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Problem 1: Structure factor (Written)

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 $\mathbf{p}_j$ and $\mathbf{m}_j$ in the atom at lattice point $\mathbf{x}_j$. The plane wave is at normal incidence to one of the surfaces of the crystal (xy-plane) and has the wave vector $\mathbf{k}_{\text{in}}$.

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

c) Take the limit $N \to \infty$ for the structure factor $S(\mathbf{q})$.

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 ?

Problem 2: Fraunhofer diffraction from a circular aperture (Written)

Learning objective

After showing that the Bessel functions obey a recurrence relation in the first part, the second part will make use of this property to calculate the diffracted intensity of a circular aperture in the Fraunhofer limit.

a) The ordinary Bessel function $J_n(x)$ is a solution to the second order differential equation

$$x^2\frac{d^2y}{dx^2} + x\frac{dy}{dx} + (x^2 - n^2)y = 0. \tag{1}$$

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

$$J_n = x^{-(n+1)} \frac{d}{dx} \left[x^{n+1} J_{n+1}(x)\right] \tag{2}$$

is a solution of order n. Conclude that

$$\int_0^x x' J_0(x') = x J_1(x). \tag{3}$$

b) 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,

$$u(p,q) = \frac{\sqrt{I_0}}{S_A} \int C(\xi,\eta) e^{-ik(p\xi+q\eta)}\, d\xi\, d\eta, \tag{4}$$

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

$$C(\xi,\eta) = \begin{cases} 1 & \text{for } \sqrt{\xi^2+\eta^2} \leq a \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

and compute the diffracted intensity $I(p,q) = |u(p,q)|^2$ in the Fraunhofer limit. Go to cylindrical coordinates and use the integral representation of the Bessel function

$$J_n(x) = \frac{1}{2\pi i^n} \int_0^{2\pi} e^{ix\cos\phi} e^{in\phi} d\phi. \tag{6}$$

Make use of the results from a).

Problem 3: Fourier optics (Bonus)

Learning objective

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. The points for this exercise do not count to the total number of points of which 80% are required to obtain the “Schein”. Students who are short on points should see this exercise as an opportunity to improve their score in order to fulfill the Schein criteria.

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.

Remark: An arbitrarily shaped aperture $A(\mathbf{r} = (\eta,\xi))$ can be replicated at positions $\{\mathbf{r}_i\}$ by a convolution operation with an array of delta functions $\Omega_\delta = \sum_i \delta(\mathbf{r}' - \mathbf{r}_i)$. Schematically:

$$\text{Tiling of apertures } A = (\Omega_\delta * A)(\mathbf{r}) \equiv \int \sum_i \delta(\mathbf{r}' - \mathbf{r}_i) A(\mathbf{r} - \mathbf{r}') d^2 r' = \sum_i A(\mathbf{r} - \mathbf{r}_i). \tag{7}$$

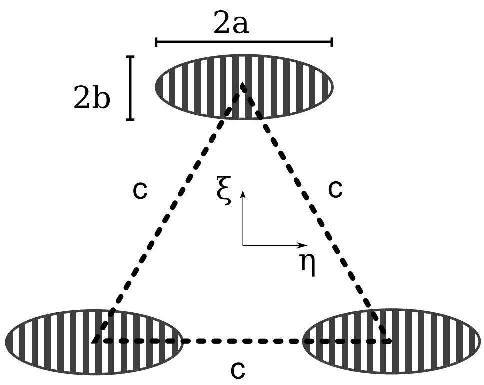
b) Let $\mathcal{A}_1$ and $\mathcal{A}_2$ be two apertures such that the extension of $\mathcal{A}_2$ in a particular direction, e.g. in ξ-direction, is μ times that of $\mathcal{A}_1$. Show by a suitable change of integration variables from (ξ, η) to (ξ', η') in the Fraunhofer integral that the diffracted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

