Solutions for Homework Set 2

1. *Kittel Problem 2.4*

Solution

(a) We are given that

$$F = \frac{1 - \exp\left[-iM(\mathbf{a}\cdot\Delta\mathbf{k})\right]}{1 - \exp\left[-i(\mathbf{a}\cdot\Delta\mathbf{k})\right]},$$

and hence multiplying by F^* gives:

$$|F|^2 = \left(\frac{1 - \exp\left[-iM(\mathbf{a}\cdot\Delta\mathbf{k})\right]}{1 - \exp\left[-i(\mathbf{a}\cdot\Delta\mathbf{k})\right]}\right)\left(\frac{1 - \exp\left[iM(\mathbf{a}\cdot\Delta\mathbf{k})\right]}{1 - \exp\left[i(\mathbf{a}\cdot\Delta\mathbf{k})\right]}\right), \tag{1}$$

where we now expand the parentheses and use $cos(x) = (e^{ix} + e^{-ix})/2$ to get

$$\begin{aligned} |F|^2 &= \frac{2 - 2\cos M(\mathbf{a}\cdot\Delta\mathbf{k})}{2 - 2\cos(\mathbf{a}\cdot\Delta\mathbf{k})}, \\ &= \frac{\sin^2\left(M\mathbf{a}\cdot\Delta\mathbf{k}/2\right)}{\sin^2\left(\mathbf{a}\cdot\Delta\mathbf{k}/2\right)}, \end{aligned} \tag{2}$$

where we use the identity $\cos(x) = 1 - 2\sin^2(x)$.

(b) The zeros of $|F|^2$ are exactly when the sin term in the numerator of (2) vanishes. We can find these points by expanding the $\sin(x)$ term in (2) above using

$$\sin(x + y) = \sin(x)\cos(y) + \sin(y)\cos(x),$$

which gives

$$\begin{aligned} \sin[(M(2\pi h + \epsilon)/2] &= \sin(M\pi h)\cos(M\epsilon/2)\sin(M\epsilon/2)\cos(\pi M h), \\ &= \sin(M\epsilon/2), \\ &= 0, \end{aligned}$$

and hence $M\epsilon/2 = \pi n$, where for the first zero $n = 1$. Hence, we get

$$\epsilon = \frac{2\pi}{M}. \tag{3}$$

2. *Kittel Problem 2.5*

Solution

(a) As the problem states, we must treat diamond as a SC lattice with an 8 point basis. The basis points are at

$$(0,0,0), \frac{a}{2}(1,1,0), \frac{a}{2}(1,0,1), \frac{a}{2}(0,1,1),$$

and

$$\frac{a}{4}(1,1,1), \frac{a}{4}(-1,1,-1), \frac{a}{4}(-1,-1,1), \frac{a}{4}(1,-1,-1).$$

For a reciprocal lattice vector of our SC lattice viz. $\mathbf{G} = (n_1\mathbf{b}_1 + n_2\mathbf{b}_2 + n_3\mathbf{b}_3)$, the structure factor is given by (assuming all scattering centres are identical)

$$\begin{aligned} S_{\mathbf{G}} = f\Big(&1 + e^{i\pi(n_1+n_2)} + e^{i\pi(n_1+n_3)} + e^{i\pi(n_2+n_3)} + \\ &e^{i\pi(n_1+n_2+n_3)/2} + e^{i\pi(-n_1-n_2+n_3)/2} + e^{i\pi(n_1-n_2-n_3)/2} + e^{i\pi(-n_1+n_2-n_3)/2}\Big). \end{aligned} \tag{4}$$

(b) Let $n = n_1 + n_2 + n_3$. Then, after some algebra:

$$S_{\mathbf{G}} \;=\; f\left(1 + e^{i\pi n/2}\right)\left(e^{i\pi(n_1+n_2)} + e^{i\pi(n_2+n_3)} + e^{i\pi(n_1+n_3)}\right). \tag{5}$$

The zeros of $S_{\mathbf{G}}$ are now easily read off. The zero for the first factor is given by $n = 4m + 2$ where m is an integer, and the second factor vanishes only when one of n_1, n_2, and n_3 is of different parity to the others. That is, one is odd and the other two even, or one even and the other two odd. For all other combinations the expression does not vanish. Hence, for reflections ($S_{\mathbf{G}}$ non-zero) the condition are either (i) n is odd, or (ii) alternatively $n = 4m$ with all of n_1, n_2, and n_3 even as required.

3. *Kittel Problem 2.6*

Solution

In this problem we examine the case where the scattering centre is not an ideal point source, but rather a distribution given by

$$n(\mathbf{r}) = \frac{e^{-2r/a_0}}{\pi a_0^3}.$$

This is spherically symmetric, and so the form factor is given (From Kittel Chapter 2, Eq (50)):

$$f = 4\pi \int_0^\infty dr n(r) r^2 \frac{\sin(Gr)}{Gr}, \tag{6}$$

and hence using our given expression for $n(r)$, one gets after integrating over r assuming G is real, the required result is:

$$f = \frac{16}{(4 + G^2 a_0^2)^2}. \tag{7}$$

4. *Kittel Problem 2.7*

Solution

(a) We orientate our axes so that the line of atoms is along the x-axis and the incident radiation is initially along the y-axis. Then, the structure factor the line of atoms is given by

$$S_{\mathbf{G}} = f_A + f_B e^{-i\mathbf{G}\cdot\mathbf{d}}, \tag{8}$$

where $\mathbf{d} = (a/2)\hat{\mathbf{x}}$, and $\mathbf{G} = n_1\hat{\mathbf{x}} + n_2\hat{\mathbf{y}}$ is the wavevector of the scattered radiation. Hence, if θ is the angle between $\mathbf{G}$ and the x-axis containing the line of atoms, we have

$$S_{\mathbf{G}} = f_A + f_B e^{-iGa\cos\theta/2}. \tag{9}$$

Condition for interference, constructive or destructive, is then clearly given by

$$\frac{Ga\cos\theta}{2} = n\pi,$$

for an integer n. Only at these points is $|S_{\mathbf{G}}|^2$ at a maximum or minimum. Hence, as G is a wavevector for the scattered radiation one has $G = 2\pi n/\lambda$, with λ the wavelength of the radiation. The condition for interference becomes

$$n\lambda = a\cos\theta. \tag{10}$$

(b) The intensity of the scattered radiation is proportional to $|S_{\mathbf{G}}|^2$. Thus constructive interference is when $|S_{\mathbf{G}}|^2$ is at a maximum, which corresponds to n being even. Thus using (9) above we have

$$|S_{\mathbf{G}}|^2 = |f_A + f_B|^2. \tag{11}$$

Destructive interference similarly is when n is odd, and the intensity is proportional to

$$|S_{\mathbf{G}}|^2 = |f_A - f_B|^2. \tag{12}$$

(c) When $f_A = f_B$ the atoms A and B are now identical, so the line of atoms scatters in a manner identical to that of a diffraction grating. Indeed this is what is observed, for we have zeros in $S_{\mathbf{G}}$ for n odd, and maxima for n odd. Using (a), we see the condition for the zeros and maxima are identical to that for a grating.