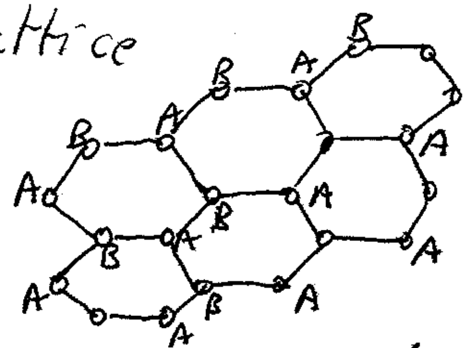
Physics 231 Homework 1 Solutions. Total (33)

1/ Honeycomb lattice



Let the atomic spacing be a.

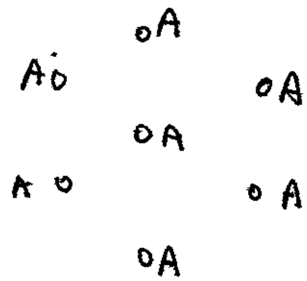
Smallest repeating unit is a nearest neighbor pair eg

↖ The basis

(It is not a Bravais lattice because, for example, starting at A there is a vector $\vec{e}$, say, to $\vec{B}$ but the vector $-\vec{e}$, starting at a, does not go to a lattice point).

(4)

The Bravais lattice is the lattice formed by, say, all the A sites, this is a triangular lattice.

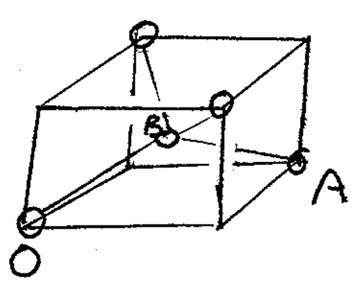


The spacing between nearest neighbor points of the Bravais lattice is $\sqrt{3}\,a$, where a is the lattice space of the Honeycomb lattice.

2/ (a) This is a bcc lattice with a, the side of the conventional cubic cell, equal to 2.

(2) (b) This is an fcc lattice with a, the side of the conventional cubic cell equal to 2.

3/



O is at $(0,0,0)$

A is at $(2,2,0)$

B is at $(1,1,1)$ so $\vec{OB} = (1,1,1)$

$\vec{BA} = (-1,-1,1)$

$$\cos(O\hat{B}A) = \frac{\vec{OB}\cdot\vec{BA}}{|OB|\cdot|BA|} = \frac{-1}{\sqrt{3}\sqrt{3}} = \frac{-1}{3}$$

(3)

$$\text{so } O\hat{B}A = \cos^{-1}\left(\frac{-1}{3}\right) = 109.47^\circ$$

4 Reciprocal lattice basis vectors $\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}$ etc.

For $\underline{b_{cc}}$, $\vec{a}_1 = \frac{a}{2}(-1,1,1)$ $\vec{a}_2 = \frac{a}{2}(1,-1,1)$, $\vec{a}_3 = \frac{a}{2}(1,1,-1)$

$\vec{a}_2 \times \vec{a}_3 = \left(\frac{a}{2}\right)^2 (0, +2, 2)$ and $\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3 = \left(\frac{a}{2}\right)^3 (2+2) = \underline{\underline{\frac{a^3}{2}}}$

Hence $\vec{b}_1 = 2\pi \frac{2}{a^3} \left(\frac{a}{2}\right)^2 (0,2,2) = \underline{\frac{2\pi}{a}(0,1,1)}$

This is a basis vector of ~~of~~ the FCC lattice.
A similar calculation shows $\vec{b}_2$ and $\vec{b}_3$ are basis vectors of the FCC lattice.
Hence reciprocal lattice of the bcc is FCC

Similarly for FCC $\vec{a}_1 = \frac{a}{2}(0,1,1)$, $\vec{a}_2 = \frac{a}{2}(1,0,1)$, $\vec{a}_3 = \frac{a}{2}(1,1,0)$

(4)

Hence $\vec{a}_2 \times \vec{a}_3 = \left(\frac{a}{2}\right)^2 [-1, 1, 1]$

and $\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3 = \left(\frac{a}{2}\right)^3 [0+1+1] = \frac{a^3}{4}$

Hence $\vec{b}_1 = 2\pi \frac{4}{a^3} \frac{a^2}{4} (-1,1,1) = \underline{\frac{2\pi}{a}(-1,1,1)}$

which is a ~~reciprocal lattice~~ basis vector of the bcc lattice.
Similarly $\vec{b}_2$ and $\vec{b}_3$ are basis vectors of the bcc lattice.

