Assignment 1

EE 698N, Advanced Semiconductor Physics
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1 Crystal Math

a) Show that if $s = 0, 1, \ldots, N-2, N-1$, and a is a lattice constant, and $S_q = \sum_{s=0}^{N-1} e^{i(qa)s}$, then

$$|S_q|^2 = \frac{\sin^2(Nqa/2)}{\sin^2(qa/2)}. \tag{1}$$

b) Plot $|S_q|^2$ for $N = 30$ against q, and identify the values of q where the peaks occur.

c) Show that the value of intensity peaks are N^2, and (Hard!) the area of each period of $|S_q|^2$ is $A = 2\pi N/a$. You might have to evaluate a complex integral.

d) (Hard!) Show that the full width at half max (FWHM) of the peaks of $|S_q|^2$ is given by $2\Delta q \approx 5.42/Na$ (assume that Δq is small).

e) What happens to the peaks (magnitude, area, and FWHM) as $N \to \infty$? What mathematical function best describes $|S_q|^2$ in this limit? Show by qualitative arguments that in this limit, you can derive a *very* useful result -

$$\sum_{s=0}^{N-1} e^{iqsa} = \frac{2\pi}{a} \sum_{m=-\infty}^{+\infty} \delta(q - \frac{2\pi}{a} m) \tag{2}$$

Note that this result is also found in books of signal processing, Fourier transforms, etc. The chain of delta functions on the right, looks like a 'bed of nails' - we will refer to this function by this name for later work.

f) Generalize this sum to the three dimensional case; it is again a very useful result that relates the real space lattice vectors $\vec{R}_l$ to reciprocal space lattice vectors $\vec{G}$ -

$$\sum_{l} e^{i\vec{q}\cdot\vec{R}} = \frac{(2\pi)^3}{a^3} \sum_{\vec{G}} \delta(\vec{q} - \vec{G}) \tag{3}$$

2 1-D Crystal

You will now make sense out of the math in the previous problem. Assume a hypothetical 'crystal', comprised of *identical* atoms periodically arranged in a line, with spacing a. There are N atoms in the line, making the length of the crystal $L = Na$. Now a wave (say X-Ray, or high-energy neutrons) is incident on the crystal. The crystal will diffract this wave; the *amplitude* of the diffracted wave (from electromagnetic theory) is proportional to

$$S_q \propto \sum_{s} f_s e^{i(qa)s}, \tag{4}$$

Table 1: Density of States (DOS) for particles with and without mass

Dispersion	d=1	d=2	d=3
$E = \hbar ck$	const.	$\sim E$	$\sim E^2$
$E = \hbar^2 k^2/2m$	$1/\sqrt{E}$	const.	$\sim \sqrt{E}$

where the quantity f_s is called an 'atomic form factor'. It is a measure of the scattering power of the atom, i.e., it is an atomic property. Hence, it is the same for all atoms of the same kind.

From the previous problem, show the following -

a) **Bragg/Laue Condition** - For a finite crystal, The diffracted beam peaks are along directions which meet the condition $qa = 2\pi m$

b) **Crystal Extent** - The 'larger' the size of the crystal is, the sharper and stronger are the diffraction peaks.

c) **Crystal with Basis** - If the crystal has two different atoms in the basis with form factors f_A and f_B, the diffraction pattern changes; some peaks disappear, and new ones appear. This is how crystal structure is revealed in diffraction measurements.

3 3D-Crystal

Consider a finite-size, simple cubic crystal of $N_x \times N_y \times N_z$ atoms, with lattice spacing a.

a) For $k_x = k_y = 0$, plot the k_z-dependence of the intensity of the scattered X-rays around the (0,0,1) point in reciprocal space. Show that there is a peak at (0,0,1) and that the peak width is finite. How is the width related to the size of the crystal N_z? Assume $N_z \gg 1$

b) What happens to the line width if we have a collection of crystallites, which are all oriented parallel to each other, but their positions are random?

4 Density of States

Calculate the density of states for particles with mass (electrons, dispersion $E = \hbar^2 k^2/2m$) and particles without mass (photons, dispersion $E = \hbar ck$) for d=1,2, and 3 dimensions (see Table 1). Show that the energy dependence is as listed in the Table. (Caution - For 1D, make sure you include both positive and negative k-values in your evaluation. Neglect of this fact gives half the correct DOS).