Assignment 2: SOLID STATE PHYSICS – RECIPROCAL LATTICE

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Problem 1

Interplanar separation Consider a plane hkl in a crystal lattice. (a) Prove that the reciprocal lattice vector $G = hb_1 + kb_2 + lb_3$ is perpendicular to this plane. (b) Prove that the distance between two adjacent parallel planes of the lattice is $d(hkl) = 2\pi/|G|$. (c) Show for a simple cubic lattice that $d^2 = a^2/(h^2 + k^2 + l^2)$.

Answer 1: a.) The two vectors that can be found in the plane are $(x_2\vec{a_2} - x_1\vec{a_1})$ and $(x_3\vec{a_3} - x_1\vec{a_1})$. Hence, the normal vector to the plane can be defined as

$$(x_2\vec{a_2} - x_1\vec{a_1}) \times (x_3\vec{a_3} - x_1\vec{a_1}) \tag{1}$$

$$= x_1x_3\vec{a_3} \times \vec{a_1} + x_1x_2\vec{a_1} \times \vec{a_2} + x_2x_3\vec{a_3} \times \vec{a_3} \tag{2}$$

$$= x_1x_2x_3(\frac{1}{x_1}\vec{a_2} \times \vec{a_3} + \frac{1}{x_2}\vec{a_3} \times \vec{a_1} + \frac{1}{x_3}\vec{a_1} \times \vec{a_2}) \tag{3}$$

$$\therefore \approx h\vec{b_1} + k\vec{b_2} + l\vec{b_3} \tag{4}$$

b.) To prove that the distance between two adjacent parallel planes of the lattice is $d(hkl) = \frac{2\pi}{||G||}$, suppose that, for any $\vec{R} = x_1\vec{a_1} + x_2\vec{a_2} + x_3\vec{a_3}$, the expression $e^{i\vec{G}\vec{R}}$ is equal to some constant. Since, the lattice contain $0\vec{a_1}+0\vec{a_2}+0\vec{a_3}$, we get $e^{i\vec{G}\vec{R}} = 1$. Therefore, $\vec{G}\vec{R} = 2\pi n \rightarrow \vec{G}\Delta\vec{R} = 2\pi\Delta n$. With that, the distance between two adjacent parallel plane $(\Delta n = 1)$ is

$$d = \frac{\vec{G}}{||\vec{G}||}\Delta\vec{R} = \frac{2\pi}{||\vec{G}||} \tag{5}$$

c.) For a simple cubic lattice, we have

$$\vec{G} = h\vec{b_1} + k\vec{b_2} + l\vec{b_3} \tag{6}$$

$$||\vec{G}|| = \sqrt{h^2 + k^2 + l^2} \times (\frac{2\pi}{a}) \rightarrow \ d = \frac{2\pi}{||G||} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \tag{7}$$

Problem 2

Hexagonal space lattice. The primitive translation vectors of the hexagonal space lattice may be taken as

$$a_1 = (\frac{\sqrt{3}}{2}a)\hat{x} + (\frac{1}{2}a)\hat{y}; \quad a_2 = -(\frac{\sqrt{3}}{2}a)\hat{x} + (\frac{1}{2}a)\hat{y}; \quad a_3 = c\hat{z} \tag{8}$$

a.) Show that the volume of the primitive cell is $\frac{\sqrt{3}}{2}a^2c$.
b.) Show that the primitive translation of the reciprocal lattice are

$$b_1 = (\frac{2\pi}{\sqrt{3}a})\hat{x} + (\frac{2\pi}{a})\hat{y}; \quad b_1 = -(\frac{2\pi}{\sqrt{3}a})\hat{x} + (\frac{2\pi}{a})\hat{y}; \quad b_3 = (\frac{2\pi}{c})\hat{z} \tag{9}$$

so that the lattice is its own reciprocal, but with a rotation of axes.
c.) Describe and sketch the first Brillouin zone of the hexagonal space lattice.

Answer 2:
a.) The volume of the primitive cell is

$$V_c = a_1 \cdot (a_2 \times a_3) = \begin{bmatrix} \frac{\sqrt{3}a}{2} & \frac{a}{2} & 0 \\ -\frac{\sqrt{3}a}{2} & \frac{a}{2} & 0 \\ 0 & 0 & c \end{bmatrix} = \frac{\sqrt{3}}{2}a^2c \tag{10}$$

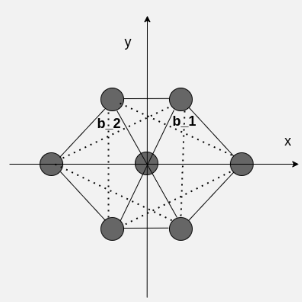
b.)

