

PHYSICS 880.06

Home Work Assignment # 2

10/4/2011

Due: Tue., Oct. 11, 2011.

1. *Sharpness of diffraction peaks:* To understand the width of diffraction peaks, consider the simple 1D model of a large crystal of *finite* size. Let there be identical point scatterers located at $x_m = ma$, where a is the lattice spacing and m is an integer in range $0 \leq m \leq M$. The scattering matrix element is given by

$$\langle k' | U | k \rangle = \int dx e^{-iqx} U(x) \quad \text{with} \quad q = k - k'$$

(a) Show within the Born approximation that the amplitude for scattering an X-ray with wavevector k to k' is proportional to

$$\mathcal{A} = \sum_{m=0}^{M-1} e^{-imqa}$$

and thus the scattered intensity goes like

$$|\mathcal{A}|^2 = \frac{\sin^2(Mqa/2)}{\sin^2(qa/2)}.$$

(b) Hence conclude that the diffraction maxima occur at $q = 2\pi h/a$, where h is an integer.

(c) Next, move slightly off the maximum by choosing $q = (2\pi h/a) + \delta q$ and show that the width of the diffraction peak is given by $\delta q = 2\pi/(Ma)$. Thus for a macroscopic crystal, the diffraction peak is extremely sharp.

Note: Read A & M (Ashcroft and Mermin) Chapter 6.

Please note a potentially confusing point of terminology.

A & M use the term “geometrical structure factor”, denoted by $S_{\mathbf{K}}$, for the F.T. of the *density* of a rigid lattice within a primitive cell, evaluated at a reciprocal lattice vector.

This is to be carefully distinguished from the standard term “Structure factor”, denoted by $S(\mathbf{q})$, which is the F.T. of the *density-density correlation* function in a condensed matter system.

2. A & M, Ch. 6, Problem 3 (a) through (e).

3. A & M, Ch. 6, Problem 5 (a) and (b).