Condensed matter physics (phy 771)

HW #6 - solution

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① $U(\vec{r}) = \sum_{\vec{K}} U_{\vec{K}} e^{i\vec{K}\cdot\vec{r}}$; $\langle r|k\rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$, $\langle k|r\rangle = \frac{1}{\sqrt{V}} e^{-i\vec{k}\cdot\vec{r}}$

$\langle k'|U|k\rangle = \int d^3\vec{r} \langle k'|U|k\rangle$, introduce $|r\rangle\langle r| = 1$

$= \int d^3\vec{r} \langle k'|r\rangle U(r) \langle r|k\rangle$

$= \frac{1}{V}\int d^3\vec{r}\, e^{-i\vec{k}'\cdot\vec{r}} \sum_{K} U_K e^{i\vec{K}\cdot\vec{r}} e^{i\vec{k}\cdot\vec{r}}$

$= \frac{1}{V}\sum_{\vec{K}} U_K \underbrace{\int d^3\vec{r}\, e^{i(\vec{k}+\vec{K}-\vec{k}')\cdot\vec{r}}}_{V\,\delta_{k', k+K}}$

$= \frac{V}{V}\sum_{K} U_K\, \delta_{k', k+K} = U_{k'-k}$

now $\langle k+K|U|k\rangle$, substitute in here and take $k' = k+K$

$\langle k+K|U|k\rangle = U_{k+K-k} = U_K$

similarly $\langle k|U|k+K\rangle = U_{k-k-K} = U_{-K}$ → when I set $k' = k$, and $k = k+K$

knowing that

$\langle k|U|k+K\rangle = \langle k+K|U|k\rangle^* = U_K^* = U_{-K}$

$\therefore U_{-K} = U_K^*$

(2)

$$U(x) = 2V_0 \cos^2\left(\frac{\pi}{a}x\right) \quad ; \quad \text{using } \cos^2 x = \frac{1+\cos 2x}{2}$$

$$= V_0\left(1 + \cos\frac{2\pi}{a}x\right)$$

$$\varepsilon_k^{(1)} = \langle k|U(x)|k\rangle \quad ; \quad \text{let } |k\rangle = \frac{1}{\sqrt{a}} e^{ikx}$$

$$= \frac{1}{a}\int_0^a e^{-ikx} V_0\left(1+\cos\frac{2\pi}{a}x\right) e^{ikx}\,dx$$

$$= \frac{V_0}{a}\left[\int_0^a dx + \underbrace{\int_0^a dx \cos\frac{2\pi}{a}x}_{\text{zero integration over its period } \frac{2\pi}{2\pi/a}=a}\right] = \frac{V_0}{a}\,a = V_0$$

$$\varepsilon_k^{(2)} = \sum_{k'\neq k} \frac{|\langle k'|U|k\rangle|^2}{\varepsilon_k^{(0)} - \varepsilon_{k'}^{(0)}} \quad ; \quad \text{using } |k'\rangle = \frac{1}{\sqrt{a}} e^{ik'x}, \text{ we have}$$

$$\langle k'|U|k\rangle = \langle k'|V_0 + V_0\cos\frac{2\pi}{a}x|k\rangle$$

$$= \langle k'|V_0|k\rangle + V_0\langle k'|\cos\frac{2\pi}{a}x|k\rangle$$

$$= V_0\underbrace{\langle k'|k\rangle}_{\text{zero orthogonal}} + V_0\int_0^a \frac{1}{\sqrt{a}} e^{-ik'x}\cos\frac{2\pi}{a}x\,\frac{1}{\sqrt{a}}e^{ikx}\,dx$$

$$= \frac{V_0}{a}\int_0^a e^{-ik'x}\left[\frac{e^{i\frac{2\pi}{a}x} + e^{-i\frac{2\pi}{a}x}}{2}\right]e^{ikx}\,dx$$

$$= \frac{V_0}{2a}\int_0^a e^{-ik'x}\left[e^{i(k+\frac{2\pi}{a})x} + e^{i(k-\frac{2\pi}{a})x}\right]$$

$$= \frac{V_0}{2a}\left[\int_0^a e^{-i(k'-(k+\frac{2\pi}{a}))x}\,dx + \int_0^a e^{-i(k'-(k-\frac{2\pi}{a}))x}\,dx\right]$$

