FY8904 Assignment 3

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Abstract

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Introduction

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Theory

The periodic surface Rayleigh equation

We will solve numerically the *periodic surface Rayleigh equation*

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

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

$$\boldsymbol{K}_\parallel = \boldsymbol{k}_\parallel + \boldsymbol{G}_\parallel \qquad\qquad \boldsymbol{K}'_\parallel = \boldsymbol{k}_\parallel + \boldsymbol{G}'_\parallel, \tag{2}$$

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

$$\boldsymbol{G}_\parallel(\boldsymbol{h}) = h_1\boldsymbol{b}_1 + h_2\boldsymbol{b}_2, \qquad h_i \in \mathbb{Z}. \tag{3}$$

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

$$\boldsymbol{G}_\parallel(\boldsymbol{h}) = h_1\frac{2\pi}{a}\hat{\boldsymbol{x}}_1 + h_2\frac{2\pi}{a}\hat{\boldsymbol{x}}_2, \qquad h_i \in \mathbb{Z}. \tag{4}$$

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

$$\boldsymbol{k} = \boldsymbol{k}_\parallel \pm \alpha_0(k_\parallel,\omega)\hat{\boldsymbol{x}}_3 \tag{5}$$

with

$$\alpha_0(k_\parallel,\omega) = \begin{cases} \sqrt{\frac{\omega^2}{c^2} - k_\parallel^2} & k_\parallel^2 < \frac{\omega^2}{c^2} \\ i\sqrt{k_\parallel^2 - \frac{\omega^2}{c^2}} & k_\parallel^2 \geq \frac{\omega^2}{c^2} \end{cases}. \tag{6}$$

The wavelength of the incident beam is denoted by λ, and is related to the angular frequency ω via $\omega/c = 2\pi/\lambda$.

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 the periodic surface $\xi(\boldsymbol{x}_\parallel$ into reflected waves characterized by the wave vector $\boldsymbol{K}'_\parallel$.

The $\hat{I}$-integrals are defined elsewhere.

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

$$\boldsymbol{K}'_\parallel(\boldsymbol{h}) = \boldsymbol{k} + \boldsymbol{G}'_\parallel(\boldsymbol{h}) \tag{7}$$

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

$$h_i \in [-H, H] \quad (h_i \in \mathbb{Z}), \tag{8}$$

where H is a positive integer. We then have a finite set of $N = n^2 = (2H)^2$ 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 evaluations of Eq. (1). We can then express Eq. (1) as a linear system of equations $\boldsymbol{Ax} = \boldsymbol{b}$, where

$$\boldsymbol{A} = \begin{pmatrix} A_{1,1} & A_{1,2} & \dots & A_{1,N} \\ A_{2,1} & A_{2,2} & \dots & A_{2,N} \\ \vdots & \vdots & \ddots & \vdots \\ A_{N,1} & A_{N,2} & \dots & A_{N,N} \end{pmatrix} \tag{9}$$

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

$$A_{i,j} = \hat{I}\Big(-\alpha_0\big(K'^{j}_\parallel, \omega\big)\big|\boldsymbol{K}^i_\parallel - \boldsymbol{K}'^{j}_\parallel\Big) M\big(\boldsymbol{K}^i_\parallel\big|\boldsymbol{K}'^{j}_\parallel\big), \tag{10}$$

and

$$\boldsymbol{K}^i_\parallel = \boldsymbol{K}_\parallel(\boldsymbol{h}_i) \tag{11}$$

$$\boldsymbol{K}'^{j}_\parallel = \boldsymbol{K}'_\parallel(\boldsymbol{h}_j) \tag{12}$$

Further we have

$$\boldsymbol{x} = \begin{pmatrix} r\Big(\boldsymbol{K}'^{1}_\parallel|\boldsymbol{k}_\parallel\Big) \\ r\Big(\boldsymbol{K}'^{2}_\parallel|\boldsymbol{k}_\parallel\Big) \\ \dots \\ r\Big(\boldsymbol{K}'^{N-1}_\parallel|\boldsymbol{k}_\parallel\Big) \\ r\Big(\boldsymbol{K}'^{N}_\parallel|\boldsymbol{k}_\parallel\Big) \end{pmatrix} \tag{13}$$

and

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

In practice this is implemented as

$$\boldsymbol{h}_i = (h_j, h_k) \quad \text{where} \quad j = i \mathbin{/\!/} n \quad \text{and} \quad k = i \bmod n, \tag{14}$$

where // is integer division and mod is the *modulo* operator.

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

$$\hat{I}\big(\gamma|\boldsymbol{G}_\parallel(\boldsymbol{h})\big) = (-i)^{h_1} \mathrm{J}_{h_1}\left(\frac{\gamma\xi_0}{2}\right)(-i)^{h_2} \mathrm{J}_{h_2}\left(\frac{\gamma\xi_0}{2}\right), \tag{15}$$

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`.

Results and discussion

Particle in a box

Conclusion

References

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