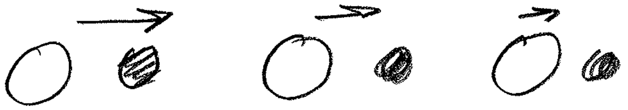
Simon 10.1

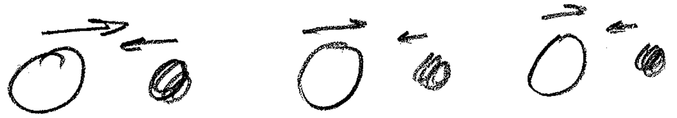
Problem Set #5

Ⓐ An acoustic mode has all the elements of the unit cell moving together, whereas an optical mode has relative motion (opposite direction) within the unit cell.

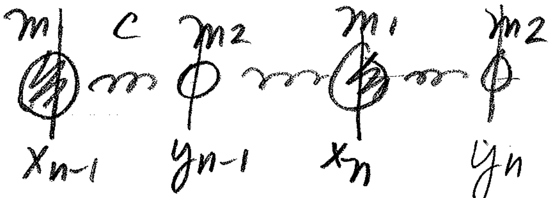
(1) acoustic



optical



Ⓑ



① $m_1 \ddot{x}_n = -c(y_n - x_n) + c(y_{n-1} - x_n)$

② $m_2 \ddot{y}_n = -c(x_{n+1} - y_n) + c(x_n - y_n)$

① ⇒ $m_1 \ddot{x}_n = c(y_n + y_{n-1}) - 2c x_n$

② ⇒ $m_2 \ddot{y}_n = c(x_{n+1} - x_n) - 2c y_n$

Try solution $x_n = A e^{i\omega t} e^{ikna}$ $y_n = B e^{i\omega t} e^{ikna}$

$$① \rightarrow m_1(-w^2) A \cancel{e^{iwt}} \cancel{e^{-ikna}}$$

$$= C B \cancel{e^{iwt}} \cancel{e^{-ikna}} \left[1 + e^{ika}\right] - 2CA \cancel{e^{iwt}} \cancel{e^{-ikna}}$$

$$m_1(-w^2) A = C B \left[1 + e^{ika}\right] - 2CA$$

$$② \rightarrow m_2(-w^2) B = C A \left[e^{-ika} + 1\right] - 2CB$$

$$\begin{bmatrix} m_1 w^2 - 2C & C\left[1+e^{ika}\right] \\ C\left[1+e^{-ika}\right] & m_2 w^2 - 2C \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = 0$$

$$(m_1 w^2 - 2C)(m_2 w^2 - 2C) = C^2 \left[1+e^{ika}\right]\left[1+e^{-ika}\right] = 0$$

$$(m_1 w^2 - 2C)(m_2 w^2 - 2C) - C^2\left[1 + \underset{\substack{\downarrow \\ C^2[2+2\cos ka]}}{e^{ika} + e^{-ika}} + 1\right] = 0$$

$$\left[m_1 m_2 w^4 - 2C m_2 w^2 - 2C m_1 w^2 + 4C^2\right] - \qquad = 0$$

$$w^2 = \frac{+\cancel{2}C[m_1+m_2] \pm \sqrt{\cancel{4}C^2(m_1+m_2)^2 - \cancel{4} m_1 m_2 \times 2C^2[1-\cos ka]}}{\cancel{2} m_1 m_2}$$

$$= C\frac{[m_1+m_2]}{m_1 m_2} \pm C\frac{\sqrt{m_1^2 + m_2^2 + 2\cos ka (m_1 m_2)}}{m_1 m_2}$$

ⓒ at $k=0$

$$w^2 = \frac{c[m_1+m_2]}{m_1 m_2} \pm \frac{c}{m_1 m_2}\sqrt{m_1^2+m_2^2+2m_1 m_2}$$

$$= \frac{c[m_1+m_2]}{m_1 m_2} \pm \frac{c}{m_1 m_2}(m_1+m_2)$$

$$w_+^2 = \frac{2c(m_1+m_2)}{m_1 m_2} = 2c\left[\frac{1}{m_1}+\frac{1}{m_2}\right]$$

$$w_-^2 = 0$$

at $k = \pi/a$

$$w^2 = \frac{c[m_1+m_2]}{m_1 m_2} \pm \frac{c}{m_1 m_2}\sqrt{m_1^2+m_2^2-2m_1 m_2}$$