Hence reciprocal lattice of FCC is bcc

5 $v = \vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3$

(4) $v_{Br} = \vec{b}_1 \cdot \vec{b}_2 \times \vec{b}_3 = 2\pi \frac{(\vec{a}_2 \times \vec{a}_3)}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \cdot (\vec{b}_2 \times \vec{b}_3)$

Now $(\vec{A} \times \vec{B}) \cdot (\vec{C} \times \vec{D}) = (\vec{A} \cdot \vec{C})(\vec{B} \cdot \vec{D}) - (\vec{A} \cdot \vec{D})(\vec{B} \cdot \vec{C})$

so $v_{Br} = \frac{2\pi}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \left((\vec{a}_2 \cdot \vec{b}_2)(\vec{a}_3 \cdot \vec{b}_3) - (\vec{a}_2 \cdot \vec{b}_3)(\vec{a}_3 \cdot \vec{b}_2) \right)$

But $a_i b_j = 2\pi \delta_{ij}$ so $V_{Br} = \frac{(2\pi)^3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} = \underline{\underline{\frac{(2\pi)^3}{v}}}$

4 6. See Ashcroft & Mermin p 90

4 7. See Ashcroft & Mermin p 99-100

8. NaCl. Bravais lattice is fcc, basis vectors
$\vec{a}_1 = \frac{a}{2}(0,1,1)$, $\vec{a}_2 = \frac{a}{2}(1,0,1)$, $\vec{a}_3 = \frac{a}{2}(1,1,0)$

Basis is 1 atom at 0 and the other at $\frac{a}{2}(1,0,0)$

As shown in problem 4 the reciprocal lattice is bcc with reciprocal lattice basis vectors
$\frac{2\pi}{a}(-1,1,1)$, $\frac{2\pi}{a}(1,-1,1)$, $\frac{2\pi}{a}(1,1,-1)$

Since the bcc is 2 interpenetrating simple cubic lattices a reciprocal lattice vector is $\frac{2\pi}{a}(m_1, m_2, m_3)$ where the m_i are either all even, or all odd, see Qu. 2(a).
Equivalently we can say
$$\vec{G} = \frac{4\pi}{a}(\nu_1, \nu_2, \nu_3)$$
where either all ν_i are integer
or all ν_i = integer + 1/2

Form factor of the unit cell is
$$\sum_i f_i e^{i\vec{G}\cdot\vec{r}_i} = f_1 + f_2 e^{i\vec{G}\cdot\vec{r}} \qquad \vec{r} = \frac{a}{2}(1,0,0)$$

4 Now $e^{i\vec{G}\cdot\vec{r}} = e^{2\pi i \nu_1} = \begin{cases} 1 & \text{if } \nu_1 = \text{integer} \\ -1 & \text{if } \nu_1 = \text{integer} + 1/2 \end{cases}$

Hence form factor of cell is $\begin{cases} f_1 + f_2 & \text{if } \nu_1 = \text{integer} \\ f_1 - f_2 & \text{if } \nu_1 = \text{integer} + \frac{1}{2} \end{cases}$

if $f_1 = f_2$ there is no difference between the atoms (as far as the scattering experiment is concerned) so we (effectively) have a sc lattice with lattice spacing $a/2$ so the reciprocal lattice is also sc with reciprocal lattice vectors
$\frac{4\pi}{a}(m_1, m_2, m_3)$ where the m_i are integers
Thus the spots with ν_i = integer + $\frac{1}{2}$ must vanish.

(4) (9)

9 Scattering amplitude from a chain of atoms

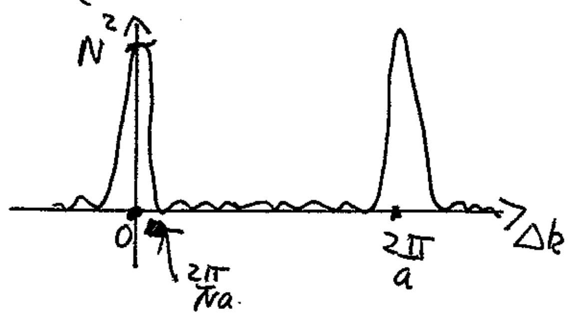
$$F = \sum_{n=0}^{N-1} e^{ina\Delta k} = \frac{1 - e^{ia\Delta k N}}{1 - e^{ia\Delta k}}$$

Scattering intensity $\propto |F|^2 = \frac{(1 - e^{-ia\Delta kN})(1 - e^{ia\Delta kN})}{(1 - e^{-ia\Delta k})(1 - e^{ia\Delta kN})}$

$$= \frac{2 - 2\cos(aN\Delta k)}{2 - 2\cos a\Delta k}$$

(4)

