Solid State Physics I, Spring 2010 — Exercise 2

Please return by Monday 8.2.2010 12:00. The exercise session will be held at Physicum D115 on the same day at 16:15. You can contact the the teaching assistant at *tuomas.pylkkanen@helsinki.fi*.

1. (a) Sketch the first four Brillouin zones of the two-dimensional square lattice ($a = b$).
   (b) Show that the areas of the first, second and third zones are equal.
   (c) Demonstrate how points in the third zone can be mapped to the first zone through appropriate reciprocal lattice vectors.

2. Assuming the following expression for the net potential energy between two adjacent atoms

$$U(r) = -\frac{C}{r} + D\exp\left(-\frac{r}{\rho}\right)$$

   (a) Calculate the binding energy in terms of the equilibrium interatomic separation r_0 and the parameters D and ρ.
   (b) What is the vibrational frequency in the harmonic approximation, if the reduced mass of the atom pair is M?

3. Suppose an infinite one-dimensional chain of atoms with a modulated period, so that the position of the nth atom is given by $r(n) = na + A\sin(2\pi na/\lambda)$. Let $\lambda \gg a$ (long wavelength modulation) and $A \ll a$ (small amplitude). Calculate the reciprocal lattice as the Fourier transform of the density. Compare with an unperturbed 1D lattice (you should see additional structure near the lattice points). Can you think of a physical example of such modulation?

4. Calculate the structure factor S for a hcp structure consisting of identical atoms. Determine the possible values of $|S|^2$.

5. X-ray diffraction from lithium. Lithium has two $1s$ electrons and one $2s$ electron. Using the following hydrogen-like wave functions

$$\psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}, \qquad \psi_{200} = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2 - \frac{Zr}{a_0}\right)e^{-Zr/2a},$$

   (a) Calculate the atomic form factor[1]

$$f = \int \rho(\mathbf{r})\exp(i\mathbf{q}\cdot\mathbf{r})\ \mathrm{d}^3\mathbf{r}$$

   assuming $f = 2f_{1\mathrm{s}} + f_{2\mathrm{s}}$.
   (b) Plot $f_{1\mathrm{s}}$, $f_{2\mathrm{s}}$ and f as a function of q. Use $Z = 3$, and $a_0 = 0.529$ Å (the Bohr radius).
   (c) Calculate the positions of the first 5 reflections of lithium (bcc, lattice constant 3.51 Å) and include them in the plot. Remember: $d_{hkl} = a/\sqrt{h^2 + k^2 + l^2}$ for cubic systems.
   (d) We can obtain experimental values of $|f^2|$ by measuring x-ray diffraction of the above reflections. Which electrons is the experiment more sensitive to?

[1] Hint: The density is spherically symmetric, so

$$\int \rho(\mathbf{r})e^{i\mathbf{q}\cdot\mathbf{r}}\ \mathrm{d}^3\mathbf{r} = \int_0^\infty r^2 dr \int_0^{2\pi} d\theta \int_0^\pi \sin\phi\ e^{iqr\cos\phi} d\phi.$$