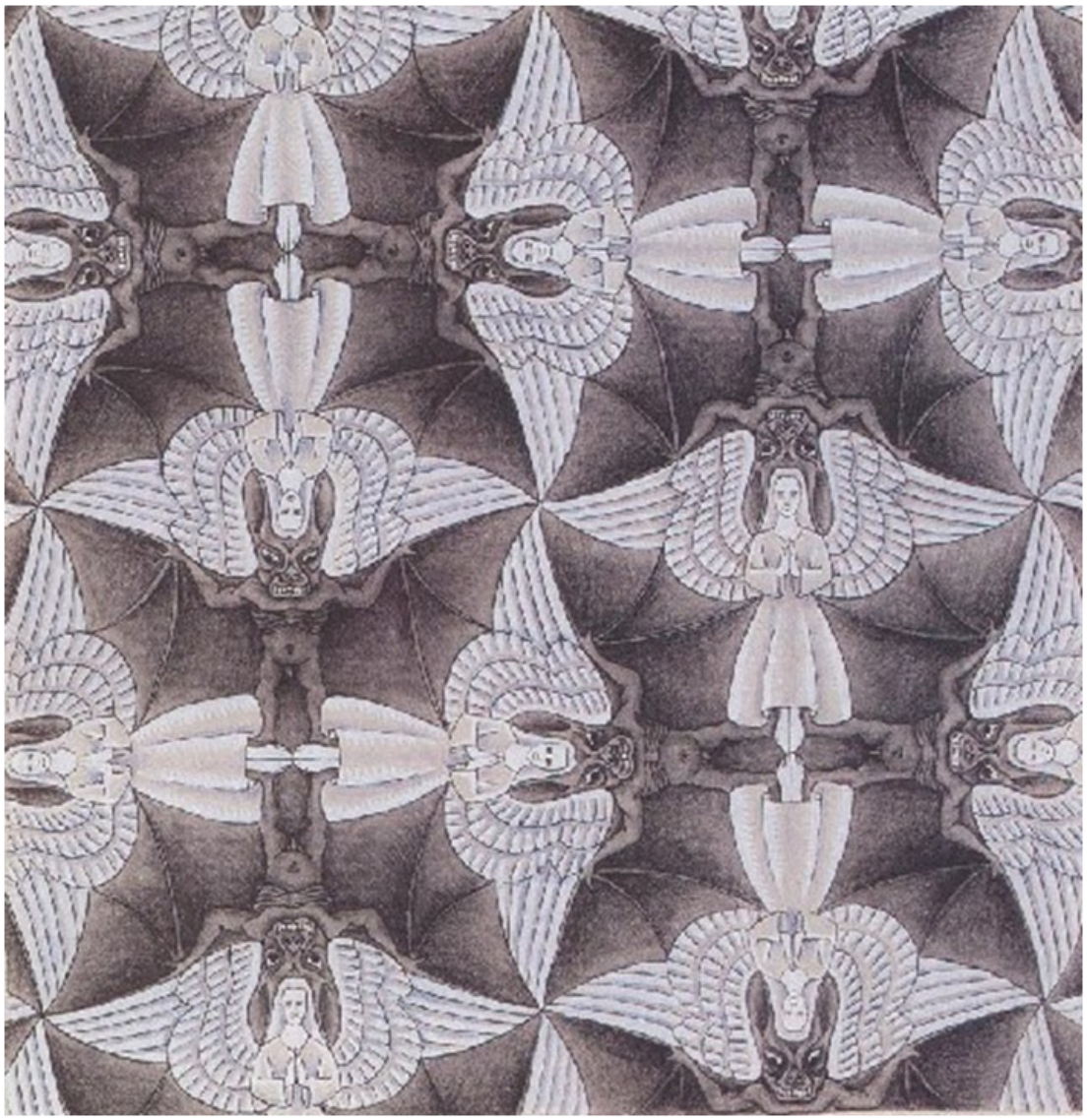
Condensed Matter Physics Option
Question Sheet 1

1. Consider the Escher drawing in the figure here below, and imagine that it would be infinitely repeated in both directions.



(a) Draw the unit cell on the figure.

(b) Identify the highest-order (smallest rotation) axes and draw them on the figure with the appropriate symbol. Are the highest-order axes related by any other symmetry? What does this tell us about (i) equivalence classes and (ii) Wyckoff letters for those positions?

(c) Draw any axes of lower order on the figure with the appropriate symbols.

(d) Draw any mirror planes on the figure with the appropriate symbol. How are they related?

(e) Are there any roto-translation operators (glides)? If so, draw them with the appropriate symbols.

(f) Using the decision tree provided in the handouts (lecture 1, page 34) determine the "wallpaper" group describing the symmetry of the drawing.

2. A monoclinic crystal has lattice parameters $a = 0.6nm$, $b = 0.7nm$ and $c = 0.8nm$ and β=110°.

(a) Find the magnitude of the length denoted by the direction $[31\overline{2}]$.

