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Condensed Matter Theory 1 — Exercise 2

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`https://ilias.studium.kit.edu/goto.php?target=crs_2219528`
To be discussed on: *Thursday 2023/11/09*

1. Fourier transformation on a 1d lattice of finite size

a) Consider a periodic function $f(x)$ with period L, i.e. $f(x) = f(x + L)$. The Fourier transform f_q is defined by the transformations,

$$f(x) = \frac{1}{L} \sum_{q_m} f_{q_m} e^{iq_m x}, \quad f_{q_m} = \int_0^L dx\, f(x) e^{-iq_m x}. \tag{1}$$

Show with the help of the first equation that the function $f(x)$ is indeed periodic if the wavevector assumes only the values $q_m = 2\pi m/L$, with $m \in \mathbb{Z}$. Confirm that the second equation holds by evaluating the x integral explicitly using the first equation.

b) Consider a function g which is defined only on discrete lattice points $x_n = n\,a$ with $n = 0, \ldots, N$, with lattice spacing $a > 0$, and the system size is $L = Na$. The function is assumed to obey periodic boundary conditions: $g(x_0) = g(x_N)$. The Fourier transform g_{q_m} is defined as follows

$$g(x_n) = \frac{1}{L} \sum_{q_m \in 1.\mathrm{BZ}} g_{q_m} e^{iq_m x_n}, \quad g_{q_m} = a \sum_{n=1}^{N} g(x_n) e^{-iq_m x_n}. \tag{2}$$

Using the second equation show that $g_{q_m} = g_{q_m + G_\ell}$ with the reciprocal lattice vector $G_\ell = \frac{2\pi\ell}{a}$ where $\ell \in \mathbb{Z}$. This periodicity of g_{q_m} allows to restrict the sum over momenta in the first equation to the *first Brillouin zone* (1. BZ): $-\pi/a < q_m \leq \pi/a$. How many different values of q_m contains the 1. BZ for an even N?

c) Verify explicitly the two formulae

$$a \sum_{n=1}^{N} e^{-i(q_m - q_{m'})x_n} = L\delta_{m,m'}, \quad \frac{1}{L} \sum_{q_m \in 1.BZ} e^{iq_m(x_n - x_{n'})} = \frac{1}{a}\delta_{n,n'}, \tag{3}$$

by performing the sum. *Hint:* The sum is a geometric series.

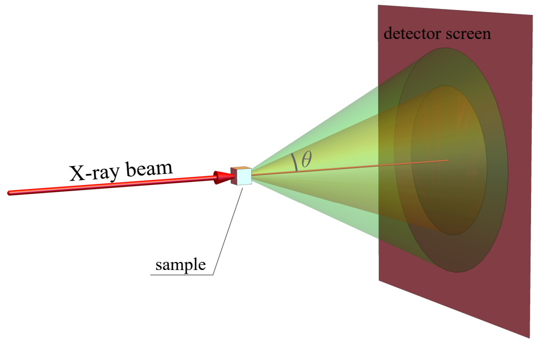

Figure 1: Debye-Scherrer diffraction of a X-ray beam.

d) Convince yourself that one recovers Eqs. (1) from Eqs. (2) in the limit $N \to \infty, a \to 0$, with $Na = L = \text{const.}$ On the other hand, in the thermodynamic limit $L \to \infty$ while keeping a constant a show that momenta within the 1. BZ become dense and that

$$g(x_n) = \int_{-\pi/a}^{\pi/a} \frac{dq}{2\pi}\, g_q\, e^{iqx_n}. \tag{4}$$

2. X-ray diffraction

In the Debye-Scherrer method the X-ray beam diffracts off a polycrystalline sample or a powder with grains that are still very large on the atomic scale and therefore capable of diffracting X-rays. Because the crystal axes of the individual grains are randomly oriented, the diffraction pattern corresponds to an average over all possible crystal orientations. When the scattered radiation is collected on a flat detector screen, this averaging leads to diffraction rings around the beam axis in contrast to the discrete spots observed in Laue diffraction off a single crystal. The angle θ between the beam axis and the ring is called the scattering angle, see Fig. 1. In accordance with Bragg's law, each ring corresponds to a particular reciprocal lattice vector $\vec{G}$ in the sample crystal.

a) Show that $|\vec{G}| = \frac{4\pi}{\lambda} \sin\frac{\theta}{2}$, where λ is the wavelength of the incident X-ray beam.

b) A Debye-Scherrer diffraction experiment is carried out for a fcc crystal lattice. Increasing the temperature from T_1 to $T_2 = T_1 + \Delta T$, a decrease of the scattering angle is observed from θ_1 to θ_2. Express the coefficient of thermal expansion $\alpha_{\mathrm{V}} = \mathscr{V}^{-1} d\mathscr{V}/dT \approx \mathscr{V}^{-1}\Delta\mathscr{V}/\Delta T$ of this material in terms of scattering angles, where $\mathscr{V}$ is volume of the sample.

c) What is the maximum number of diffraction cones that appear for a silver sample (lattice constant $a = 4.086$ $\mathring{A}$) for the X-Ray wavelength $\lambda = 1.789$ $\mathring{A}$?

3. Cohesion of solids

Consider a simple cubic crystal where the nearest neighbour interaction between atoms positioned at $\vec{r}_1$ and $\vec{r}_2$ can be approximated by the Morse potential

$$v(r) = D\left[e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)}\right], \tag{5}$$

where $r = |\vec{r}_1 - \vec{r}_2|$.

a) Find the equilibrium lattice constant and compute the total binding energy V_{eff} of the crystal consisting of a large number $N \gg 1$ of atoms.

b) Calculate the bulk modulus $K = -\mathscr{V} dP/d\mathscr{V}$ where P is the hydrostatic pressure, that is applied to the sample uniformly from all directions, and $\mathscr{V}$ is the sample volume. *Hint*: Use the relation $P = -\partial V_{\text{eff}}/\partial \mathscr{V}$.