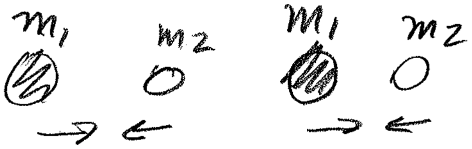
$$= \frac{c[m_1+m_2]}{m_1 m_2} \pm \frac{c}{m_1 m_2}[m_1-m_2]$$

$$w_+^2 = \frac{2m_1 c}{m_1 m_2} = \frac{2c}{m_2}$$

$$w_-^2 = \frac{2m_2 c}{m_1 m_2} = \frac{2c}{m_1}$$

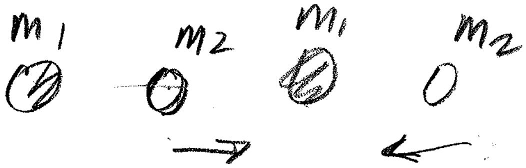
Motion

For ω_+ at $k=0$

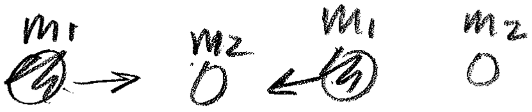


ω_- at $k=0$

For ω_+ at $k=\pi/a$



ω_- at $k=\pi/a$



Sound velocity → Group Velocity for ω_- at small k

$$\omega_-^2 = C\frac{[m_1+m_2]}{m_1 m_2} - \frac{C}{m_1 m_2}\sqrt{m_1^2+m_2^2+2\cos ka\,(m_1 m_2)}$$

for k small $\cos Ka = 1-\frac{(ka)^2}{2}$

$$\omega_-^2 \approx C\frac{[m_1+m_2]}{m_1 m_2} - \frac{C}{m_1 m_2}\sqrt{\underbrace{m_1^2+m_2^2+2m_1m_2}_{\downarrow\;(m_1+m_2)^2} - (ka)^2 \times m_1 m_2}$$

also $\sqrt{1-x^2} \approx 1-\frac{x^2}{2}$

so $\omega_-^2 \approx \frac{C[\cancel{m_1+m_2}]}{\cancel{m_1 m_2}} - \frac{C}{m_1 m_2}(m_1+m_2)\left[\cancel{1} - \frac{(ka)^2}{2}\frac{m_1 m_2}{(m_1+m_2)^2}\right]$

$$= \frac{C}{\cancel{m_1 m_2}}(\cancel{m_1+m_2})\frac{(ka)^2\,\cancel{m_1 m_2}}{2\,(m_1+m_2)^{\cancel{2}}}$$

$$\omega_- = \sqrt{\frac{c}{2(m_1+m_2)}}\;ka$$

$$\boxed{\frac{\partial\omega}{\partial k} = \sqrt{\frac{c}{2(m_1+m_2)}}\;a = V_{sound}}$$

at B.Z boundary

$$\omega^2 = c\frac{[m_1+m_2]}{m_1+m_2} \pm c\frac{\sqrt{m_1^2+m_2^2+2\cos ka(m_1 m_2)}}{m_1 m_2}$$

$$\frac{\partial\omega^2}{\partial k} = 2\omega\frac{\partial\omega}{\partial k} \quad \therefore \quad \frac{\partial\omega}{\partial k} = \frac{\partial\omega^2}{\partial k}\frac{1}{2\omega}$$

$$\frac{\partial\omega^2}{\partial k} = \frac{c}{m_1 m_2}\frac{a(\tfrac{1}{2})(2\sin ka(m_1 m_2))}{\sqrt{m_1^2+m_2^2+2\cos ka(m_1 m_2)}}(-1)$$

$$\therefore \left.\frac{\partial\omega}{\partial k}\right|_{k=\frac{\pi}{a}} = 0 \text{ as } \sin ka \to 0.$$

