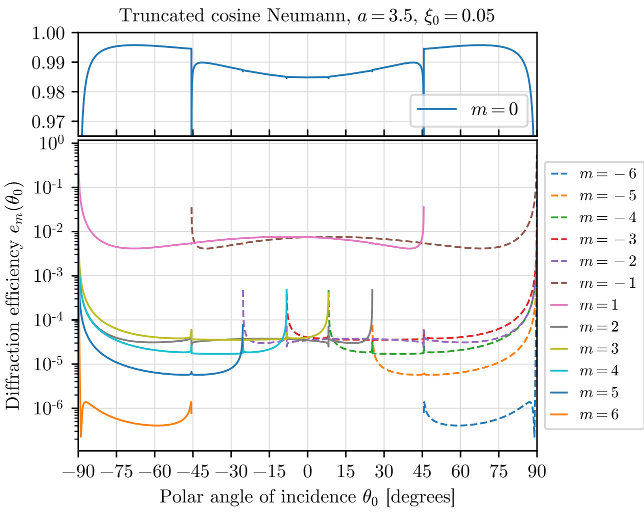
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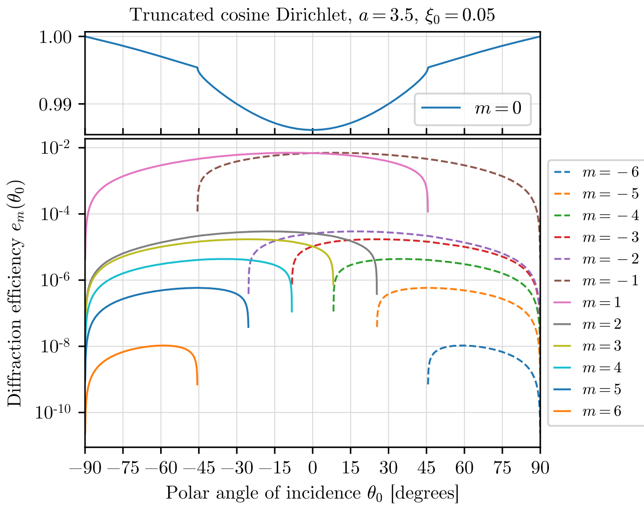
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Polar angle of incidence θ_0 [degrees]

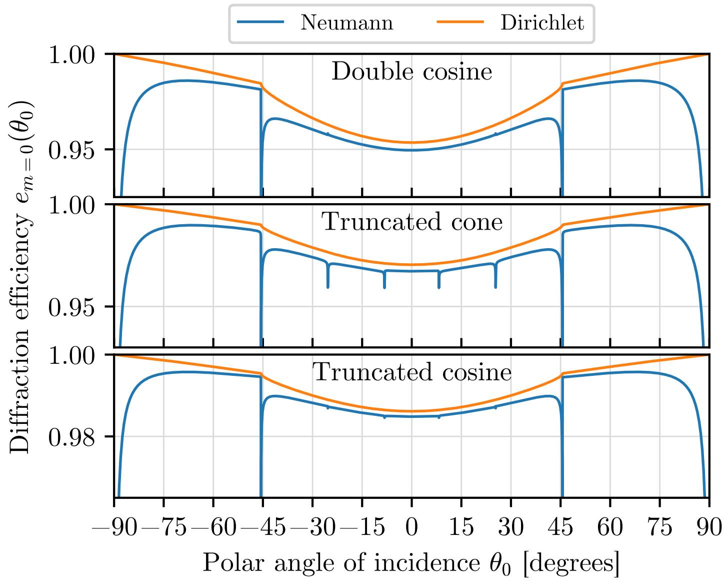

Figure 5: Diffraction efficiency as function of angle of incidence for $m = 0$, for three types of surface profile functions and both Dirichlet and Neumann boundary conditions.

Conclusion

References

[1] A. A. Maradudin, V. Pérez-Chávez, A. Jędrzejewski, and I. Simonsen. "Features in the diffraction of a scalar plane wave from doubly-periodic Dirichlet and Neumann surfaces". In: *Low Temperature Physics* 44.7 (2018), pp. 733–743.

[2] M. J. Powell. "A hybrid method for nonlinear equations". In: *Numerical methods for nonlinear algebraic equations* (1970).