$$\langle k'|U|k\rangle = \frac{V_0}{2a}\left[a\delta_{k',k+\frac{2\pi}{a}} + a\,\delta_{k',k-\frac{2\pi}{a}}\right]$$ two contributions

only from $k' = k+\frac{2\pi}{a}$ and $k' = k-\frac{2\pi}{a}$

$$\Rightarrow \langle k'|U|k\rangle = \frac{V_0}{2}\left[\delta_{k',k+\frac{2\pi}{a}} + \delta_{k',k-\frac{2\pi}{a}}\right]$$

$$\Rightarrow \varepsilon_k^{(2)} = \sum_{k'\neq k} \frac{|\langle k'|U|k\rangle|^2}{\varepsilon_k^{(0)} - \varepsilon_{k'}^{(0)}} = \frac{|V_0|^2/4}{\varepsilon_k^{(0)} - \varepsilon_{k+\frac{2\pi}{a}}} + \frac{|V_0|^2/4}{\varepsilon_k^{(0)} - \varepsilon_{k-\frac{2\pi}{a}}}$$

now $\varepsilon_k^{(0)} - \varepsilon_{k+\frac{2\pi}{a}}^{(0)} = \frac{\hbar^2}{2m}k^2 - \frac{\hbar^2}{2m}\left(k+\frac{2\pi}{a}\right) = \frac{\hbar^2}{2m}\left(-\frac{4\pi^2}{a^2} - \frac{4\pi k}{a}\right)$

and $\varepsilon_k^{(0)} - \varepsilon_{k-\frac{2\pi}{a}}^{(0)} = \frac{\hbar^2 k^2}{2m} - \frac{\hbar^2}{2m}\left(k-\frac{2\pi}{a}\right) = \frac{\hbar^2}{2m}\left(\frac{-4\pi^2}{a^2} + \frac{4\pi k}{a}\right)$

$$\Rightarrow \varepsilon_k^{(2)} = \frac{V_0^2}{4}\frac{2m}{\hbar^2}\left[\frac{1}{-\frac{4\pi^2}{a^2} - \frac{4\pi k}{a}} + \frac{1}{-\frac{4\pi^2}{a^2} + \frac{4\pi k}{a}}\right]$$

$$= -\frac{V_0^2 m}{4\hbar^2}\left[\frac{1}{\frac{2\pi^2}{a^2} + \frac{2\pi k}{a}} + \frac{1}{\frac{2\pi^2}{a^2} - \frac{2\pi k}{a}}\right]$$

$$= \frac{-mV_0^2}{4\hbar^2}\left[\frac{4\pi^2/a^2}{4\pi^2/a^2\left(\frac{\pi}{a}+k\right)\left(\pi/a - k\right)}\right]$$

$$= \frac{-mV_0^2}{4\hbar^2}\,\frac{1}{\left(\frac{\pi}{a}\right)^2 - k^2}$$; which diverges at $k = \pm\frac{\pi}{a}$

so this does not work. To find the $\varepsilon_k^{(2)}$, we use the degenerate perturbation theory as follows → at $k = \pm\pi/a$

let $H = \begin{pmatrix} \langle k|H|k\rangle & \langle k|H|k-\pi\rangle \\ \langle k-\pi|H|k\rangle & \langle k-\pi|H|k-\pi\rangle \end{pmatrix}$;

now $\langle k|H|k\rangle = \langle k|H_0+U|k\rangle = \langle k|\underbrace{H_0|k\rangle}_{\varepsilon_k^{(0)}} + \langle k|U|k\rangle$

$= \varepsilon_k^{(0)}\underbrace{\langle k|k\rangle}_{1} + \underbrace{\langle k|U|k\rangle}_{V_0} = \varepsilon_k^{(0)} + V_0$

similarly

$\langle k-\pi|H|k-\pi\rangle = \langle k-\pi|H_0+U|k-\pi\rangle$

$= \langle k-\pi|\underbrace{H_0|k-\pi\rangle}_{\varepsilon_{k-\pi}^{(0)}} + \langle k-\pi|U|k-\pi\rangle$

$= \varepsilon_{k-\pi}^{(0)}\underbrace{\langle k-\pi|k-\pi\rangle}_{1} + \underbrace{\langle k-\pi|U|k-\pi\rangle}_{V_0}$

$= \varepsilon_{k-\pi}^{(0)} + V_0$; but at $k = \pi/2$, we have $\varepsilon_k^{(0)} = \varepsilon_{k-\pi}^{(0)}$

