(1)

19) It was shown in the lectures (equation (33)) that the crystal energy is

$$U_{TOT} = 2N\varepsilon\left\{A_{12}\left(\frac{\sigma}{R}\right)^{12} - A_6\left(\frac{\sigma}{R}\right)^6\right\}$$

For BCC: $A_{12} = 9.11418$, $A_6 = 12.2533$

For FCC: $A_{12} = 12.13188$ $A_6 = 14.45392$

(the numbers for FCC were given in the lectures.)

In equilibrium $U'_{TOT} = 0$ where $U_{TOT} = \sum_{\text{lattice sites}} U(r)$

$$U'_{TOT} = 2\varepsilon N\left\{-12A_{12}\frac{\sigma^{12}}{r^{13}} + 6A_6\frac{\sigma^6}{r^7}\right\}$$

$$= \frac{12\varepsilon\sigma^6}{r^{13}}\left\{-2A_{12}\sigma^6 + A_6 r^6\right\}$$

$U' = 0 \Rightarrow$ equilibrium spacing is $r_0^6 = \frac{2A_{12}}{A_6}\sigma^6 \Rightarrow r_0 = \left(\frac{2A_{12}}{A_6}\right)^{1/6}\sigma$

$$U(r_0) = 2\varepsilon N\left\{A_{12}\left(\frac{\sigma}{r_0}\right)^{12} - A_6\left(\frac{\sigma}{r_0}\right)^6\right\}$$

$$= 2\varepsilon N\left\{A_{12}\left(\frac{A_6}{2A_{12}}\right)^2 - A_6\cdot\left(\frac{A_6}{2A_{12}}\right)\right\}$$

$$= 2\varepsilon N\frac{A_6^2}{2A_{12}}\left(\frac{1}{2} - 1\right)$$

$$= -\varepsilon N\frac{A_6^2}{2A_{12}}$$

$$= \begin{cases} -8.236\,\varepsilon N & \text{for BCC} \\ -8.610\,\varepsilon N & \text{for FCC}\end{cases}$$

$$\Rightarrow U/N = \begin{cases} -41.18 \times 10^{-22}\ \text{J for BCC} \\ -43.05 \times 10^{-22}\ \text{J for FCC}\end{cases}$$

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2)

The binding energy for FCC is lower than that of BCC, hence FCC is the more stable configuration and Neon freezes into a FCC crystal structure

(3)

(2a) The dispersion relation is given at the bottom of p. 45 of the notes:

$$\omega^2 = \frac{C(M_1+M_2) \pm C\sqrt{(M_1+M_2)^2 - 4M_1M_2\sin^2\left(\frac{Ka}{2}\right)}}{M_1M_2}$$

Phase velocity is

$$v_p = \frac{\omega}{K} = \frac{\left\{C(M_1+M_2) \pm C\sqrt{(M_1+M_2)^2 - 4M_1M_2\sin^2\left(\frac{Ka}{2}\right)}\right\}^{1/2}}{\sqrt{M_1M_2}\cdot K}$$

When K is small, $\sin\left(\frac{Ka}{2}\right) \simeq \frac{Ka}{2}$

$$v_p \simeq \begin{cases} \sqrt{\frac{2C(M_1+M_2)}{M_1M_2}}\,\frac{1}{\sqrt{K}} & : \text{upper sign (divergent as } K\to 0) \\ \sqrt{\frac{C}{2(M_1+M_2)}}\cdot a & : \text{lower sign.} \end{cases}$$

When $K = \frac{\pi}{a}$, $\sin^2\left(\frac{Ka}{2}\right) = 1$

$$v_p = \frac{\{C(M_1+M_2) \pm C(M_1-M_2)\}^{1/2}}{\sqrt{M_1M_2}\cdot K} \quad (\text{If } M_1 > M_2)$$

$$= \begin{cases} \sqrt{\frac{2C}{M_2}}\cdot\frac{2a}{\pi} & \text{upper sign} \\ \sqrt{\frac{2C}{M_1}}\cdot\frac{2a}{\pi} & \text{lower sign.} \end{cases}$$

The upper sign for v_p diverges as $K\to 0$ (optical mode). v_p is not a physical velocity.

