Assignment due on December 1, **before** the beginning of the lecture

1 Heat capacity of quantum harmonic oscillators (12 points)

Calculate the heat capacity $C(T) = \partial U/\partial T$ of a system of N quantum harmonic oscillators, all having the *same* frequency ω (unlike the situation we have for phonons, where every phonon mode has a different frequency). Then determine the limiting behavior of $C(T)$ for low temperatures, $T \ll \hbar\omega/k_\mathrm{B}$ and compare it to the behavior we obtained for phonons at low temperatures. Finally, explain what is the difference between the definition of the heat capacity of an object and the definition of the specific heat of the material of which the object consists.

2 X-ray diffraction from multilayers (18 points)

In class we discussed that the intensity measured at the detector in an X-ray diffraction experiment is proportional to the absolute square of the electric field, $|E|^2$. The electric field, in turn, is proportional to the Fourier transform of the electron density distribution in the sample. For a crystal

$$E(\mathbf{Q}) \propto \int e^{i\mathbf{Qr}}\rho(\mathbf{r})d^3\mathbf{r} = \underbrace{\sum_{n_1=1}^{N_1}\sum_{n_2=1}^{N_2}\sum_{n_3=1}^{N_3} e^{i\mathbf{Q}(n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3)}}_{L(\mathbf{Q})}\underbrace{\sum_j^D f_j(\mathbf{Q})e^{i\mathbf{Qd}_j}}_{S(\mathbf{Q})} \tag{1}$$

where $L(\mathbf{Q})$ is the lattice sum whose absolute square $|L(\mathbf{Q})|^2$ mainly determines the position of intensity maxima and $S(\mathbf{Q})$ is the structure factor responsible their intensity; $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$ are the primitive unit vectors.

We will study a single crystal. One can write (you do not need to show that) $|L(\mathbf{Q})|^2$ as

$$I \propto |L(\mathbf{Q})|^2 = \frac{\sin^2(N_1\mathbf{Qa_1}/2)}{\sin^2(\mathbf{Qa_1}/2)}\frac{\sin^2(N_2\mathbf{Qa_2}/2)}{\sin^2(\mathbf{Qa_2}/2)}\frac{\sin^2(N_3\mathbf{Qa_3}/2)}{\sin^2(\mathbf{Qa_3}/2)} \tag{2}$$

We assume a cubic lattice for conceptual simplicity, i.e. $a = |\mathbf{a}_1| = |\mathbf{a}_2| = |\mathbf{a}_3|$ and $\mathbf{a}_1 = (1,0,0)$, $\mathbf{a}_2 = (0,1,0)$, $\mathbf{a}_3 = (0,0,1)$.

Let us regard a thin film $N_3 \ll N_1, N_2$, with a surface normal $\mathbf{n}_0||\mathbf{a}_3$, $\mathbf{a}_1$ and $\mathbf{a}_2$ being "in plane", Fig. 1. Let us discuss the intensity along the $[0,0,L]$ direction, that means $\mathbf{Q}_0 = \mathbf{Q} = (0,0,L)$. How does (2) simplify for $\mathbf{Q} = (0,0,L)$? Hint: when you just put $\mathbf{Q}$ into (2), you get terms "0/0" which is a problem; but you can expand the sine function...

Next argue that for a cubic crystal for the primitive reciprocal unit vectors $\mathbf{b}_i||\mathbf{a}_i$ holds.

Then assume $N_3 = 10$ and $a = 0.2$ nm and sketch the resulting intensity pattern along $\mathbf{Q}_0$. Use, if possible, a computer program to plot the sketch. Don't forget to label the axes. What do you learn from this sketch about how to determine N_3 from a measured pattern if you were to investigate an unknown layer? Hint: You can play around and change N_3 from 10 to higher and lower values – how does the pattern change?

Experimentally, one measures the intensity at the detector in a so-called $\theta - 2\theta$-scan. Explain why keeping the angle between $\mathbf{k}_i$ and $\mathbf{k}_f$ twice as large as the angle between $\mathbf{k}_i$ and the surface (Fig. 1a)) will result in a scan along the surface normal.

From a $\theta - 2\theta$-scan one obtains the intensity versus the angle θ, Fig. 1b). What is the relation between θ and $\mathbf{Q}$? Hint: Think of Bragg's law... Keeping in mind that $\mathbf{Q} = (0,0,L)$, write down the simplified $|L(\mathbf{Q})|^2$ you have obtained above in terms of θ instead of $\mathbf{Q}$. Why are the maxima not equidistant in θ?

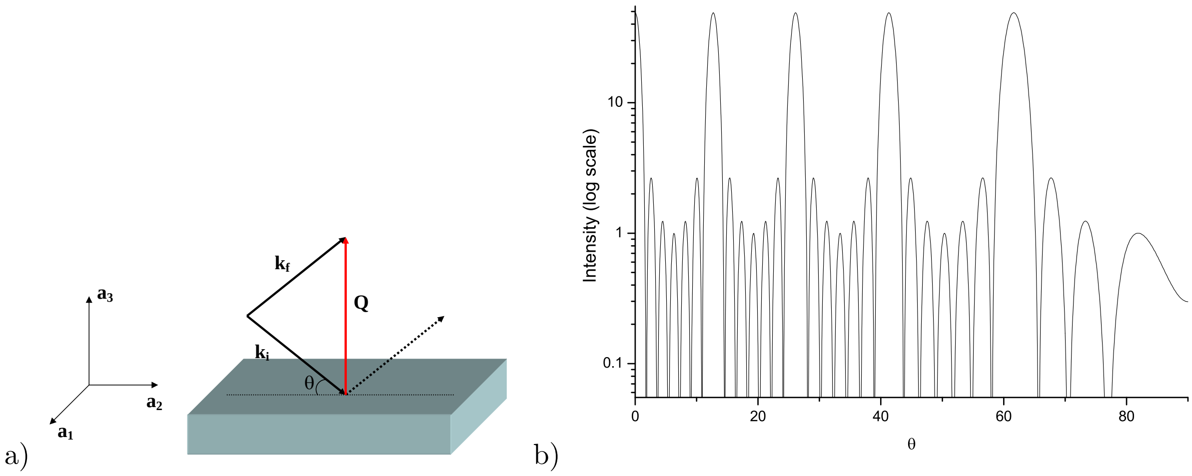

Figure 1: a) Sketch of the "scattering triangle" formed by $\mathbf{k}_i$, $\mathbf{k}_f$ and $\mathbf{Q}$ in a diffraction experiment from a thin film. b) Scattering intensity pattern from a $\theta - 2\theta$-scan plotted versus θ measured with Cu K-α radiation, $\lambda = 0.154$ nm. The intensity axis is logarithmic.

For the given example in Fig. 1b), determine the thickness of the layer and the lattice constant a.

3 Papers (doubled participation points)

Read the papers of the other groups (the final versions will be distributed after Tuesday's lecture). Prepare for a discussion and also prepare some questions.