$= \varepsilon_k^{(0)} + V_0$,

now

$\langle k-\pi|H|k\rangle = \langle k-\pi|H_0+U|k\rangle = \langle k-\pi|\underbrace{H_0|k\rangle}_{\varepsilon_k^{(0)}|k\rangle} + \langle k-\pi|U|k\rangle$

$= \varepsilon_k^{(0)}\underbrace{\langle k-\pi|k\rangle}_{\text{zero}} + \underbrace{\langle k-\pi|U|k\rangle}_{U_\pi}$

$= U_\pi$, where $\pi = -\frac{2\pi}{a}$; $\frac{2\pi}{a}x$

$U_\pi = \frac{1}{a}\int_0^a dx\, U(x)\, e^{-i\pi x} = \frac{1}{a}\int_0^a dx\, V_0\left(1+\cos\frac{2\pi}{a}x\right) e$

$$U_\pi = \frac{V_0}{a}\left[\underbrace{\int_0^a dx\, e^{i\frac{2\pi}{a}x}}_{\text{Zero integrate over the Period}} + \int_0^a dx \left[\frac{e^{i\frac{2\pi}{a}x} + e^{-i\frac{2\pi}{a}x}}{2}\right] e^{i\frac{2\pi}{a}x}\right]$$

$$= \frac{V_0}{2a}\int_0^a dx \left[e^{i\frac{4\pi}{a}x} + 1\right] = \frac{V_0}{2a}\left[\int_0^a dx + \int_0^a dx\, e^{i\frac{4\pi}{a}x}\right]$$

$$= \frac{V_0}{2a}\left[a + \frac{a}{i4\pi} e^{i\frac{4\pi}{a}x}\Big|_0^a\right] = \frac{V_0}{2a}\left[a + \frac{a}{i4\pi}\underbrace{(e^{i4\pi} - 1)}_{=1}\right] = \frac{V_0}{2}$$

similarly $\langle k|H|k-\pi\rangle = \langle k-\pi|H|k\rangle^* = \frac{V_0^*}{2} = \frac{V_0}{2}$ as V_0 is real

$$\Rightarrow H = \begin{pmatrix} \varepsilon_k^{(0)} + V_0 & V_0/2 \\ V_0/2 & \varepsilon_k^{(0)} + V_0 \end{pmatrix} \Rightarrow H\psi = \varepsilon\psi$$

$$\Rightarrow \begin{pmatrix} \varepsilon_k^{(0)} + V_0 & V_0/2 \\ V_0/2 & \varepsilon_k^{(0)} + V_0 \end{pmatrix} \begin{pmatrix} |k\rangle \\ |k-\pi\rangle \end{pmatrix} = \varepsilon \begin{pmatrix} |k\rangle \\ |k-\pi\rangle \end{pmatrix}$$

$$\Rightarrow \begin{vmatrix} \varepsilon_k^{(0)} + V_0 - \varepsilon & V_0/2 \\ V_0/2 & \varepsilon_k^{(0)} + V_0 - \varepsilon \end{vmatrix} = 0 \Rightarrow \left(\varepsilon_k^{(0)} + V_0 - \varepsilon\right)^2 = \frac{V_0^2}{4}$$

$$\Rightarrow \varepsilon_k^{(0)} + V_0 - \varepsilon = \pm\frac{V_0}{2} \Rightarrow \varepsilon = \underbrace{\varepsilon_k^{(0)}}_{\text{Zeroth}} + \underbrace{V_0}_{1^{st}} \pm \underbrace{\frac{V_0}{2}}_{2nd}$$

$$\Rightarrow \varepsilon_k^+ = \varepsilon_k^{(0)} + V_0 + \frac{V_0}{2}$$

$$\varepsilon_k^- = \varepsilon_k^{(0)} + V_0 - \frac{V_0}{2}$$

$$\Rightarrow \Delta\varepsilon = \varepsilon_k^+ - \varepsilon_k^- = V_0 \equiv \text{band gap at } k = \pm\pi/a$$

