Homework 2 Solutions

4. (a) This follows by forming

$$|F|^2 = \frac{1-\exp[-iM(a\cdot\Delta k)]}{1-\exp[-i(a\cdot\Delta k)]}\cdot\frac{1-\exp[iM(a\cdot\Delta k)]}{1-\exp[i(a\cdot\Delta k)]}$$
$$= \frac{1-\cos M(a\cdot\Delta k)}{1-\cos(a\cdot\Delta k)} = \frac{\sin^2 \frac{1}{2}M(a\cdot\Delta k)}{\sin^2\frac{1}{2}(a\cdot\Delta k)}.$$

(b) The first zero in $\sin\frac{1}{2}M\varepsilon$ occurs for $\varepsilon = 2\pi/M$. That this is the correct consideration follows from

$$\sin M(\pi h + \frac{1}{2}\varepsilon) = \underbrace{\sin\ \pi Mh}_{\substack{\text{zero,}\\ \text{as Mh is}\\ \text{an integer}}}\ \cos\ \frac{1}{2}M\varepsilon + \underbrace{\cos\ \pi Mh}_{\pm 1}\ \sin\ \frac{1}{2}M\varepsilon.$$

5. $S\,(v_1v_2v_3) = f\ \sum_j\ e^{-2\pi i(x_jv_1+y_jv_2+z_jv_3)}$

Referred to an fcc lattice, the basis of diamond is $000; \frac{1}{4}\frac{1}{4}\frac{1}{4}$. Thus in the product

$$S(v_1v_2v_3) = S(\text{fcc lattice}) \times\ S\,(\text{basis}),$$

we take the lattice structure factor from (48), and for the basis

$$S\,(\text{basis}) = 1 + e^{-i\frac{1}{2}\pi(v_1+v_2+v_3)}.$$

Now S(fcc) = 0 only if all indices are even or all indices are odd. If all indices are even the structure factor of the basis vanishes unless $v_1 + v_2 + v_3 = 4n$, where n is an integer. For example, for the reflection (222) we have $S(\text{basis}) = 1 + e^{-i3\pi} = 0$, and this reflection is forbidden.

6.
$$f_G = \int_0^\infty 4\pi r^2\,(\pi a_0^{\ 3}\ Gr)^{-1}\ \sin Gr\ \exp\,(-2r/a_0)\ dr$$
$$= (4/G^3a_0^{\ 3})\int dx\ x\ \sin x\ \exp\,(-2x/Ga_0)$$
$$= (4/G^3a_0^{\ 3})\ (4/Ga_0)/(1+r/G^2a_0^{\ 2})^2$$
$$16/(4+G^2a_0^{\ 2})^2.$$

The integral is not difficult; it is given as Dwight 860.81. Observe that f = 1 for G = 0 and $f \propto 1/G^4$ for $Ga_0 >> 1$.

7. (a) The basis has one atom A at the origin and one atom B at $\frac{1}{2}a$. The single Laue equation $\mathbf{a}\cdot\Delta\mathbf{k} = 2\pi\times$ (integer) defines a set of parallel planes in Fourier space. Intersections with a sphere are a set of circles, so that the diffracted beams lie on a set of cones. (b) $S(n) = f_A + f_B\, e^{-i\pi n}$. For n odd, $S = f_A - f_B$; for n even, $S = f_A + f_B$. (c) If $f_A = f_B$ the atoms diffract identically, as if the primitive translation vector were $\frac{1}{2}$ a and the diffraction condition $(\frac{1}{2}\mathbf{a}\cdot\Delta\mathbf{k}) = 2\pi\times$ (integer).