$$V_s = \sqrt{\frac{c}{2(m_1+m_2)}}\,a$$

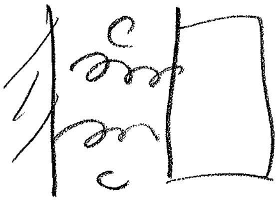
2 springs per unit cell

$$\beta = \text{compressibility} = \frac{2}{c\,a} \quad \text{(see equation 8.1)}$$

$$\rho = \text{density} = \frac{m_1+m_2}{a} \quad \text{in 1D}$$

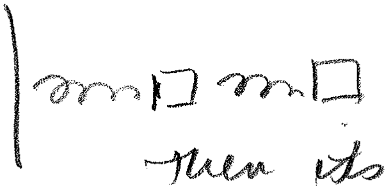
$$V_s = \sqrt{\frac{c\,a^2}{2(m_1+m_2)}} = \sqrt{\frac{1}{\beta\rho}}$$

If the two springs were in parallel



then 2c is the new spring constant

If they are in series



then its 1/2 as much

Ⓓ See attached for sketch

\# of modes $K_{max} = \frac{2\pi}{\lambda_{min}} = \frac{2\pi}{2a} = \frac{\pi}{a}$

each branch has $$\frac{\overset{(+\pi/a \text{ to } -\pi/a)}{2\,\pi/a}}{K_{min} = \frac{2\pi}{L}} = \frac{2\pi/a}{2\pi/Na} = N\text{mode}$$

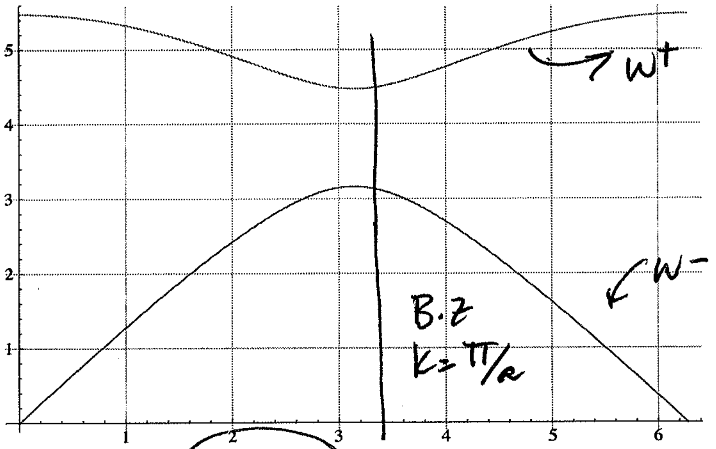
and there are 2 branches for $\underline{2N}$ modes!

there are 2 branches [1 optical + 1 acoustic]

Ⓔ see attached

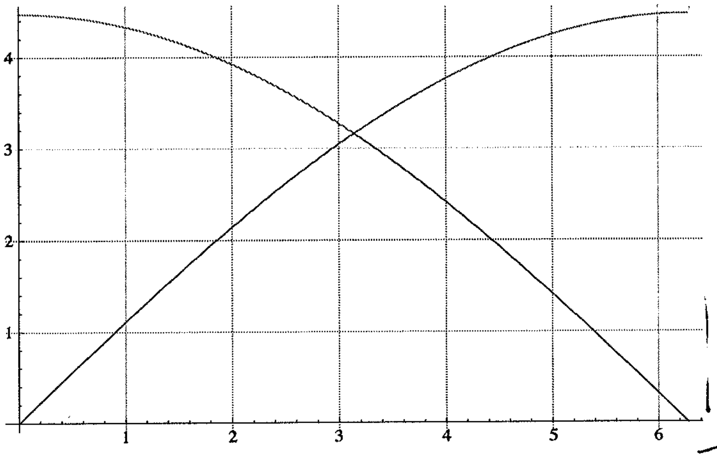
```
In[42]:= SprC = 10; m1 = 1; m2 = 2; a = 1;

In[43]:= Plot[{Sqrt[SprC (m1 + m2)/(m1 m2) - SprC/(m1 m2) Sqrt[m1^2 + m2^2 + 2 m1 m2 Cos[k a]]],
           Sqrt[SprC (m1 + m2)/(m1 m2) + SprC/(m1 m2) Sqrt[m1^2 + m2^2 + 2 m1 m2 Cos[k a]]]},
          {k, 0, 2 Pi}, GridLines → Automatic]
```