(3)

$$U(x,y) = -4U_0 \cos\left(\frac{2\pi}{a}x\right)\cos\left(\frac{2\pi}{a}y\right),$$

using $\cos A \cos B = \frac{1}{2}\left[\cos(A+B) + \cos(A-B)\right]$; where $A = \frac{2\pi}{a}x$, $B = \frac{2\pi}{a}y$

$$\Rightarrow U(x,y) = -2U_0\left[\cos\frac{2\pi}{a}(x+y) + \cos\frac{2\pi}{a}(x-y)\right]$$

$$= -2U_0\left[\frac{e^{i\frac{2\pi}{a}(x+y)} + e^{-i\frac{2\pi}{a}(x+y)}}{2} + \frac{e^{i\frac{2\pi}{a}(x-y)} + e^{-i\frac{2\pi}{a}(x-y)}}{2}\right]$$

$$= -U_0\left[e^{i\frac{2\pi}{a}(x+y)} + e^{-i\frac{2\pi}{a}(x+y)} + e^{i\frac{2\pi}{a}(x-y)} + e^{-i\frac{2\pi}{a}(x-y)}\right] \quad \text{---- (1)}$$

let us compare this result with

$$U(x,y) = \sum_{K} U_K e^{i\vec{K}\cdot\vec{r}} \quad ; \ \vec{K} \text{ is reciprocal lattice vectors}$$

$$= \sum_{K} U_K e^{iK_x x + iK_y y}, \text{ we see that the}$$

Fourier components U_K are the coefficients of the Plane waves $e^{iK_x x + iK_y y}$. From (1), we see that $U_K = -U_0$ and this corresponds to the following reciprocal lattice vectors

$$e^{i\frac{2\pi}{a}(x+y)} \longrightarrow \vec{K_1} = (K_x, K_y) = \left(\frac{2\pi}{a}, \frac{2\pi}{a}\right)$$

$$e^{-i\frac{2\pi}{a}(x+y)} \longrightarrow \vec{K_2} = (K_x, K_y) = \left(-\frac{2\pi}{a}, -\frac{2\pi}{a}\right)$$

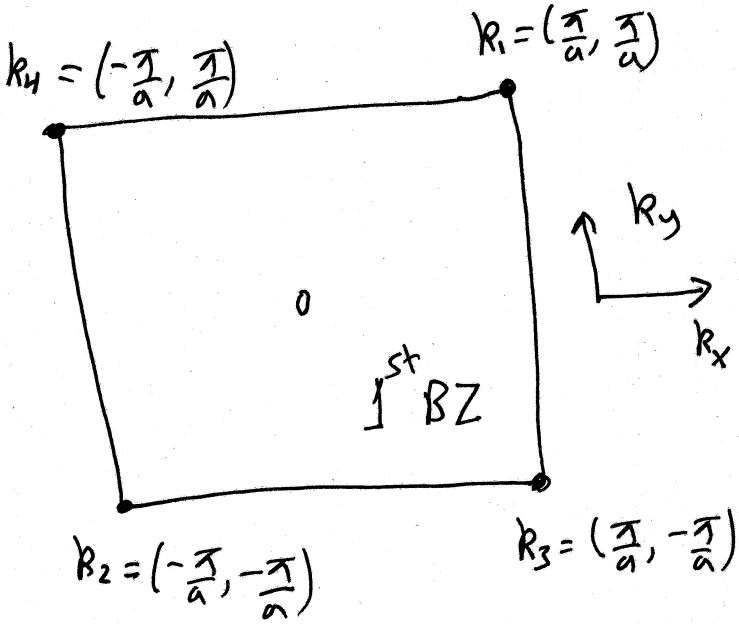
$e^{i\frac{2\pi}{a}(x-y)} \longrightarrow \vec{K_3} = (K_x, K_y) = \left(\frac{2\pi}{a}, -\frac{2\pi}{a}\right)$, and finally

$e^{-i\frac{2\pi}{a}(x-y)} \longrightarrow \vec{K_4} = (K_x, K_y) = \left(-\frac{2\pi}{a}, \frac{2\pi}{a}\right)$.

$\Rightarrow$ the Fourier components U_K are non-zero only at the reciprocal lattice vectors $\vec{K} = \left(\pm\frac{2\pi}{a}, \pm\frac{2\pi}{a}\right)$, and for each $\vec{K}$, the Fourier comp is $U_K = -U_0$.