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(4)

$$\frac{d}{dK}(\omega^2) = \pm\frac{c}{2M_1M_2}\frac{\left(-4M_1M_2\, a \sin(Ka/2)\cos(\frac{Ka}{2})\right)}{\sqrt{(M_1+M_2)^2-4M_1M_2\sin^2(\frac{Ka}{2})}}$$

$$= 2\omega\frac{d\omega}{dK}$$

$$\Rightarrow \omega\frac{d\omega}{dK} = \mp\frac{ca\sin(\frac{Ka}{2})\cos(\frac{Ka}{2})}{\sqrt{(M_1+M_2)^2-4M_1M_2\sin^2(\frac{Ka}{2})}}$$

$$= \mp\frac{ca\sin(Ka)}{2\sqrt{(M_1+M_2)^2-4M_1M_2\sin^2(\frac{Ka}{2})}}$$

$$\Rightarrow \frac{d\omega}{dK} = \mp\frac{a\sqrt{cM_1M_2}\,\sin(Ka)}{2\left\{(M_1+M_2)\pm\sqrt{(M_1+M_2)^2-4M_1M_2\sin^2(\frac{Ka}{2})}\right\}^{1/2}}$$

$$\times\frac{1}{\sqrt{(M_1+M_2)^2-4M_1M_2\sin^2(\frac{Ka}{2})}}$$

$$\therefore v_g = \mp\frac{a\sqrt{cM_1M_2}\,\sin(Ka)}{2\left\{(M_1+M_2)\pm\sqrt{(M_1+M_2)^2-4M_1M_2\sin^2(\frac{Ka}{2})}\right\}^{1/2}}\frac{1}{\sqrt{(M_1+M_2)^2-4M_1M_2\sin^2(\frac{Ka}{2})}}$$

as $K\to 0$ the upper sign gives $v_g \to 0$, which is the correct physical velocity of the optical mode.
The lower sign gives

$$v_g \simeq \frac{a\sqrt{cM_1M_2}\cdot Ka}{2\left[(M_1+M_2)-(M_1+M_2)\left\{1-\frac{4M_1M_2}{(M_1+M_2)^2}\cdot\frac{K^2a^2}{4}\right\}^{1/2}\right]^{1/2}}\cdot\frac{1}{\sqrt{(M_1+M_2)^2}}$$

$$\simeq \frac{a\sqrt{cM_1M_2}\;Ka}{2\sqrt{\frac{M_1M_2}{(M_1+M_2)}\cdot\frac{Ka}{2}}}\;\frac{1}{(M_1+M_2)} = \frac{1}{\sqrt{2}}\sqrt{\frac{c}{(M_1+M_2)}}\cdot a$$

(5)

at the Brillouin zone boundary $K = \pi/a$

$\Rightarrow \sin(Ka) = 0$

$$(m_1+m_2)^2 - 4m_1m_2\sin^2\left(\frac{Ka}{2}\right) = (m_1-m_2)^2$$

$$m_1+m_2 \pm \sqrt{(m_1+m_2)^2 - 4m_1m_2\sin^2\left(\frac{Ka}{2}\right)}$$

$$= m_1+m_2 \pm \sqrt{(m_1-m_2)^2} = \begin{cases} 2m_1, & \text{upper sign} \\ 2m_2, & \text{lower sign} \end{cases}$$

with $m_1 > m_2$.

$\Rightarrow v_g \to 0$ as $K \to \pi/a$, provided $m_1 \neq m_2$

The group velocity agrees with the phase velocity for the acoustic mode at small K, but not otherwise.

(6)

(21) With periodic boundary conditions an integral no. of wavelengths must fit into a length $L = \mathcal{N}a$ where $\mathcal{N}$ = no. of lattice sites.

$$\Rightarrow \quad \lambda = \frac{\mathcal{N}a}{p} \Rightarrow K = \frac{2\pi}{\lambda} = \frac{2\pi p}{\mathcal{N}a}, \quad p = 0, \pm1, \pm2, \ldots, \mathcal{N}.$$

The spacing in wavevector space between states is

$\Delta K = \frac{\pi}{\mathcal{N}a}$. The density of states is the number of modes between w and $w + \delta w$

$$\delta N = \frac{dN}{dw}\delta w = \frac{dN}{dK}\frac{dK}{dw}\delta w = D(w)\,\delta w$$

$$\frac{dN}{dK} = \frac{1}{\Delta K} = \frac{\mathcal{N}a}{2\pi}, \text{ for each direction of } K$$

$$\text{So} \quad D(w)\,\delta w = \frac{\mathcal{N}a}{2\pi}\frac{dK}{dw}\delta w$$

$$D(w) = \frac{\mathcal{N}a}{2\pi}\frac{dK}{dw} = \frac{2L}{2\pi}\,dK/dw$$

The extra factor of 2 is to allow for propagation in either direction.

$$\text{With } w = w_0 \sin\left(\frac{Ka}{2}\right), \quad \frac{dw}{dK} = w_0\frac{a}{2}\cos w/2$$