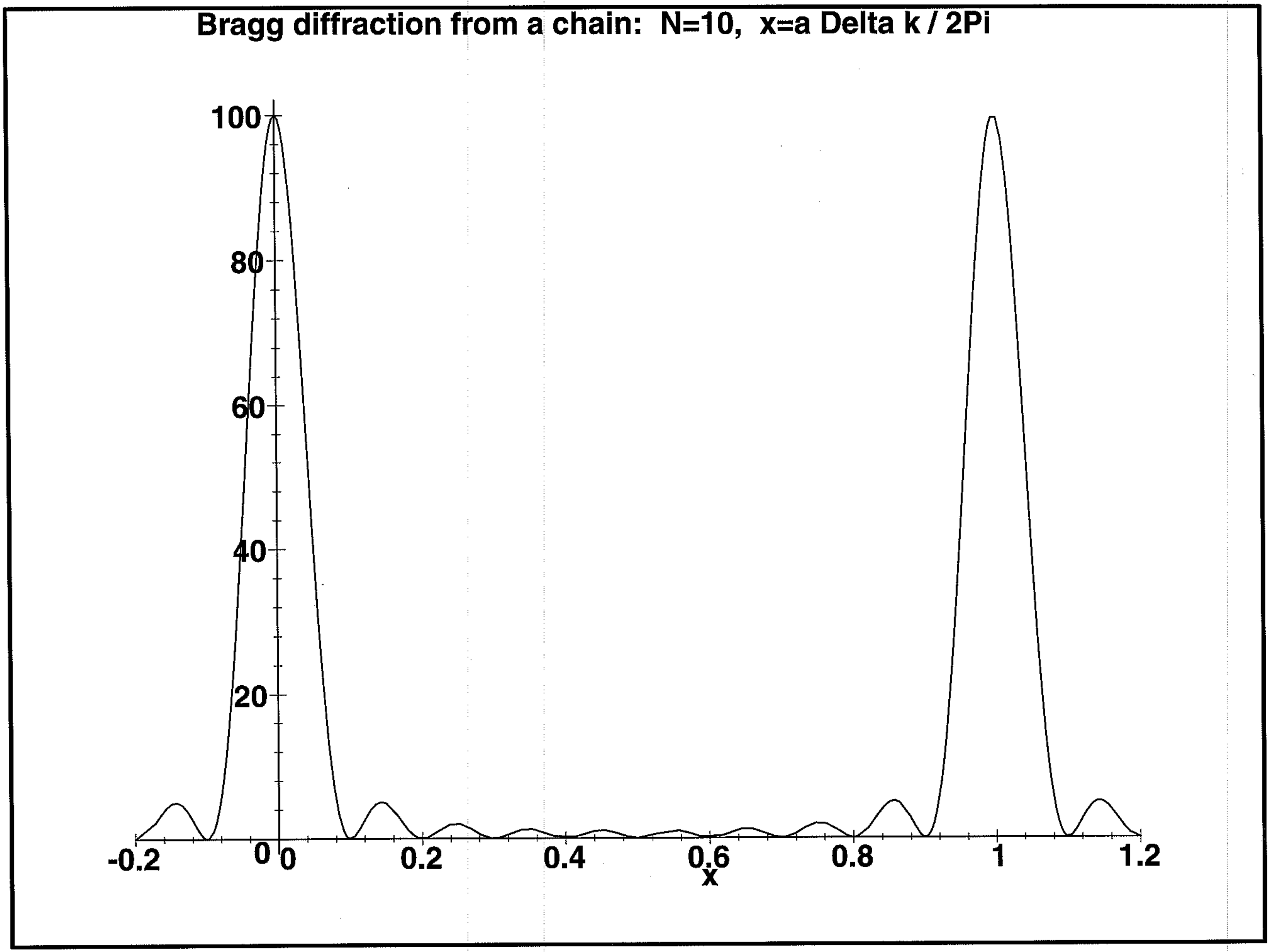
$$= \frac{\sin^2(\frac{1}{2}Na\Delta k)}{\sin^2(\frac{1}{2}a\Delta k)}$$



$\Delta k \to 0$ $\quad |F|^2 = N^2$ i.e. very large if N is large.

1st zero is at $\Delta k = \frac{2\pi}{Na}$ so width of peak $\propto \frac{1}{N}$.

i.e. very sharp if N large.


Bragg diffraction from a chain: N=10, x=a Delta k / 2Pi
100
80
60
40
20
0
-0.2
0
0.2
0.4
0.6
0.8
1
1.2
x

Bragg diffraction from a chain: N=10, x=a Delta k / 2Pi