No to find the energy gap at $K_1 = \left(\frac{\pi}{a}, \frac{\pi}{a}\right)$, we need to couple it to another points that have same energy. Now using

$$\varepsilon = \frac{\hbar^2 K^2}{2m} = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2\right),$$



we see that all points $K_1 \to K_4$, have same energy, i.e

$$\varepsilon_{K_1} = \varepsilon_{K_2} = \varepsilon_{K_3} = \varepsilon_{K_4} = \frac{\hbar^2}{2m}\left(\frac{\pi^2}{a^2} + \frac{\pi^2}{a^2}\right) = \frac{\hbar^2}{2m}\left(\frac{2\pi^2}{a^2}\right) = \frac{\hbar^2\pi^2}{ma^2}.$$

Now there is another condition, which says that when any two k points are coupled, the difference between the two points must be a reciprocal lattice vector $\left(\pm\frac{2\pi}{a}, \pm\frac{2\pi}{a}\right)$,

let us check that

couple k_1 with $k_2 \Rightarrow \vec{k}_2 - \vec{k}_1 = (-\frac{\pi}{a}, -\frac{\pi}{a}) - (\frac{\pi}{a}, \frac{\pi}{a}) = (-\frac{2\pi}{a}, -\frac{2\pi}{a})$ ✓

" k_1 with $k_3 \Rightarrow \vec{k}_3 - \vec{k}_1 = (\frac{\pi}{a}, -\frac{\pi}{a}) - (\frac{\pi}{a}, \frac{\pi}{a}) = (0, -\frac{2\pi}{a})$ ✗

" k_1 with $k_4 \Rightarrow \vec{k}_4 - \vec{k}_1 = (-\frac{\pi}{a}, \frac{\pi}{a}) - (\frac{\pi}{a}, \frac{\pi}{a}) = (-\frac{2\pi}{a}, 0)$ ✗

see that coupling k_1 to (k_3 and k_4) results in reciprocal lattice vectors $(0, -\frac{2\pi}{a})$, $(-\frac{2\pi}{a}, 0)$ that have zero Fourier components, so the only choice is to mix $\vec{k}_1$ with $\vec{k}_2$, i.e we need to mix $\vec{\kappa}_1 = (\frac{2\pi}{a}, \frac{2\pi}{a})$ with $\vec{\kappa}_2 = (-\frac{2\pi}{a}, -\frac{2\pi}{a})$

- now schrodinger eq^n in reciprocal space reads

$$\left[\frac{\hbar^2}{2m}(k-\kappa)^2 - \varepsilon\right]\psi(k-\kappa) + \sum_{\kappa'} U_{\kappa'-\kappa}\,\psi(k-\kappa') = 0 \quad \text{---- (2)}$$

at κ_1, it becomes

$$\left[\underbrace{\frac{\hbar^2}{2m}(k-\kappa)^2}_{\downarrow \varepsilon_{k_1}} - \varepsilon\right]\psi(k-\kappa_1) + \sum_{\kappa'} U_{\kappa'-\kappa_1}\,\psi(k-\kappa') = 0$$

$$\left[\varepsilon_{k_1} - \varepsilon\right]\psi(k-\kappa_1) + U_{\kappa_1-\kappa_1}\psi(k-\kappa_1) + U_{\kappa_2-\kappa_1}\psi(k-\kappa_2) = 0$$

but $U_{\kappa_1-\kappa_1} = U_{\kappa_2-\kappa_2} = 0$ as the Fourier components vanish at (0,0) reciprocal lattice vectors, and

$$U_{\kappa_2-\kappa_1} = U_{\kappa_1-\kappa_2} = -U_0 \Rightarrow$$

$$\boxed{\left[\varepsilon_{k_1} - \varepsilon\right]\psi(k-\kappa_1) - U_0\,\psi(k-\kappa_2) = 0} \quad \text{---- (3)}$$

similarly at K_2, we have

$$\left[\underbrace{\frac{\hbar^2}{2m}(k-K_2)^2}_{\varepsilon_{k_2}} - \varepsilon\right]\psi(k-K_2) + \sum_{K'} U_{K'-K_2}\,\psi(k-K') = 0$$

$$\left(\varepsilon_{k_2} - \varepsilon\right)\psi(k-K_2) + \underbrace{U_{K_1-K_2}}_{-U_0}\psi(k-K_1) + \underbrace{U_{K_2-K_2}}_{\text{zero}}\psi(k-K_2) = 0$$

$$\boxed{\left(\varepsilon_{k_2} - \varepsilon\right)\psi(k-K_2) - U_0\,\psi(k-K_1) = 0} \quad \text{---- (4)}$$