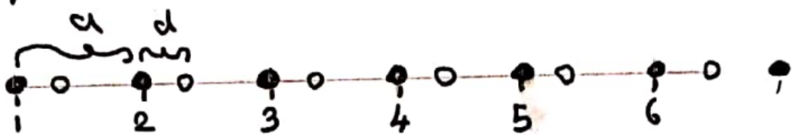
$$= w_0\frac{a}{2}\sqrt{1 - \sin^2 w/2}$$

$$\frac{dw}{dK} = \frac{a}{2}\sqrt{w_0^2 - w^2} \Rightarrow D(w) = \frac{\mathcal{N}a}{2\pi}\cdot\frac{2}{a\sqrt{w_0^2 - w^2}}$$

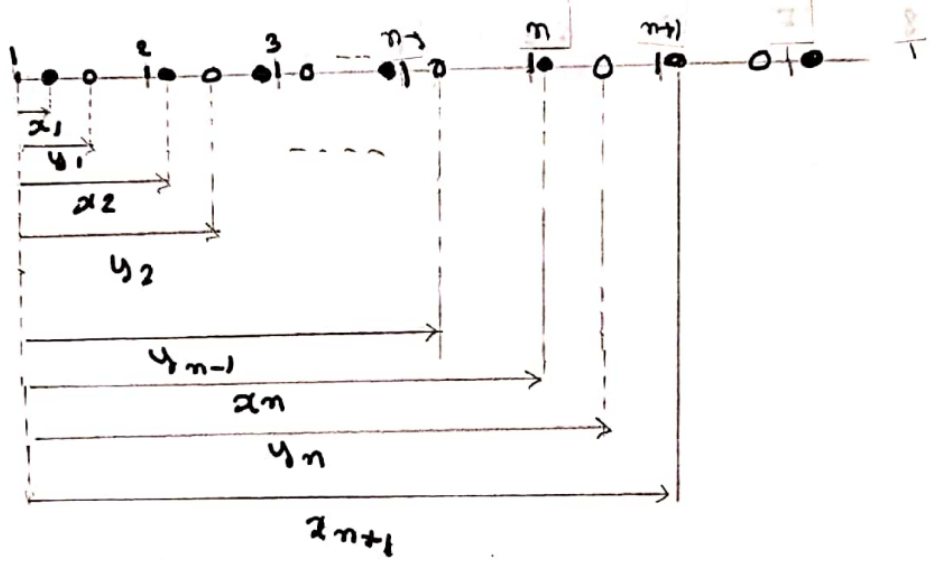
$$\Rightarrow D(w) = \frac{\mathcal{N}}{\pi}\frac{1}{\sqrt{w_0^2 - w^2}}$$

(7)

22) Equilibrium position is



when atoms are displaced from equilibrium



denote the distance of the black atom associated with lattice site n from lattice site 1 by x_n and the distance of the white atom associated with lattice site n from lattice site 1 by y_n

From Hookes law the force on the black atom associated with lattice site n is

$$F_n = C(y_n - x_n) - D(x_n - y_{n-1})$$

The force on the white atom associated with lattice site n is

$$F_n' = D(x_{n+1} - y_n) - C(y_n - x_n)$$

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(8)

Newton's 2ND law gives

$$m\ddot{x}_n = C(y_n - x_n) - D(x_n - y_{n-1})$$
$$m\ddot{y}_n = D(x_{n+1} - y_n) - C(y_n - x_n)$$

Look for a solution of the form

$$x_n = \varepsilon_1 e^{-i\omega t + iKan} = an + u_n$$
$$y_n = \varepsilon_2 e^{-i\omega t + iKan} = an + d + v_n$$

with ε_1 and ε_2 constant amplitudes

$$-\omega^2 m \varepsilon_1 e^{-i\omega t + iKan}$$
$$= C(\varepsilon_2 - \varepsilon_1) e^{-i\omega t + iKan} - D(\varepsilon_1 - \varepsilon_2 e^{-iKa}) e^{-i\omega t + iKan}$$

$$-\omega^2 m \varepsilon_2 e^{-i\omega t + iKan} = D(\varepsilon_1 e^{iKa} - \varepsilon_2) e^{-i\omega t + iKan}$$
$$- C(\varepsilon_2 - \varepsilon_1) e^{-i\omega t + iKan}$$

$$\Rightarrow -\omega^2 m \varepsilon_1 = (C + D e^{-iKa})\varepsilon_2 - (C+D)\varepsilon_1$$
$$-\omega^2 m \varepsilon_2 = (C + D e^{iKa})\varepsilon_1 - (C+D)\varepsilon_2$$

$$\Rightarrow \boxed{\begin{array}{l} (\omega^2 m - (C+D))\varepsilon_1 + (C + D e^{-iKa})\varepsilon_2 = 0 \\ (\omega^2 m - (C+D))\varepsilon_2 + (C + D e^{iKa})\varepsilon_1 = 0 \end{array}}$$

