Physics 481: Condensed Matter Physics - Homework Solutions 3

Homework 3.1

a) $\vec{a}_1 = \begin{pmatrix} a \\ 0 \\ 0 \end{pmatrix}, \quad \vec{a}_2 = \begin{pmatrix} a/2 \\ a\sqrt{3}/2 \\ 0 \end{pmatrix}, \quad \vec{a}_3 = \begin{pmatrix} 0 \\ 0 \\ c \end{pmatrix}$

- primitive cell volume

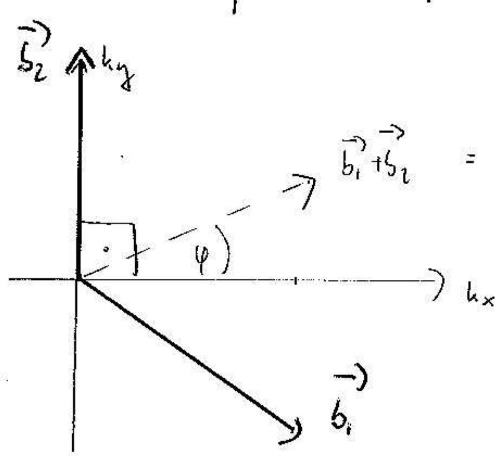
$$\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = \begin{vmatrix} a & 0 & 0 \\ a/2 & a\sqrt{3}/2 & 0 \\ 0 & 0 & c \end{vmatrix} = \frac{\sqrt{3}}{2} a^2 c$$

$$\vec{b}_1 = \frac{4\pi}{\sqrt{3}a^2c} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ a/2 & a\sqrt{3}/2 & 0 \\ 0 & 0 & c \end{vmatrix} = \frac{4\pi}{\sqrt{3}a^2c}\left(\frac{\sqrt{3}}{2}ac\,\hat{x} - \frac{1}{2}ac\,\hat{y}\right)$$

$$= \frac{2\pi}{a}\begin{pmatrix} 1 \\ -1/\sqrt{3} \\ 0 \end{pmatrix}$$

$$\vec{b}_2 = \frac{4\pi}{\sqrt{3}a^2c} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 0 & c \\ a & 0 & 0 \end{vmatrix} = \frac{4\pi}{\sqrt{3}a^2c}\left(\hat{y}\,ac\right) = \frac{2\pi}{a}\begin{pmatrix} 0 \\ 2/\sqrt{3} \\ 0 \end{pmatrix}$$

$$\vec{b}_3 = \frac{4\pi}{\sqrt{3}a^2c} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ a & 0 & 0 \\ a/2 & a\sqrt{3}/2 & 0 \end{vmatrix} = \hat{z}\,a^2\frac{\sqrt{3}}{2}\,\frac{4\pi}{\sqrt{3}a^2c} = \frac{2\pi}{c}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$



$$\vec{b}_1 + \vec{b}_2 = \frac{2\pi}{a}\begin{pmatrix} 1 \\ 1/\sqrt{3} \\ 0 \end{pmatrix} \qquad \tan\varphi = \frac{1}{\sqrt{3}}$$

$$\underline{\varphi = 30^\circ}$$

b) basis $\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$ $\begin{pmatrix} a/2 \\ a/(2\sqrt{3}) \\ c/2 \end{pmatrix}$

$$F(\vec{q}) = \left| \sum_j e^{i\vec{q}\cdot\vec{v}_j} \right|^2 =$$

$$= \left| 1 + e^{i(n_1\vec{b}_1 + n_2\vec{b}_2 + n_3\vec{b}_3)\cdot(a/2,\, a/(2\sqrt{3}),\, c/2)} \right|^2$$

$$= \left| 1 + e^{i\left\{\frac{2\pi}{a}n_1\left(\frac{a}{2}-\frac{a}{6}\right) + \frac{2\pi}{a}n_2\frac{a}{3} + \frac{2\pi}{c}n_3\frac{c}{2}\right\}} \right|^2$$

$$= \left| 1 + e^{i2\pi\left(\frac{1}{3}(n_1+n_2) + \frac{1}{2}n_3\right)} \right|^2$$

c) extinction when

$\frac{1}{3}(n_1+n_2) + \frac{1}{2}n_3$ is $\left(\text{integer} + \frac{1}{2}\right)$

e.g. n_1+n_2 multiple of 3, n_3 odd

3.2 Debye-Waller factor

$$\langle S(\vec{q})\rangle = \left\langle \frac{1}{N} \left| \sum_{l} e^{i\vec{q}\cdot(\vec{R}_l+\vec{u}_l)}\right|^2 \right\rangle$$

$$= \left\langle \frac{1}{N} \sum_{lj} e^{i\vec{q}\cdot(\vec{R}_l+\vec{u}_l)} e^{-i\vec{q}\cdot(\vec{R}_j+\vec{u}_j)} \right\rangle$$

$$= \frac{1}{N} \sum_{lj} e^{i\vec{q}(\vec{R}_l-\vec{R}_j)} \left\langle e^{i\vec{q}\cdot(\vec{u}_l-\vec{u}_j)} \right\rangle$$

Now deal with the average

$$\left\langle e^{i\vec{q}\cdot(\vec{u}_l-\vec{u}_j)} \right\rangle = 1 \quad \text{for} \quad l = j$$

for $l \neq j$

$$\left\langle e^{i\vec{q}\cdot(\vec{u}_l-\vec{u}_j)} \right\rangle = \left(\frac{1}{2\pi\Delta^2}\right)^3 \int d^3u_l\, d^3u_j\, e^{-(u_l^2+u_j^2)/2\Delta^2} e^{i\vec{q}(\vec{u}_l-\vec{u}_j)}$$

$$= \left(\frac{1}{2\pi\Delta^2}\right)^{3/2} \int d^3u_l\, e^{-\frac{u_l^2}{2\Delta^2}} e^{i\vec{q}\cdot\vec{u}_l} \int d^3u_j\, e^{-\frac{u_j^2}{2\Delta^2}} e^{-i\vec{q}\cdot\vec{u}_j}$$

Complete the square in the exponents

$$\left\langle e^{i\vec{q}\cdot(\vec{u}_l-\vec{u}_j)} \right\rangle = e^{-\frac{\Delta^2}{2}q^2} \; e^{-\frac{\Delta^2}{2}q^2} = e^{-\Delta^2 q^2}$$

$$\langle S(\vec{q})\rangle = S^0(q) \quad e^{-\Delta q^2} \quad (+\text{ const (from } j=l))$$

ideal case — Debye-Waller factor

peaks still sharp