Question 1. (Kittel Ch.2 Problem 5) Structure factor of diamond

(a)

diamond structure \equiv fcc \text{ Bravais lattice} + \left[ \vec{0}, \frac{a}{4}(\hat{x} + \hat{y} + \hat{z}) \right]

(1)

That is, at \( x_jy_jz_j = 000; 0\frac{1}{2}\frac{1}{2}\frac{1}{2}; 0\frac{1}{2}\frac{1}{2}\frac{3}{4}\frac{3}{4}\frac{3}{4}; 0\frac{1}{2}\frac{3}{4}\frac{3}{4}\frac{3}{4}\frac{3}{4}; \) there are 8 identical atoms.

Recall that

\[ \vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3, \]
\[ \vec{r}_j = x_j\vec{a}_1 + y_j\vec{a}_2 + z_j\vec{a}_3. \]

(2)

The structure factor is given with

\[ S = \sum_j f_j e^{-i\vec{G} \cdot \vec{r}_j}. \]

(3)

Since \( f_j \) is an atomic property, we can replace all \( f_j \) by \( f \), because all atoms are identical. Furthermore there are 8 atoms in the primitive cell of the diamond structure, so the structure factor should consist of 8 terms. Then, \( S(hkl) \) is equal to

\[ S(hkl) = \left[ 1 + e^{-i\pi(k+l)} + e^{-i\pi(h+l)} + e^{-i\pi(h+k)} + e^{-\frac{i\pi}{2}(h+k+l)} \right]^{(4)} \]

(4)

(b) When all of \( hkl \) is even and simultaneously satisfy \( h + k + l = 4n \), then \( S \) is finite. When they are all odd, \( e^{-\frac{i\pi}{2}(h+k+l)} \) is either equal to \( i \) or \( -i \), so \( S \) can be considered of the form \( z = x + iy \) where \( x, y \) are real numbers and \( z \) is complex. Again the scattered intensity \( S^*S \) is going to be finite. When only one of them is even or only one of them is odd, then \( S \) is equal to 0.

Question 2. (Kittel Ch.3 Problem 5) Linear ionic crystal

(a) The total potential energy of a linear diatomic system is equal to \( U_{\text{total}} = NU_i \), because \( 2N \) ions is equal to \( N \) molecules. Here,
\[ U_i = \sum_{i \neq j} U_{ij} \, . \]  

Let the repulsive potential energy for the nearest neighbors be:

\[ U_{\text{rep.}} = \frac{A}{R^n} \, . \] (6)

Then,

\[ U_{ij} = \frac{A}{R^n} - \frac{q^2}{R} \text{ for nearest neighbors} \]
\[ U_{ij} = \pm \frac{q^2}{p_{ij} R} \text{ otherwise} \] (7)

\[ U_{\text{total}} = N U_i = N \sum_{i \neq j} U_{ij} = \frac{N z A}{R^n} - \frac{q^2 N \alpha}{R} \, , \text{ where } \alpha \equiv \sum_{i \neq j} \frac{(\pm)}{p_{ij}} \, . \] (8)

At the equilibrium separation:

\[ \left[ \frac{dU_{\text{total}}}{dR} \right]_{R_0} = 0 \, , \]
\[ \frac{-n N z A}{R_0^{n+1}} + \frac{q^2 N \alpha}{R_0^2} = 0 \Rightarrow \frac{z A}{R_0^n} = \frac{q^2 \alpha}{n R_0} \]

\[ U(R_0) = \frac{N z A}{R_0^n} - \frac{q^2 N \alpha}{R_0} = -\frac{q^2 N \alpha}{R_0} \left( 1 - \frac{1}{n} \right) \, . \] (10)

(b) Consider the Taylor expansion for \( U_i \), (we deal with \( U_i \) instead of \( U \), because we want to obtain the work done in compressing a unit length):

\[ U_i(R_0 - \delta R_0) = U_i(R_0) - U'_i(R_0) \delta R_0 + \frac{1}{2} U''_i(R_0) \delta^2 R_0^2 + \ldots \] (11)

The work done is equal to

\[ W = U_i(R_0 - \delta R_0) - U_i(R_0) = -U'_i(R_0) \delta R_0 + \frac{1}{2} U''_i(R_0) \delta^2 R_0^2 + \ldots \] (12)

Since in equilibrium \( U''_i(R_0) = 0 \),

\[ W = U_i(R_0 - \delta R_0) - U_i(R_0) \simeq \frac{1}{2} U''_i(R_0) \delta^2 R_0^2 \, . \] (13)
\[
\left[ \frac{d^2 U_i}{dR^2} \right]_{R_0} = \frac{n(n+1)zA}{R_0^{n+2}} - \frac{2q^2 \alpha}{R_0^3}.
\]  

(14)

From the equilibrium condition we have found that

\[
\frac{zA}{R_0^3} = \frac{q^2 \alpha}{n R_0},
\]

(15)

\[
\left[ \frac{d^2 U_i}{dR^2} \right]_{R_0} = \frac{(n+1)q^2 \alpha}{R_0^3} - \frac{2q^2 \alpha}{R_0^3} = \frac{(n-1)q^2 \alpha}{R_0^3}.
\]

(16)

The work \( W \) done is then equal to:

\[
W = \frac{\delta^2}{2} \frac{(n-1)q^2 \alpha}{R_0}.
\]

(17)