Physics 481: Condensed Matter Physics - Homework Solutions 6

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Problem 1: Noble gas crystal

a) 12 nearest neighbors in f.c.c. lattice

nearest neighbor distance $r = \sqrt{2}\,\frac{1}{2}a = \frac{a}{\sqrt{2}}$

b) $\frac{E}{N} = \frac{1}{2} \cdot 12 \cdot U(r_{min}) = 6\,U(r_{min})$

to minimize U : $x = \left(\frac{\sigma}{r}\right)^6$

$U = -4\varepsilon\,(x - x^2)$

$\frac{dU}{dx} = -4\varepsilon\,(1 - 2x) \Rightarrow x_{min} = \frac{1}{2}$

$r_{min} = 2^{1/6}\,\sigma = 3.81\,\mathring{A}$

$U_{min} = U(x = \frac{1}{2}) = -\varepsilon$

$\frac{E}{N} = -6\varepsilon = -0.0624\ \text{eV/atom}$

less strong than exp (further neighbors neglected)

$a = \sqrt{2}\,r_{min} = 5.39\,\mathring{A}$ very close to exp

c) $\frac{E}{N} = 6\,U(r)$ expand about $r = r_{min}$

$$= 6\,U(r_{min}) + 6\,\frac{1}{2}\,\delta^2 r_{min}^2 \left.\frac{\partial^2 U}{\partial r^2}\right|_{r_{min}}$$

$$\frac{\Delta E}{N} = 3\delta^2 r_{min}^2 \left[-4\varepsilon \left(\frac{42\sigma^6}{r^8} \right) + 4\varepsilon \left(\frac{156\,\sigma^{12}}{r^{14}} \right) \right]_{r_{min}}$$

$$= 12\,\delta^2 \varepsilon \left[-42 \left(\frac{\sigma}{r_{min}} \right)^6 + 156 \left(\frac{\sigma}{r_{min}} \right)^{12} \right] = -12\,\delta^2 \varepsilon \left(-21 + 39 \right)$$

$$\boxed{\frac{\Delta E}{N} = 216\,\delta^2 \varepsilon}$$

d)

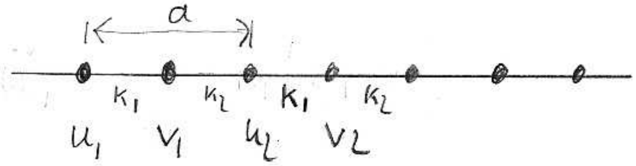
$$\Delta E = -p\,\Delta V \qquad \Delta V = \frac{N}{4} \left(a^3 (1-\delta)^3 - a^3 \right) = -\frac{N a^3}{4}\, 3\delta$$

4 atoms per unitcell

$$216\,\delta^2 \varepsilon = p\,\frac{3}{4}\,a^3 \delta$$

$$\delta = \frac{1}{288}\,\frac{p a^3}{\varepsilon} = \frac{1}{288}\,\frac{10^7 \frac{N}{m^2} \left(5.4 \cdot 10^{-10}\,m \right)^3}{0.01 \cdot 1.6 \cdot 10^{-19}\,Nm} = 0.0034$$

Problem 6.2



$$M\ddot{u}_n = -K_1(u_n - v_n) - K_2(u_n - v_{n-1})$$

$$M\ddot{v}_n = -K_1(v_n - u_n) - K_2(v_n - u_{n+1})$$

$$u_n = u_0 e^{i(qan - wt)}$$

$$v_n = v_0 e^{i(qan - wt)}$$

$$-w^2 M u_0 e^{iqan} = -K_1(u_0 e^{iqan} - v_0 e^{iqan}) - K_2(u_0 e^{iqan} - v_0 e^{iqa(n-1)})$$

$$-w^2 M v_0 e^{iqan} = -K_1(v_0 e^{iqan} - u_0 e^{iqan}) - K_2(v_0 e^{iqan} - u_0 e^{iqa(n+1)})$$

$$0 = [Mw^2 - (K_1 + K_2)]u_0 + (K_1 + K_2 e^{-iqa})v_0$$

$$0 = (K_1 + K_2 e^{iqa})u_0 + [Mw^2 - (K_1 + K_2)]v_0$$

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homogeneous system has solutions if coefficient determinant vanishes

$$\left[M\omega^2 - (K_1+K_2)\right]^2 = \left(K_1 + K_2 e^{-iqa}\right)\left(K_1 + K_2 e^{iqa}\right)$$

$$= K_1^2 + K_2^2 + 2K_1K_2 \cos qa$$

$$\omega^2 = \frac{K_1+K_2}{m} \pm \sqrt{\frac{K_1^2+K_2^2+2K_1K_2\cos qa}{m^2}}$$

two branches (+) : optical branch

(−) : acoustic branch

small q :

$$\omega^2 = \frac{K_1+K_2}{m} - \frac{1}{m}\sqrt{K_1^2+K_2^2+2K_1K_2\left(1-\tfrac{1}{2}q^2a^2\right)}$$

$$= \frac{K_1+K_2}{m} - \frac{1}{m}\sqrt{(K_1+K_2)^2 - K_1K_2q^2a^2}$$

$$= \frac{K_1+K_2}{m} - \frac{K_1+K_2}{m}\sqrt{1 - \frac{K_1K_2q^2a^2}{(K_1+K_2)^2}}$$

$$\omega^2 = \frac{1}{2m}\frac{K_1K_2}{K_1+K_2}q^2a^2 \Rightarrow c = \sqrt{\frac{a^2}{2m}\frac{K_1K_2}{K_1+K_2}}$$

c) $K_1 \gg K_2$ $\quad \omega^2 = \frac{K_1+K_2}{m} \pm \frac{K_1}{m}\sqrt{1+2\frac{K_2}{K_1}\cos qa}$

$$\omega^2 = \frac{K_1+K_2}{m} \pm \frac{K_1}{m}\left(1+\frac{K_2}{K_1}\cos qa\right)$$

$$\omega^2 = \begin{cases} \frac{2K_1}{m} + O(K_2/K_1) \\ \frac{K_2}{m}(1-\cos qa) = \frac{2K_2}{m}\sin^2\frac{qa}{2} \end{cases}$$

Optical branch: independent molecular vibrations with strong bond K_1

accoustic branch: linear chain of atoms of mass $2m$, coupled by weak bond K_2

d) $K_1 = K_2$

$$\omega^2 = \frac{2K}{m} \pm \frac{1}{m}\sqrt{2K^2(1+\cos qa)}$$

$$= \frac{2K}{m} \pm \frac{1}{m}\sqrt{4K^2\cos^2\frac{qa}{2}}$$

$$\omega^2 = \frac{2K}{m}\left(1 \pm \cos\frac{qa}{2}\right)$$

$a = 2d$

$\hat{=}$ nearest neighbor distance

$$\omega^2 = \frac{2K}{m}(1 \pm \cos qd)$$

identical to mon-atomic chain

(optical branch $\hat{=}$ higher q)