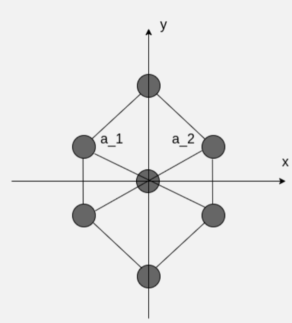
$$b_1 = \frac{2\pi}{V_c}(a_2 \times a_3) = \frac{2\pi}{\frac{\sqrt{3}}{2}a^2c} \begin{bmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{\sqrt{3}a}{2} & \frac{a}{2} & 0 \\ 0 & 0 & c \end{bmatrix} = \frac{2\pi}{a}(\frac{1}{\sqrt{3}}\hat{x} + \hat{y}) \tag{11}$$

$$b_2 = \frac{2\pi}{V_c}(a_3 \times a_1) = \frac{2\pi}{\frac{\sqrt{3}}{2}a^2c} \begin{bmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 0 & c \\ \frac{\sqrt{3}a}{2} & \frac{a}{2} & 0 \end{bmatrix} = \frac{2\pi}{a}(-\frac{1}{\sqrt{3}}\hat{x} + \hat{y}) \tag{12}$$

$$b_3 = \frac{2\pi}{V_c}(a_1 \times a_2) = \frac{2\pi}{\frac{\sqrt{3}}{2}a^2c} \begin{bmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{\sqrt{3}a}{2} & \frac{a}{2} & 0 \\ \frac{-\sqrt{3}a}{2} & \frac{a}{2} & 0 \end{bmatrix} = \frac{2\pi}{c}\hat{z} \tag{13}$$

c.)





Problem 3

Volume of Brillouin zone. Show that the volume of the first Brillouin zone is $(2\pi)^3/V_c$ where V_c is the volume of a crystal primitive cell. Hint: The volume of a Brillouin zone is equal to the volume of the primitive parallelepiped in Fourier space. Recall the vector identity $(c \times a) \times (a \times b) = (c \cdot a \times b)a$

Answer 3: Based on the given hint, the volume of the Brillouin zone i equal to the volume of the primitive parallelepiped in Fourier space which was described by

$$\vec{b_1} = 2\pi \frac{\vec{a_2} \times \vec{a_3}}{\vec{a_1} \cdot \vec{a_2} \times \vec{a_3}} \tag{14}$$

$$\vec{b_2} = 2\pi \frac{\vec{a_3} \times \vec{a_1}}{\vec{a_1} \cdot \vec{a_2} \times \vec{a_3}} \tag{15}$$

$$\vec{b_3} = 2\pi \frac{\vec{a_1} \times \vec{a_2}}{\vec{a_1} \cdot \vec{a_2} \times \vec{a_3}} \tag{16}$$

With that, the volume of the first Brillouin zone $V_{BZ} = \vec{b_1} \cdot \vec{b_2} \times \vec{b_3}$ and $V_c = \vec{a_1} \cdot \vec{a_2} \times \vec{a_3}$

$$V_{BZ} = \frac{(2\pi)^3}{V_c^3} \vec{a_2} \times \vec{a_3} \cdot (\vec{a_3} \times \vec{a_1}) \times (\vec{a_1} \times \vec{a_2}) \tag{17}$$

$$= \frac{(2\pi)^3}{V_c^3} \vec{a_2} \times \vec{a_3} \cdot (\vec{a_3} \cdot \vec{a_1} \times \vec{a_2}) \vec{a_1} \tag{18}$$

$$= \frac{(2\pi)^3}{V_c^3} (\vec{a_1} \cdot \vec{a_2} \times \vec{a_3})^2 = \frac{(2\pi)^3}{V_c} \tag{19}$$

Problem 4

Structure factor of diamond. The crystal structure of diamond is described in previous discussion. The basis consists of eight atoms if the cell is taken as the conventional cube. (a) Find the structure factor S of this basis. (b) Find the zeros of S and show that the allowed reflections of the diamond structure satisfy $v_1 + v_2 + v_3 = 4n$, where all indices are even and n is any integer, or else all indices are odd (see figure below). Notice that h, k, l may be written for v_1, v_2, v_3 and this is often done.

Answer 4:
a.) Let

$$S = \sum_{i=1}^{n} exp(i\vec{G} \cdot \vec{R_j}) \tag{20}$$

where $\vec{R_1}$, $\vec{R_2}$, $\vec{R_3}$, $\vec{R_4}$, , are the four atoms in a fcc cubic cell. Also, $\vec{R_5}$, $\vec{R_6}$, $\vec{R_7}$, $\vec{R_8}$, are the four atoms in another fcc cubic cell which is shifted by $\vec{R_0} = (\vec{x}+\vec{y}+\vec{z})a/4$. Therefore, $\vec{R_5} = \vec{R_1} + \vec{R_0}$, $\vec{R_6} = \vec{R_2} + \vec{R_0}$, $\vec{R_7} = \vec{R_3} + \vec{R_0}$, and $\vec{R_8} = \vec{R_4} + \vec{R_0}$.