Out[43]=



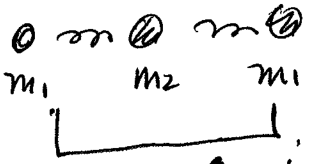
```
In[44]:= SprC = 10; m1 = 2; m2 = 2; a = 1;
         Plot[{Sqrt[SprC (m1 + m2)/(m1 m2) - SprC/(m1 m2) Sqrt[m1^2 + m2^2 + 2 m1 m2 Cos[k a]]],
           Sqrt[SprC (m1 + m2)/(m1 m2) + SprC/(m1 m2) Sqrt[m1^2 + m2^2 + 2 m1 m2 Cos[k a]]]},
          {k, 0, 2 Pi}, GridLines → Automatic]
```

Out[44]=



⟵ masses the same.

This is edge of B.Z because



a is really 2x what it should be so edge B.Z is at $\pi/a/2$ $= 2\pi/a$

Simon 11.1

Density of States $= g(E) = \frac{\#\text{ modes}}{dk}\,\frac{dk}{dE}$

$$E = \epsilon_0 - 2t\cos ka$$

$$\frac{\partial E}{\partial k} = 2ta\sin ka \qquad \frac{\#\text{ mode}}{dk} = \frac{\overset{\downarrow\text{spin}}{2}\ \overset{\downarrow\text{direction}}{2}}{2\pi/L} = \frac{2L}{\pi}$$

$$g(E) = \frac{2L}{\pi}(2ta\sin ka)^{-1} = \frac{2Na}{\pi}\,\frac{1}{\cancel{2}t\cancel{a}\sin ka}$$

but $2t\cos ka = \epsilon_0 - E \rightarrow 4t^2\cos^2 ka = (\epsilon_0 - E)^2$

$$= 4t^2(1-\sin^2 ka)$$

$$4t^2\sin^2 ka = 4t^2 - (\epsilon_0 - E)^2$$

$$2t\sin ka = \sqrt{4t^2 - (\epsilon_0 - E)^2}$$

$$\boxed{g(E) = \frac{2N}{\pi}\,a\,\sqrt{4t^2 - (\epsilon_0 - E)^2}^{\;-1}}$$

If monovalent

$K_{min} = \frac{2\pi}{L}$ where $L = Na$

Put in 2 electrons ↑↓ into each of $\pm n\frac{2\pi}{Na}$

so that $n = N/4$ $\qquad K_F = \frac{\cancel{N}}{4}\,\frac{2\pi}{\cancel{N}a} = \frac{\pi}{2a}$

$$g(E) = \frac{N}{\pi t}(\sin ka)^{-1}\Big|_{K_F = \frac{\pi}{2a}} \Rightarrow \boxed{g(E_F) = \frac{N}{\pi t}}$$

Simon 11.1

continued.

See 4.2

in 1D this is L

$$C = \gamma K_B \, g(E_F) \, K_B T \quad \checkmark$$

$$g(E_F) = \frac{N}{\pi t}$$

$$C = \gamma K_B \frac{N}{\pi t} K_B T L$$

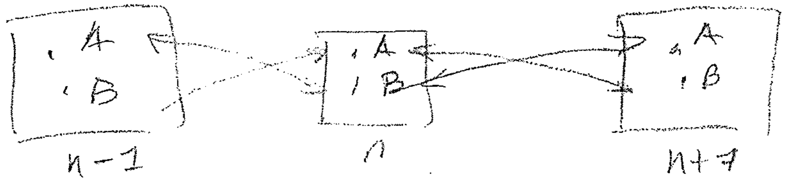
$$\boxed{\frac{C}{L} = \gamma K_B^2 \frac{N}{\pi t} T}$$

units correct

equivalent of per unit volume in 1D

If the atoms are divalent then the band is completely full and there is a gap to excitations so you can't change E very easily with temperature $\frac{\partial E}{\partial T} = 0 = C$.