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(9)

As a matrix equation

$$\begin{pmatrix} m\omega^2-(C+D) & C+De^{-ika} \\ C+De^{ika} & m\omega^2-(C+D) \end{pmatrix}\begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \end{pmatrix} = 0 \quad \text{---} (1)$$

If ε_1 and ε_2 are not both zero then the matrix cannot have an inverse $\Rightarrow$ it must have determinant zero

$$\Rightarrow \det \begin{pmatrix} m\omega^2-C-D & C+De^{-ika} \\ C+De^{ika} & m\omega^2-C-D \end{pmatrix} = 0$$

$$\Rightarrow (m\omega^2-(C+D))^2 - (C+De^{-ika})(C+De^{ika}) = 0$$

$$\Rightarrow m^2\omega^4 - 2m\omega^2(C+D) + (C+D)^2 - (C^2+D^2+CDe^{ika}+CDe^{-ika}) = 0$$

$$\Rightarrow \omega^2 = \frac{2m(C+D) \pm \sqrt{4m^2(C+D)^2 - 4m^2[(C+D)^2-(C^2+D^2+2CD\cos ka)]}}{2m^2}$$

$$= \frac{(C+D)}{m} \pm \frac{\sqrt{4m^2(C^2+D^2+2CD\cos ka)}}{2m^2}$$

$$\Rightarrow \boxed{\omega^2 = \frac{C+D}{m} \pm \frac{\sqrt{C^2+D^2+2CD\cos ka}}{m}} \quad \text{---} (2)$$

(10)

Using this in (1) gives the ratio between ε_1 and ε_2

$$\left\{(C+D) - (C+D) \pm \sqrt{C^2+D^2+2CD\cos ka}\right\}\varepsilon_1 + \left(C+De^{-ika}\right)\varepsilon_2 = 0$$

$$\Rightarrow \quad \varepsilon_2 = \frac{\pm\sqrt{C^2+D^2+2CD\cos ka}}{\left(C+De^{-ika}\right)}\,\varepsilon_1$$

$$= \frac{\pm\sqrt{\left(C+De^{ika}\right)\left(C+De^{-ika}\right)}}{\left(C+De^{-ika}\right)}\,\varepsilon_1$$

$$= \pm\sqrt{\frac{C+De^{ika}}{C+De^{-ika}}}\;\varepsilon_1$$

$$= \pm\frac{C+De^{ika}}{\sqrt{\left(C+De^{-ika}\right)\left(C+De^{ika}\right)}}\,\varepsilon_1$$

$$= \pm\frac{C+De^{ika}}{\left|C+De^{ika}\right|}\,\varepsilon_1$$

(11)

From (2)

$$2\omega \frac{d\omega}{dk} = \pm \frac{1}{2m} \frac{(-4aCD\sin Ka)}{\sqrt{C^2+D^2+2CD\cos Ka}}$$

$$\frac{d\omega}{dk} = v_g = \mp \frac{aCD\sin(Ka)}{\omega m\sqrt{C^2+D^2+2CD\cos Ka}} \quad \cdots\cdots (3)$$

{ as a check: when $C = D$ this is the same as in Q 20 with $M_1 = M_2 = m$ }

Near the Brillouin zone boundary $K = \frac{\pi}{a} - \frac{\varepsilon}{a}$

with $\varepsilon << 1$, $\sin Ka = \sin(\pi - \varepsilon)$

$$= -\cos\pi \sin\varepsilon = \varepsilon + o(\varepsilon^3)$$

$$\cos Ka = \cos(\pi - \varepsilon) = \cos\pi\cos\varepsilon = -\cos\varepsilon$$

$$= -(1 - \varepsilon^2/2 + \ldots) \simeq -1$$

$$(2) \Rightarrow \omega^2 = \frac{C+D}{m} \pm \frac{\sqrt{C^2+D^2-2CD+o(\varepsilon^2)}}{m}$$

$$\simeq \frac{C+D}{m} \pm \frac{\sqrt{(C-D)^2}}{m} = \begin{cases} 2C/m \\ 2D/m, \end{cases}$$

assuming $C > D$ (other way round if $C < D$).

$(3) \Rightarrow$

$$v_g = \mp \frac{aCD \cdot \varepsilon}{\omega m\sqrt{(C-D)^2}} = \begin{cases} \sqrt{\frac{C}{2m}} \cdot \frac{aD\varepsilon}{(C-D)} \\ \sqrt{\frac{D}{2m}} \cdot \frac{aC\varepsilon}{(C-D)} \end{cases}$$

$v_g \to 0$ as $\varepsilon \to 0$ provided $C \neq D$.

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