recall again that $\varepsilon_{k_1} = \varepsilon_{k_2}$

$$\varepsilon_{k_1} = \frac{\hbar^2}{2m}(k_1-K_1)^2 = \frac{\hbar^2}{2m}\left(\left(\frac{\pi}{a},\frac{\pi}{a}\right)-\left(\frac{2\pi}{a},\frac{2\pi}{a}\right)\right)^2 = \frac{\hbar^2}{2m}\left(\left(-\frac{\pi}{a},-\frac{\pi}{a}\right)\right)^2 = \frac{\hbar^2}{2m}\left(\frac{\pi^2}{a^2}+\frac{\pi^2}{a^2}\right)$$

$$= \frac{\hbar^2 2\pi^2}{2ma^2}$$

$$= \frac{\hbar^2\pi^2}{ma^2}$$

similarly

$$\varepsilon_{k_2} = \frac{\hbar^2}{2m}(k_2-K_2)^2 = \frac{\hbar^2}{2m}\left(\left(-\frac{\pi}{a},-\frac{\pi}{a}\right)-\left(-\frac{2\pi}{a},-\frac{2\pi}{a}\right)\right)^2$$

$$= \frac{\hbar^2}{2m}\left(\left(\frac{\pi}{a},\frac{\pi}{a}\right)\right)^2 = \frac{\hbar^2}{2m}\left(\frac{\pi^2}{a^2}+\frac{\pi^2}{a^2}\right) = \frac{\hbar^2 2\pi^2}{2ma^2} = \frac{\hbar^2\pi^2}{ma^2}$$

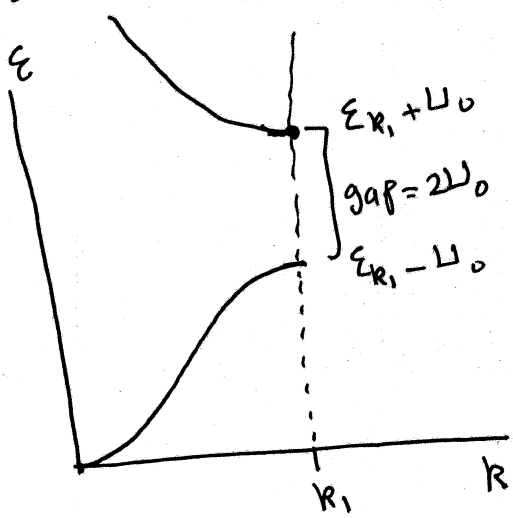
in matrix form, eqns (3) and (4) can be written as

$$\begin{pmatrix} \varepsilon_{k_1}-\varepsilon & -U_0 \\ -U_0 & \varepsilon_{k_1}-\varepsilon \end{pmatrix}\begin{pmatrix} \psi(k-K_1) \\ \psi(k-K_2) \end{pmatrix} = 0$$

set $\det(\,) = \text{zero} \Rightarrow$

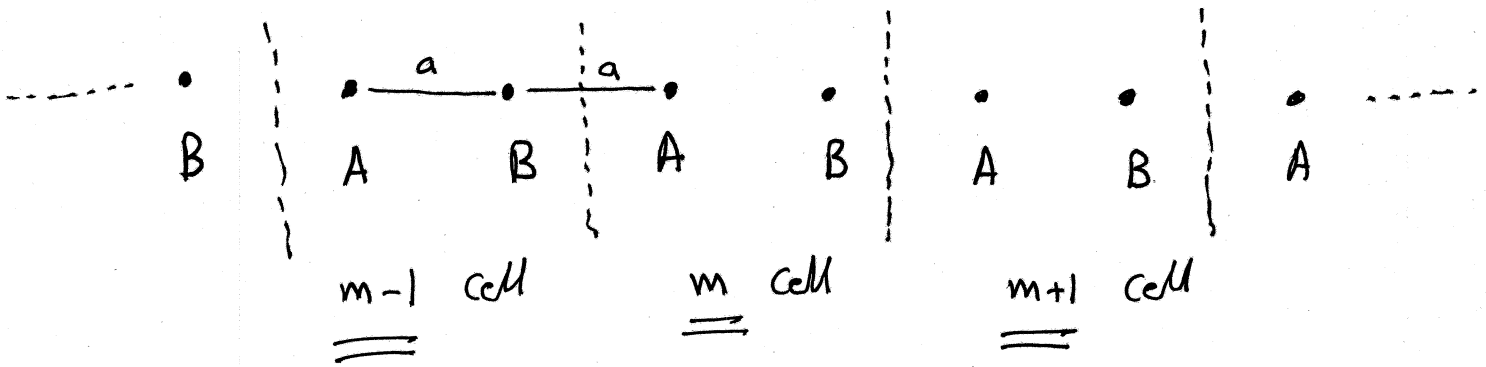
$$(\varepsilon_{k_1}-\varepsilon)^2 - U_0^2 = 0 \Rightarrow \varepsilon_{k_1}-\varepsilon = \pm U_0$$

$$\Rightarrow \varepsilon = \varepsilon_{k_1} \pm U_0 \Rightarrow \text{gap} = 2U_0$$