Session 11.2



We have $H_{atomic}(\sigma, n)\,\psi_{\sigma,n}(x) = \epsilon_A\, \psi_{A,n}(x)$

$= \epsilon_B\, \psi_{B,n}(x)$

σ is = to either A, or B

And nearest neighbor interactions such that

$\langle n | V | n+1 \rangle = -t$ [with $A \to B / B \to A$]

$\langle n-1 | V | n \rangle = -t$ " " "

and zero otherwise

let $\psi_k(x) = \sum_n e^{-ikna} \sum_\sigma \underset{\downarrow}{c_\sigma}\, \psi_{\sigma n}(x)$

Complex coefficients

$$H = \sum_{\sigma,n} H_{atomic}(\sigma, n) + \sum_n \left(V_{n,n-1} + V_{n,n+1}\right)$$

$$\langle \psi_{A,n} | H | \psi_k(x) \rangle = E_k \langle \psi_{AN} | \psi_k \rangle = E_k C_A e^{-ikna}$$

$$= \langle \psi_{A,n} | H_{atomic} | e^{-ikna} C_A | \psi_{A,n} \rangle$$

$$+ \langle \psi_{A,n} | V_{n,n-1} | e^{-ik(n-1)a} C_B | \psi_{B,n-1} \rangle$$

$$+ \langle \psi_{A,n} | V_{n,n+1} | e^{-i(n+1)a} C_B | \psi_{B,n+1} \rangle$$

$$= \epsilon_A C_A e^{-ikna} - t C_B e^{-i(n-1)ka} - t C_B e^{-ik(n+1)} a$$

$$E_k C_A \cancel{e^{-ikna}} = \epsilon_A C_A \cancel{e^{-ikna}} - t C_B \cancel{e^{-ikna}} \left[e^{ika} + e^{-ik}\right.$$

$$E_k C_A = \epsilon_A C_A - t c_B \left[e^{ika} + e^{-ika} \right]$$

$$\boxed{E_k C_A = \epsilon_A C_A - t C_B \, 2\cos ka}$$

Likewise

$$\langle \psi_{B,n} | H | \psi_k(x) \rangle = E_k \langle \psi_{B,n} | \psi_k \rangle = E_k C_B e^{-ikna}$$

$$= \langle \psi_{B,n} | H_{atomic} | e^{ikna} C_B | \psi_{B,n} \rangle$$

$$+ \langle \psi_{B,n} | V_{n,n-1} | e^{ik(n-1)a} C_A | \psi_{A,n-1} \rangle$$

$$+ \langle \psi_{B,n} | V_{n,n+1} | e^{-ik(n+1)a} C_A | \psi_{A,n+1} \rangle$$

$$E_k C_B e^{-ikna} = \epsilon_B C_B e^{-ikna} - t C_A e^{-ik(n-1)a} - t C_A e^{-i(n+1)}$$

$$\boxed{\begin{aligned} E_K C_B &= \epsilon_B C_B \underbrace{- t C_A [e^{ika} - e^{-ika}]} \\ &= \epsilon_B C_B - 2t C_A \cos ka \end{aligned}}$$

$$0 = (\varepsilon_A - E_K) C_A - t C_B 2\cos ka$$

$$0 = (\epsilon_B - E_K) C_B - t C_A 2\cos ka$$

$$\begin{bmatrix} (\varepsilon_A - E_K) & -t 2\cos ka \\ -t 2\cos ka & (\varepsilon_B - E_K) \end{bmatrix} \begin{bmatrix} C_A \\ C_B \end{bmatrix} = 0$$

$$(\varepsilon_A - E_K)(\varepsilon_B - E_K) - t^2 4\cos^2 ka = 0$$

$$\epsilon_A \epsilon_B - E_K(\varepsilon_B + \varepsilon_A) + E_K^2 - t^2 4\cos^2 ka = 0$$

$$E_K^2 - E_K(\varepsilon_A + \varepsilon_B) + \varepsilon_A\varepsilon_B - t^2 4\cos^2 ka = 0$$

Oops. There is a sign error here the t term in the sqrt should be positive. I will fix and post in future.

