# Condensed Matter Physics (I): Homework 2
# Due: October 28, 2019

**Ex.1 10%** Suppose that all atomic form factors $f_i$ are real. Show that the X-ray scattering data will make all crystals appear to be centrosymmetric.

**Ex.2 10% Effect of surface**

Consider x-ray scattering from an orthorhombic lattice terminated by a surface at $z = 0$. The lattice constant of the lattice along $z$-axis is $c$, while the lattice constants along $x$ and $y$ axes are $a$ and $b$ respectively. Furthermore, the size of the lattice is $N_x \times N_y \times N_z$. If the wavenumber change of the x-ray is $\vec{q} = (q_x, q_y, q_z)$ and the ratio of x-ray amplitudes scattered from successive planes perpendicular to $z$-axis is $\alpha$ ($0 \le \alpha \le 1$), find the scattering intensity $I(\vec{q}) \equiv |\sum_i e^{i\vec{q}\cdot\vec{r}_i}|^2$ with $\vec{r}_i$ being positions of lattice points. Sketch how shapes of scattering peaks change when $\alpha$ goes from 1 (x-ray can penetrate the sample 100%) to 0 (x-ray can not penetrate the sample).

**Ex.3** Consider a collection of $N_p$ polymers each with $N + 1$ identical monomer units connected by $N$ identical flexible links. Let $\vec{R}_\alpha$ be the position of the initial monomer in polymer $\alpha$. If we denote the position of the $i$th ($i = 1, 2, \cdots, N$) monomer in polymer $\alpha$ by $\vec{r}_{\alpha,i} = \vec{R}_\alpha + \vec{R}_{\alpha,i}$, the structure factor for polymer $\alpha$ is

$$f_\alpha(\vec{q}) = 1 + \sum_i^N e^{-i\vec{q}\cdot\vec{R}_{\alpha,i}}. \tag{1}$$

(a) 5% Find the scattering intensity for a dilute solution of the above polymers in terms of $N_p$ and averages over polymer configurations related to $f(\vec{q})$ (such as $\langle f_\alpha(\vec{q})\rangle$ and $\langle |f_\alpha(\vec{q})|^2\rangle$).

(b) 5% If we use identical polymers to decorate lattice points of a simple cubic lattice, find the scattering intensity by assuming that the polymer configurations on each lattice point are identical.

(c) 10% Following (b), assume that each lattice point is decorated by the same polymer but polymer's configurations are not identical. Polymers in each cell perform independent random walks with their initial monomer at the centers of the cubic cells. Find the intensity in this case.

**Ex.4 10%** Consider $N$ atoms in one dimension with positions $x_n = na + F(na)$, where $F$ is a periodic function of period $b$ with $b/a$ being irrational. Show that the Fourier transformation for density of atoms is given by

$$n_k = N \sum_{p,q} A_q(k) \delta_{k,2\pi p/a + 2\pi q/b}, \tag{2}$$

where $p$ and $q$ are integers and $A_q(k) = \frac{1}{b}\int_0^b dy e^{2\pi i q y/b} e^{ikF(y)}$.

**Ex.5 10%** Consider an array of atoms in one dimension with positions $x_n = na + u_n$, where $u_n = u_0 \cos qna$ with $q < 2\pi/a$ and $u_0 \ll a$. Calculate the first correction (to $O(u_0^2)$) to the magnitude of the main peaks and the magnitude of the strongest side peaks. (Assume that number of atoms $N \to \infty$ and focus on the leading terms of order $N^2$.)

**Ex.6** Consider a two-dimensional honeycomb lattice of atoms. Let the honeycomb lattice to be aligned in the $xy$-plane with the $y$-axis parallel to one of the nearest-neighbour atomic spacings. Call the distance between nearest-neighbours $a$.

(a) 7% Treating the atoms as identical scatterers, determine the intensity of all the Bragg peaks, which are normalized so that the strongest peak has unit intensity. Plot a diagram to illustrate the intensity of Bragg peaks.

(b) 6% Consider the cases where the two atoms in the unit cell are distinct and are denoted by $A$ and $B$. The scattering amplitudes from $A$ and $B$ are $f_A$ and $f_B$, which are assumed to be real. What condition on the relative scattering amplitudes will cause the intensities of some of the Bragg peaks to vanish?

(c) 7% Now consider fully three-dimensional graphite which has a simple hexagonal Bravais lattice. Show that the reciprocal lattice of a simple hexagonal Bravais lattice is also a simple hexagonal lattice. For graphite, show that the internal symmetries of the basis gives rise to the vanishing of certain Bragg scattering directions and list which reciprocal lattice vectors showing this complete interference.

**Report: hand-in before final** (1) Find appropriate references and write a brief report (less than 4 pages) on how DNA double-helix structure was found by using x-ray.

(2) Find approriate references and write a report (less than 4 pages) on the 3D atomic arrangement of the quasi-crystal that shows the same symmetry as the icosahedron (such as $Al_{86}Mn_{14}$.).