Physics 481: Condensed Matter Physics - Homework Solutions 7

1

Problem 7.1

a) radius of atom spheres:

$$r \leq \frac{a}{2} \quad (\text{distance along } x\text{-axis})$$

$$r < \sqrt{\left(\frac{a}{4}\right)^2 + \left(\frac{a}{4}\right)^2 + \frac{9a^2}{64}} = \frac{a}{8}\sqrt{17} > \frac{a}{2}$$

$$\Rightarrow \quad r_{max} = \frac{a}{2}$$

$$f = \frac{2 \cdot \frac{4}{3}\pi\left(\frac{a}{2}\right)^3}{3/2\, a^3} = \frac{16}{9}\pi\frac{1}{8} = \frac{2}{9}\pi = 69.8\,\%$$

b) Conventional cell

$$\frac{2\pi}{a}\begin{pmatrix}1\\0\\0\end{pmatrix}, \quad \frac{2\pi}{a}\begin{pmatrix}0\\1\\0\end{pmatrix}, \quad \frac{4\pi}{3a}\begin{pmatrix}0\\0\\1\end{pmatrix}$$

c)

$$\vec{q} = \frac{2\pi}{a}\begin{pmatrix}n_1\\n_2\\2n_3/3\end{pmatrix}, \quad \vec{v}_1 = \begin{pmatrix}0\\0\\0\end{pmatrix}, \quad \vec{v}_2 = \begin{pmatrix}a/2\\a/2\\3a/4\end{pmatrix}.$$

$$F(\vec{q}) = 1 + e^{i2\pi\left(\frac{n_1}{2} + \frac{n_2}{2} + \frac{n_3}{2}\right)} = 1 + e^{i\pi(n_1+n_2+n_3)}$$

extinction if $n_1+n_2+n_3$ odd

shortest $\vec{q}$ with even $h_1+h_2+h_3$

101, 011: $|\vec{q}| = \frac{2\pi}{a}\sqrt{1+(2/3)^2} = \frac{2\pi}{a}\frac{\sqrt{13}}{3} = 1.80\,\text{Å}^{-1}$ (1)

002: $|\vec{q}| = \frac{2\pi}{a}\frac{4}{3} = 1.99\,\text{Å}^{-1}$ (2)

110: $|\vec{q}| = \frac{2\pi}{a}\sqrt{2} = 2.11\,\text{Å}^{-1}$ (3)

200, 020: $|\vec{q}| = \frac{2\pi}{a}\,2$

112: $\vec{q} = \frac{2\pi}{a}\sqrt{1+1+\frac{16}{9}} = \frac{2\pi}{a}\frac{\sqrt{34}}{3} = 2.90\,\text{Å}^{-1}$ (4)

$$q = 2k_0 \sin\frac{\vartheta}{2} \Rightarrow \sin\frac{\vartheta}{2} = \frac{q}{2k_0} = \frac{q}{2}\frac{\lambda}{2\pi} = \frac{q\lambda}{4\pi}$$

(1) $24.81°$

(2) $27.48°$

(3) $29.18°$

(4) $40.5°$

Problem 7.2

a) $$M\ddot{u}_n = -\sum_{m>0} K_m(u_n - u_{n+m}) - \sum_{m>0} K_m(u_n - u_{n-m})$$

$$u_n = u_0 e^{iqan - i\omega t}$$

$$-M\omega^2 e^{iqan} = -\sum_m K_m\left(e^{iqan} - e^{iqa(n+m)}\right)$$
$$-\sum_m K_m\left(e^{iqan} - e^{iqa(n-m)}\right)$$

$$M\omega^2 = \sum_{m>0} K_m\left\{2 - 2\cos(qam)\right\}$$

$$\boxed{M\omega^2 = \sum_{m>0} K_m\, 4\sin^2\left(\frac{qam}{2}\right)}$$

b) $K_m = K_0/m^p \qquad p > 3$

Expand sin

$$M\omega^2 = K_0 \sum_{m>0} \frac{1}{m^p} q^2 a^2 m^2$$

$$\omega^2 = \left(\frac{K_0}{M} a^2 \sum_{m>0} \frac{1}{m^{p-2}}\right) q^2$$

Sum converges for $p-2 > 1$

$$c = \sqrt{\frac{K_0}{M} a^2 \sum_{m>0} \frac{1}{m^{p-2}}}$$

c) For $p < 3$, $\sum_{m>0} \frac{1}{m^{p-2}}$ diverges,

$\Rightarrow$ one cannot expand the sin

$\Rightarrow$ approximate sum by integral

$$\omega^2 = \frac{K_0}{M} \int_1^\infty dm \, \frac{1}{m^p} \, 4 \sin^2\left(\frac{qam}{2}\right)$$