$$E_K = +\frac{(\varepsilon_A + \varepsilon_B)}{2} \pm \frac{\sqrt{(\varepsilon_A + \varepsilon_B)^2 - 4(\varepsilon_A \varepsilon_B - t^2 4\cos^2 ka)}}{2}$$

$$E = \frac{\varepsilon_A + \varepsilon_B}{2} \pm \sqrt{\frac{(\varepsilon_A - \varepsilon_B)^2}{4} - t^2 4\cos^2 ka}$$

at $k=0$

$$E_K = \frac{\varepsilon_A + \varepsilon_B}{2} \pm \sqrt{\frac{(\varepsilon_A - \varepsilon_B)^2}{4} - 4t^2}$$

at $k=\pi/a$

$$E_K = \frac{\varepsilon_A + \varepsilon_B}{2} \pm \sqrt{\frac{(\varepsilon_A - \varepsilon_B)^2}{4} + 4t^2}$$

lets do this for $4t^2 << \frac{(\varepsilon_A - \varepsilon_B)^2}{4}$

then $\sqrt{1 \pm x} = 1 \pm \frac{x}{2}$

So at $k=0$

$$E_k = \frac{\varepsilon_A + \varepsilon_B}{2} \pm \left[\frac{(\varepsilon_A - \varepsilon_B)}{2} - \frac{4t^2}{\left(\frac{\varepsilon_A - \varepsilon_B}{2}\right)} \frac{1}{2} \right]$$

$$= \varepsilon_A - \frac{4t^2}{\varepsilon_A - \varepsilon_B}$$

$$= \varepsilon_B + \frac{4t^2}{\varepsilon_A - \varepsilon_B}$$

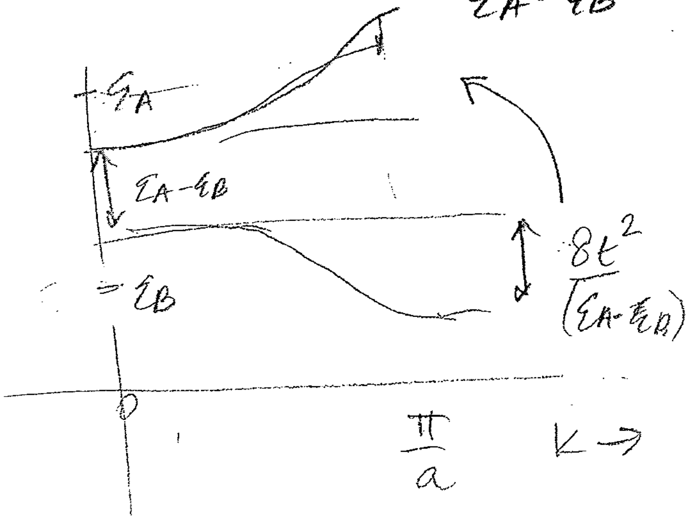
and @ $k = \frac{\pi}{a}$

$$E_k = \frac{\varepsilon_A + \varepsilon_B}{2} \pm \left[\frac{(\varepsilon_A - \varepsilon_B)}{2} + \frac{4t^2}{(\varepsilon_A - \varepsilon_B/2)} \frac{1}{2} \right]$$

$$= \varepsilon_A + \frac{4t^2}{\varepsilon_A - \varepsilon_B}$$

$$= \varepsilon_B - \frac{4t^2}{\varepsilon_A - \varepsilon_B}$$

let $\varepsilon_A > \varepsilon_B$



$E = \frac{\hbar^2 k^2}{2m^*}$ so $m^* = \left(\frac{\partial^2 E}{\partial k^2}\right)^{-1} \hbar^2$

$\frac{\partial E}{\partial k} = \frac{\hbar^2 k}{m^*} \rightarrow \frac{\partial^2 E}{\partial k^2} = \frac{\hbar^2}{m^*}$

$$E_k = \frac{(\varepsilon_A + \varepsilon_B)}{2} \pm \sqrt{\frac{(\varepsilon_A - \varepsilon_B)^2}{4} - t^2 4\cos^2 ka}$$

near bottom of band $\cos ka \approx 1 - \frac{(ka)^2}{2}$

$$\therefore \cos^2 ka \cong \left(1 - \frac{(ka)^2}{2}\right)^2 = 1 - (ka)^2 + \frac{ka^4}{4}$$