(b) Find the interplanar spacing d for planes given by $(31\overline{2})$.

(c) Find the angle between the $[31\overline{2}]$ direction and the normal to the plane $(31\overline{2})$.

(d) Draw to scale the *h0l* section of the reciprocal lattice.

(e) Suppose that initially an X-ray beam of wavelength $0.154nm$ is incident along the [100] direction. The crystal is then rotated through an angle α about [010] until the 002 reflection is obtained at a suitably placed detector. By construct the elastic scattering triangle, show how this arises with your drawing of the reciprocal lattice and calculate the angle of rotation of the crystal.

3. USi crystallises in space group *Pbnm,* with $a = 0.565nm$, $b = 0.765nm$ and $c = 0.390nm$ and Z = 4 (i.e. four USi groups per unit cell). For this space group the general equivalent positions are

$$\begin{array}{llll} x,y,z & x,y,\frac{1}{2}-z & \frac{1}{2}+x,\frac{1}{2}-y,\overline{z} & \frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z \\ \overline{x},\overline{y},\overline{z} & \overline{x},\overline{y},\frac{1}{2}+z & \frac{1}{2}-x,\frac{1}{2}+y,z & \frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}-z \end{array}$$

Given that all four U atoms have z = $\pm\frac{1}{4}$, satisfy for yourself that the four U atoms lie at the positions

$$\pm\left\{x,y,\tfrac{1}{4};\tfrac{1}{2}-x,\tfrac{1}{2}+y,\tfrac{1}{4}\right\}$$

(a) Show that the structure factor for the U atoms alone and for a general *hkl* is given by.

$$F_{hkl} = 4f_U \cos 2\pi\left[hx_U - \left(\frac{h+k}{4}\right)\right]\cos 2\pi\left[ky_U + \left(\frac{h+k+l}{4}\right)\right] \qquad (1)$$

(b) We are now interested in using diffraction data to determine the exact location of the U atoms. Because of the arbitrariness in the choice of the origin, it is sufficient to limit our search to the range $x < \frac{1}{4}$ and $y < \frac{1}{4}$. Given that the 200 and 040 reflections have zero intensities, would measuring the intensities of the , 111, 231 be sufficient to determine the solution uniquely?

(c) A powder diffraction experiment is performed on USi using copper K_α radiation (1.542 Å). From the measured intensity data below, determine approximate values for the positions x_U and y_U (the Si contributions can be neglected — why is this?). In the table, f_U is the uranium form factor at the appropriate value of

$\sin\theta/\lambda$, "LPGA" is the combined Lorentz, polarization, geometrical and attenuation factor, *including* the term (d^3/v_0). The reflection multiplicity (number of RL points contributing to the same powder peak) can be calculated from the Miller indices.

hkl	111	200	211	040	231
I	612	~ 0	150	~ 0	233
2θ (deg.)	30.12	31.6	40.09	47.41	53.70
$\mathrm{f}_U(\sin\theta/\lambda)$	81	79	75	71	69
LPGA	13.4	12.8	6.8	4.9	3.7

(d) Draw to scale the positions of the U atoms in the unit cell projected on (001). Calculate and mark on your diagram the shortest U-U distance in nm.

4. A crystal contains two atoms at general positions in the unit cell. Suppose one of then has a real atomic scattering factor f_1, while the second has a scattering factor f_2 with real and imaginary components viz: $f_2 = f' + if"$. Write down the formulae for the structure amplitude for the hkl and $\overline{hkl}$ reflections, showing that Friedel's law is untrue, i.e. show that $I(hkl) \neq I(\overline{hkl})$. Illustrate your answer on an Argand diagram. This is an example of anomalous dispersion, which can be used to tell whether a polar crystal is pointing up or down, or whether a chiral crystal is left or right-handed.

5. Consider Space Group no. 126 in the International Table, symbol $P4/nnc$.

   (a) Without looking it up in the ITC volume A, derive the crystal class from the space group symbol and explain your reasoning. How many operators does the crystal class point group have? For this part, you may use the point group tables on the course web site.

   (b) Derive the multiplicity of a general site x, y, z in this space group. What would change in your derivation if the lattice were I-centred (e.g., $I4/mcm$, no. 140)?

   (c) A special position in Space Group no. 126 — $P4/nnc$ is labelled "4 d $\bar{4}$..". What is the site symmetry point group of this special position? What is its multiplicity? Derive the multiplicity independently by comparing the number of elements in the crystal class with that of the site symmetry point group.

   (d) In Space Group no. 126 — $P4/nnc$, there is a symmetry element $\bar{4}$ at position $0, \frac{1}{2}, \frac{1}{4}$. Write the symmetry operator $\bar{4}$ in normal form, i.e., as an *improper* rotation matrix about the origin *followed by* a translation, and write its Seitz symbol. Show explicitly that the point $0, \frac{1}{2}, \frac{1}{4}$ is invariant by application of this operator.