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Problem 12.1: Structure factor

[**Written** | 4 pt(s)]

ID: ex_structure_factor:edyn23

Learning objective

We will investigate how light is scattered on a crystal and how its diffraction pattern can give insight on the structure of the crystal.

We model a simple crystal by identical little dielectric spheres of the size of an atom (radius $\propto 1\text{Å} = 10^{-10}\,\text{m}$) placed in a regular fashion on the points of a lattice. An incident monochromatic plane wave gets scattered on the crystal. We want to compute the differential scattering cross section of the scattered radiation. Of paramount importance is the *structure factor* for the distribution of scatterers. For a crystalline arrangement, a characteristic pattern of diffraction angles (points of scattered light on a screen) is obtained. This is the *Laue diffraction pattern*, which allows to determine the crystal structure.

a) Compute the differential scattering cross section for a simple cubic (sc) crystal of edge length Na where a is the distance between two atoms. Assume that the incident electric field induces dipole moments $\boldsymbol{p}_j$ and $\boldsymbol{m}_j$ in the atom at lattice point $\boldsymbol{x}_j$. The plane wave is at normal incidence to one of the surfaces of the crystal (xy-plane) and has the wave vector $\boldsymbol{k}_{\text{in}}$. **1**pt(s)

b) Compute the structure factor $S(\boldsymbol{q}) = |\sum_{\boldsymbol{x}\in\Gamma} e^{i\boldsymbol{q}\cdot\boldsymbol{x}}|^2$, where Γ denotes the set of lattice points. The scattering vector $\boldsymbol{q} = \boldsymbol{k}_{\text{in}} - |\boldsymbol{k}_{\text{in}}|\hat{\boldsymbol{r}}$ depends on the position of the observer; $\hat{\boldsymbol{r}}$ is a unit vector pointing towards the observer. In which direction will the observer see maxima of diffracted intensity? Use spherical coordinates (θ, ϕ). **1**pt(s)

c) Take the limit $N \to \infty$ for the structure factor $S(\boldsymbol{q})$. **1**pt(s)

d) Now compute the structure factor for a body centered cubic (bcc) crystal, which is a cubic crystal where an additional atom is placed in the center of each cubic unit cell. Which scattering peaks appear or disappear compared to the simple cubic lattice? **1**pt(s)

Problem 12.2: Fraunhofer diffraction from a circular aperture

[**Oral** | 3 pt(s)]

ID: ex_fraunhofer_diffraction_circular_aperture:edyn23

Learning objective

In this exercise, we will make use of the special properties of the Bessel functions to calculate the diffracted intensity of a circular aperture in the Fraunhofer limit.

a) In the Fraunhofer limit the diffracted scalar amplitude $u(p,q)$ is the 2D Fourier transform of the characteristic function $C(\xi,\eta)$ of the aperture, **1** pt(s)

$$u(p,q) = \frac{\sqrt{I_0}}{S_A} \int C(\xi,\eta) e^{-ik(p\xi+q\eta)}\, \mathrm{d}\xi\, \mathrm{d}\eta, \tag{1}$$

with wave vector $k \equiv \frac{2\pi}{\lambda}$ and $p \equiv \alpha - \alpha_0$, $q \equiv \beta - \beta_0$ denoting the difference of directional cosines (see lecture notes). S_A is the surface area of the aperture and $I_0 = |u(0,0)|^2$. Consider a circular aperture of radius a whose characteristic function is

$$C(\xi,\eta) = \begin{cases} 1 & \text{for } \sqrt{\xi^2+\eta^2} \le a \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

and compute the diffracted intensity $I(p,q) = |u(p,q)|^2$ in the Fraunhofer limit.

Hint: Go to cylindrical coordinates and use the integral representation of the Bessel function

$$J_n(x) = \frac{1}{2\pi i^n} \int_0^{2\pi} e^{ix\cos\phi} e^{in\phi} \mathrm{d}\phi, \tag{3}$$

which holds for any $n \in \mathbb{Z}$. Furthermore use the following relation:

$$\int_0^x x' J_0(x')\, \mathrm{d}x' = x J_1(x). \tag{4}$$

In the following subtasks, we will prove the relations in Eq. (4) and Eq. (3) to verify that our calculations in part a) are correct.

b) The ordinary Bessel function $J_n(x)$ is a solution to the second order differential equation **1** pt(s)

$$x^2 \frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + x\frac{\mathrm{d}y}{\mathrm{d}x} + (x^2 - n^2) y = 0. \tag{5}$$

Show that if $J_{n+1}(x)$ is a solution of the Bessel equation of order $n+1$, then

$$J_n = x^{-(n+1)} \frac{\mathrm{d}}{\mathrm{d}x} \left[x^{n+1} J_{n+1}(x) \right] \tag{6}$$

is a solution of order n. Conclude that

$$\int_0^x x' J_0(x')\, \mathrm{d}x' = x J_1(x). \tag{7}$$

c) For $n \in \mathbb{Z}$, we can write the Bessel function $J_n(x)$ as an integral **1**pt(s)

$$J_n(x) = \frac{1}{2\pi i^n} \int_0^{2\pi} e^{ix\cos\phi} e^{in\phi} \mathrm{d}\phi. \tag{8}$$

Show, that this indeed solves Eq. (5).

Problem 12.3: Fourier optics

[**Oral** | 3 pt(s)]

ID: ex_fourier_optics:edyn23

> **Learning objective**
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> In this exercise we are going to use the properties of Fourier transforms to obtain the Fraunhofer diffraction pattern of more complicated structures in a systematic way.

a) Show that an aperture consisting of two circular holes of radius a with their centers located at $(\eta, \xi) = (-\frac{d}{2}, 0)$ and $(\eta, \xi) = (+\frac{d}{2}, 0)$, respectively, can be written as a convolution of one circular hole with two delta functions located at $(\eta, \xi) = (-\frac{d}{2}, 0)$ and $(\eta, \xi) = (+\frac{d}{2}, 0)$. Write down the Fraunhofer diffraction pattern of this aperture using the convolution theorem for Fourier transforms. **Hint:** An arbitrarily shaped aperture $A(\boldsymbol{r} = (\eta, \xi))$ can be replicated at positions $\{\boldsymbol{r}_i\}$ by a convolution operation with an array of delta functions $\Omega_\delta = \sum_i \delta(\boldsymbol{r} - \boldsymbol{r}_i)$. Schematically: **1**pt(s)

$$\text{Tiling of apertures } A = (\Omega_\delta * A)(\boldsymbol{r}) \equiv \int \sum_i \delta(\boldsymbol{r'} - \boldsymbol{r}_i) A(\boldsymbol{r} - \boldsymbol{r}')\, \mathrm{d}^2 r' = \sum_i A(\boldsymbol{r} - \boldsymbol{r}_i). \tag{9}$$

b) Let $\mathcal{A}_1$ and $\mathcal{A}_2$ be two apertures such that the extension of $\mathcal{A}_2$ in a particular direction, e.g. in ξ-direction, is μ times that of $\mathcal{A}_1$. Show by a suitable change of integration variables from (ξ, η) to (ξ', η') in the Fraunhofer integral that the diffracted amplitudes obey **1**pt(s)

$$u_2(p, q) = \mu u_1(\mu p, q). \tag{10}$$

Using this result, write down the Fraunhofer diffraction pattern of an aperture which has the shape of an ellipse.

c) Using the results of a) and b), write down the Fraunhofer diffraction pattern of the aperture shown in the figure below, which consists of three elliptical holes placed at the vertices of an equilateral triangle. **1**pt(s)