$$\approx 1 - (ka)^2$$

$$E_k = \frac{(\varepsilon_A + \varepsilon_B)}{2} \pm \sqrt{\frac{(\varepsilon_A - \varepsilon_B)^2}{4} - t^2 4\left[1 - (ka)^2\right]}$$

$$= \frac{\varepsilon_A + \varepsilon_B}{2} \pm \sqrt{\frac{(\varepsilon_A - \varepsilon_B)^2}{4} - 4t^2 + 4t^2 (ka)^2}$$

for k small (at bottom of band)

$$\sqrt{1 + x} \approx 1 + \frac{x}{2}$$

$$E_k = \frac{\varepsilon_A + \varepsilon_B}{2} \pm \sqrt{\frac{(\varepsilon_A - \varepsilon_B)^2}{4} - 4t^2}\left[1 + \frac{2t^2 k^2 a^2}{\frac{(\varepsilon_A - \varepsilon_B)^2}{4} - 4t^2}\right]$$

$$\frac{\partial^2 E_k}{\partial k^2} = 4t^2 a^2 \Big/ \left[\frac{(\varepsilon_A - \varepsilon_B)^2}{4} - 4t^2\right]^{1/2}$$

$$\boxed{m^* = \frac{\hbar^2 \sqrt{\frac{(\varepsilon_A-\varepsilon_B)^2}{4} - 4t^2}}{4\, t^2 a^2}}$$

If monovalent then each site has 2 electron for a total of 2N in sample where $N = \frac{L}{a}$

$$K_{min} = \frac{2\pi}{L}$$

Each band has $\frac{\overset{\swarrow \text{spin}}{(2)}\left(\frac{\pi}{a}\right)\overset{\swarrow \text{direction } \pm k)}{(2)}}{2\pi/L}$ allowed states

$$= \frac{4\pi}{a}\,\frac{L}{2\pi} = \frac{2L}{a} = 2N$$

So the lower band is completely filled and the upper band is completely empty. So this is an insulator w/ a gap!

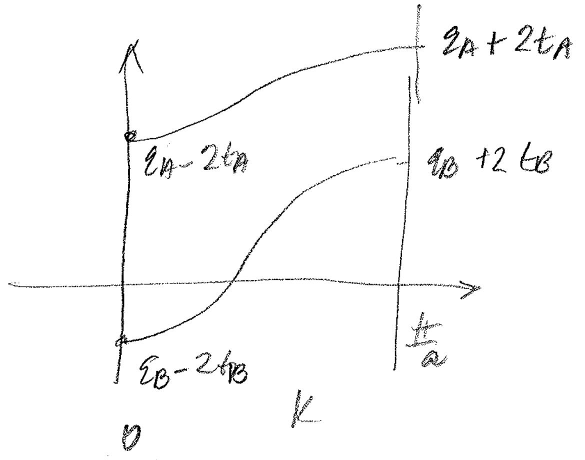
LiF is an insulator because t is small (bonds are strong and $\varepsilon_A > \varepsilon_B$ where ε_A – F ε_B – Li so the gap is large.

Simon 11.4

For 2 orbitals with t_{AA} and t_{BB} only

(a) This is identical to just Simon 11.1 done 2x (separately) such that there are 2 dispersion curves. (A and B)

$$E_1 = \varepsilon_A - 2t_A \cos ka$$
$$E_2 = \varepsilon_B - 2t_B \cos ka$$



(B) now allow $t_{AB} \neq 0$

$$\sum_{m'} H_{mn}\phi_m = \varepsilon_A \frac{e^{-ikna}}{\sqrt{N}} - t_{AA}\left[\frac{e^{-ik(n+1)a}}{\sqrt{N}} + \frac{e^{-ik(n-1)a}}{\sqrt{N}}\right] - t_{AB}\left[\frac{e^{-ik(n+1)a}}{\sqrt{N}} + \frac{e^{-ik(n-1)a}}{\sqrt{N}}\right]$$

Ignore this

$$E_1 \frac{e^{-ikna}}{\sqrt{N}} = \quad ''$$

$$\therefore\ E_1 = \varepsilon_A - t_{AA}\, 2\cos ka - t_{AB}\, 2\cos ka$$

whereas $E_2 = \varepsilon_B - t_{BB}\, 2\cos ka - t_{AB}\, 2\cos ka$