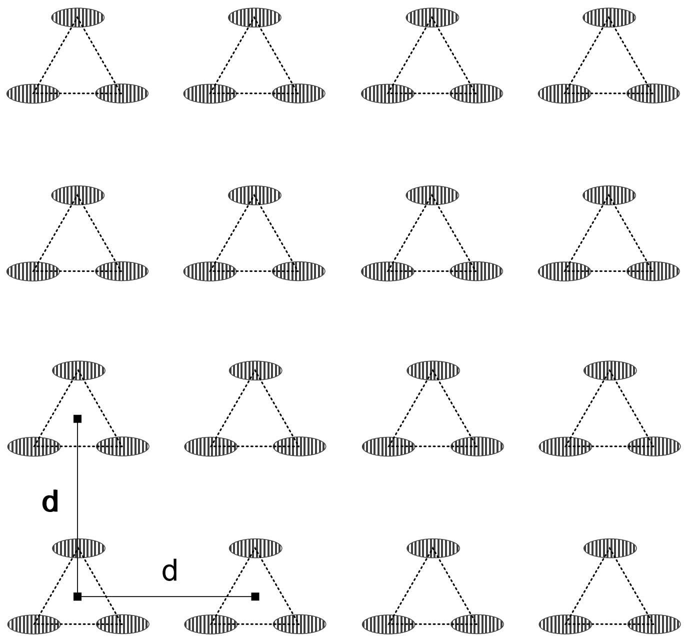
$$u_2(p, q) = \mu u_1(\mu p, q). \tag{8}$$

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 on the left, which consists of three elliptical holes placed at the vertices of an equilateral triangle.

d) Write down the Fraunhofer diffraction pattern for the aperture shown in the figure below on the right. There, the three holes have been replicated on a 4×4 square grid to give a regular arrangement of holes.





Problem 4: Lorentz Group (Written)

Learning objective

This exercise serves to become familiar with groups and their properties. Groups play a fundamental role in all fields of physics and can tremendously simplify otherwise very challenging problems. In this exercise we will explicitly show that Lorentz transformations form a group and further analyze the properties of this group. Since the group elements are matrices here, this is a good example to understand the abstract properties of groups in an easy way.

First, let us revise the definition of a group.

Definition: A group is a set G together with an operation $\bullet$ (called the *group law* of G) that combines any two elements a and b to form another element, denoted by $a \bullet b$. To qualify as a group, the set and the operation, $(G, \bullet)$, must satisfy four requirements known as the *group axioms*:

1) **Closure**: For all $a, b \in G$, the result of the operation $a \bullet b$ is also an element of G.
2) **Associativity**: For all $a, b, c \in G$ the following relation is satisfied $(a \bullet b) \bullet c = a \bullet (b \bullet c)$.
3) **Identity element**: There exists an element $e \in G$, such that for every element $a \in G$, the equality $e \bullet a = a \bullet e = a$ holds. Such an element is unique, and thus called *the* identity element.
4) **Inverse element**: For each $a \in G$, there exists an element $b \in G$ such that $a \bullet b = b \bullet a = e$, where e is the identity element.

For Lorentz transformations, we define G as the set of matrices characterized by the invariance of the metric tensor g of Minkowski spacetime, i.e.

$$G := \{\Lambda \in \mathbb{R}^{4\times 4} \quad | \quad \Lambda^t g \Lambda = g\}\,, \tag{9}$$

and the group operation $\bullet$ as the multiplication of matrices.

a) Show that the Lorentz group is a group.
b) Depending on $\det(\Lambda)$ and $\operatorname{sign}(\Lambda^0{}_0)$ the Lorentz group can be divided into four components. Show that *proper orthochronous Lorentz transformations*, i.e. $\det(\Lambda) = 1$ and $\operatorname{sign}(\Lambda^0{}_0) = 1$, form a group.
c) Next, proof that the other three components do not form a group on their own. Give an example of a combination of two components which again gives a proper group.