scale $\frac{qam}{2} = x$ $\qquad m = \frac{2x}{qa}$

$$\omega^2 = \frac{K_0}{M} \int_{\frac{qa}{2}}^\infty \frac{2dx}{qa} \left(\frac{qa}{2x}\right)^p 4 \sin^2(x)$$

$$\omega^2 = \left(\frac{qa}{2}\right)^{p-1} \frac{4K_0}{M} \underbrace{\int_{\frac{qa}{2}}^\infty dx \, x^{-p} \sin^2(x)}_{I(q)}$$

For $p < 3$, integral $I(q)$ converges for $q \to 0$

$$\boxed{\omega^2 = \left(\frac{qa}{2}\right)^{p-1} \frac{4K_0}{M} I(0)}$$

Problem 7.3

a) $$E = E_C + E_{rep} = -N\alpha \frac{e^2}{r} + \frac{1}{2} N\, 6 \cdot \frac{A}{r^{12}}$$

$$E = N\left(-\alpha \frac{e^2}{r} + 3\frac{A}{r^{12}}\right)$$

$$\frac{\partial E}{\partial r} = N\left(\frac{\alpha e^2}{r^2} - \frac{36A}{r^{13}}\right) \overset{!}{=} 0$$

$$\alpha e^2 = \frac{36A}{r^{11}}$$

$$r^{11} = \frac{36A}{\alpha e^2} \qquad r = \left(\frac{36A}{\alpha e^2}\right)^{\frac{1}{11}}$$

$$E = N\left(-\alpha e^2 \left(\frac{\alpha e^2}{36A}\right)^{\frac{1}{11}} + 3A\left(\frac{\alpha e^2}{36A}\right)^{\frac{12}{11}}\right)$$

$$= N(\alpha e^2)^{12/11} (36A)^{-\frac{1}{11}} \left(-1 + \frac{1}{12}\right)$$

$$= -\frac{11}{12} N (\alpha e^2)^{12/11} (36A)^{-\frac{1}{11}}$$

b) $$E = -N\alpha \frac{e^2}{r} + \frac{1}{2} N \cdot 8 \frac{A}{r^{12}} = N\left(-\alpha\frac{e^2}{r} + \frac{4A}{r^{12}}\right)$$

$$\frac{\partial E}{\partial r} = N\left(\frac{\alpha e^2}{r^2} - \frac{48}{r^{13}} A\right) \overset{!}{=} 0$$

$$\alpha e^2 = \frac{48}{r^{11}} A \qquad r = \left(\frac{48A}{\alpha e^2}\right)^{\frac{1}{11}}$$

$$E = N\left(-\alpha e^2 \left(\frac{\alpha e^2}{48A}\right)^{\frac{1}{11}} + 4A\left(\frac{\alpha e^2}{48A}\right)^{\frac{12}{11}}\right)$$

$$= N(\alpha e^2)^{12/11} (48A)^{-\frac{1}{11}} \left(-1 + \frac{1}{12}\right)$$

$$= -\frac{11}{12} N (\alpha e^2)^{12/11} (48A)^{-\frac{1}{11}}$$

(2)

c) NaCl $E = -\frac{11}{12}\frac{\alpha e^2}{r}$ $r = \left(\frac{36A}{\alpha e^2}\right)^{\frac{1}{11}}$

CsCl $E = -\frac{11}{12}\frac{\alpha e^2}{r}$ $r = \left(\frac{48A}{\alpha e^2}\right)^{\frac{1}{11}}$

NaCl: $\alpha^{12/11}\ 36^{-\frac{1}{11}} = 1.3274$

CsCl $\alpha^{12/11}\ 48^{-\frac{1}{11}} = 1.3053$

NaCl structure has lower energy