$$S = \sum_{i=1}^{n} exp(i\vec{G}\cdot\vec{R_0}) = \sum_{i=1}^{4} exp(i\vec{G}\cdot\vec{R_0}) + \sum_{i=1}^{4} exp[i\vec{G}\cdot(\vec{R_i}+\vec{R_0})] \tag{21}$$

$$= [1 + exp(i\vec{G}\cdot\vec{R_0})]\sum_{i=1}^{4} exp(i\vec{G}\cdot\vec{R_i}) \tag{22}$$

where the $\sum_{i=1}^{4} exp(i\vec{G}\cdot\vec{R_i})$ is the fcc structure factor. For $\vec{G} = h\vec{b_1} + k\vec{b_2} + l\vec{b_3} = \frac{2\pi}{a}(h\vec{x} + k\vec{y} + l\vec{z})$, $\vec{G}\cdot\vec{R_0} = \pi(h+k+l)/4$.

$$\therefore S = (1 + exp[\pi(h+k+l)/2])(1 + exp[i\pi(h+k)] + exp[i\pi(k+l)] + exp[i\pi(l+h)]) \tag{23}$$

b.) Due to the fcc structure factor, the zero of S occurs when h, k, l are not all even nor odd. Such that

When $h+k+l = 4n$ and all $h,\ k,\ ,l$ are even, $= 8$.

Also, when $h+k+l = 4n \pm 1$ and all $h,\ k,\ ,l$ are odd $S = 4(1 \pm i)$.

Problem 5

Form factor of atomic hydrogen. For the hydrogen atom in its ground state, the number density is $n(r) = (\pi a_0^3)^{-1} exp(-2r/a_0)$, where a_0 is the Bohr radius. Show that the form factor is $f_G = 16/(4 + G^2a_0^2)^2$.

Answer 5: The atomic form factor is

$$f_G = \int n(r)e^{-i\vec{G}\cdot\vec{r}}d\tau = \int \frac{1}{\pi a_0^3}e^{-i\vec{G}\cdot\vec{r}}d\tau \tag{24}$$

where $d\tau = r^3 sin\theta dr d\theta d\phi$

$$f_0 = \frac{1}{\pi a_0^3}\int e^{-\frac{2r}{a_0}}e^{-iGrws\theta}r^2 sin\theta dr d\theta d\phi \tag{25}$$

$$= \frac{1}{\pi a_0^3}\int_{r=0}^{\infty} r^2 e^{-\frac{2r}{a_0}}dr \int_{\theta=0}^{\pi} e^{-iGrws\theta}\dots sin\theta d\theta \int_{\phi=0}^{2\pi} d\phi \tag{26}$$

$$= \frac{1}{\pi a_0^3}2\pi \int_0^{\infty} r^2 e^{-\frac{2r}{a_0}}dr \cdots \int_0^{\pi} e^{-iGrcos\theta} sin\theta d\theta \tag{27}$$

let $u = -iGrcos\theta;\ du = iGrsin\theta d\theta$

$$f_G = \frac{2}{a_0^3}\int_0^{\infty} r^2 e^{-\frac{2r}{a_0}}dr \int \frac{e^4}{iGr}du = -\frac{2i}{a_0^3 G}\int_0^{\infty} re^{-\frac{2r}{a_0}}dr(e^4) \tag{28}$$

$$= -\frac{2i}{a_0^3 G}\int_0^\infty re^{-\frac{2r}{a_0}}dr(e^{-iGrws\theta})|_0^\pi \tag{29}$$

$$f_G = -\frac{2i}{a_0^3 G}\int_0^\infty re^{-\frac{2r}{a_0}}(e^{iGr} - e^{-iGR})dr \tag{30}$$

$$= \frac{2i}{a_0^3 G}[\int_0^\infty re^{-r(\frac{2}{a_0}-iG)}dr - \int_0^\infty re^{-r(\frac{2}{a_0}+iG)}dr] \tag{31}$$

Using the identity

$$\int_0^\infty e^{-ar}rdr = \frac{1}{a^2};\ a > 0 \tag{32}$$

$$f_G = -\frac{2i}{a_0^3 G}[\frac{1}{(\frac{2}{a_0} - iG)^2} - \frac{1}{(\frac{2}{a_0} + iG)^2}] = \frac{2i}{a_0^3 G}[\frac{\frac{8iG}{a_0}}{(\frac{4}{a_0^2} + G^2)^2}] \tag{33}$$

rewriting the denominator

$$f_G = -\frac{2i}{a_0^4 G}[\frac{8iG}{\frac{1}{a_0^4(4+a_0^2G^2)^2}}] = \frac{16}{(4 + g^2a_0^2)^2} \tag{34}$$

$$\therefore f_G = \frac{16}{4 + G^2a_0^2)^2} \tag{35}$$

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