(4)

Diatomic chain ABABAB---- (Period = 2a)



Let on-site energies be ε_A and ε_B. Now need to write the two tight-binding equations for atoms A and B.

for atom A: in the m^{th} cell

$\varepsilon_A C_m^A - t(C_m^B + C_{m-1}^B) = \varepsilon C_m^A$, where electron on A can hope to Atom B on same m^{th} cell and/or to Atom B in the previous cell $(m-1)$

for atom B: in the m^{th} cell

$\varepsilon_B C_m^B - t(C_m^A + C_{m+1}^A) = \varepsilon C_m^B$, where electron on atom B can hop to A on same m^{th} cell and/or to A in the next cell $(m+1)$.

Now let $C_m^A = u_A e^{ik2ma}$ and $C_m^B = u_B e^{ik2ma}$

substitute C_m^A and C_m^B in the above two equations,

$\Rightarrow \varepsilon_A u_A e^{i2kam} - t(u_B e^{i2kma} + u_B e^{i2k(m-1)a}) = \varepsilon u_A e^{i2kma}$, divide by e^{i2kma}

$\Rightarrow \boxed{\varepsilon_A u_A - t u_B (1 + e^{-i2ka}) = \varepsilon u_A}$ ---(1)

and $\varepsilon_B u_B e^{i2kma} - t(u_A e^{i2kma} + u_A e^{i2k(m+1)a}) = \varepsilon u_B e^{i2kma}$, divide by e^{i2kma}

$$\Rightarrow \boxed{\varepsilon_B u_B - t u_A (1 + e^{i2ka}) = \varepsilon u_B} \quad \text{---(2)}$$

in matrix form

$$\begin{pmatrix} \varepsilon_A & -t(1+e^{-2ika}) \\ -t(1+e^{2ika}) & \varepsilon_B \end{pmatrix} \begin{pmatrix} u_A \\ u_B \end{pmatrix} = \varepsilon \begin{pmatrix} u_A \\ u_B \end{pmatrix}$$

the two equations have non-trivial solution when

$$\begin{vmatrix} \varepsilon_A - \varepsilon & -t(1+e^{-2ika}) \\ -t(1+e^{2ika}) & \varepsilon_B - \varepsilon \end{vmatrix} = 0$$

$$\Rightarrow (\varepsilon_A - \varepsilon)(\varepsilon_B - \varepsilon) - t^2 \underbrace{(1+e^{-2ika})(1+e^{2ika})}_{\hookrightarrow = 1 + e^{2ika} + e^{-2ika} + 1 = 2 + 2\cos 2ka} = 0$$

$$= 2(1+\cos 2ka)$$

$$= 2 \cdot 2\cos^2(ka), \text{ where I used } \cos^2 x = \frac{1}{2}(1+\cos 2x)$$

$$\Rightarrow \varepsilon_A \varepsilon_B - \varepsilon_A \varepsilon - \varepsilon_B \varepsilon + \varepsilon^2 - 4t^2\cos^2 ka = 0$$

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

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

$$= \frac{\varepsilon_A + \varepsilon_B}{2} \pm \frac{1}{2}\sqrt{\varepsilon_A^2 + \varepsilon_B^2 + 2\varepsilon_A\varepsilon_B - 4\varepsilon_A\varepsilon_B + 16t^2\cos^2 ka}$$

$$= \left(\frac{\varepsilon_A + \varepsilon_B}{2}\right) \pm \frac{1}{2}\sqrt{\varepsilon_A^2 + \varepsilon_B^2 - 2\varepsilon_A\varepsilon_B + 16t^2\cos^2 ka}$$

$$\varepsilon = \left(\frac{\varepsilon_A + \varepsilon_B}{2}\right) \pm \sqrt{\left(\frac{\varepsilon_A - \varepsilon_B}{2}\right)^2 + 4t^2\cos^2 ka} \quad \cdots (3)$$

let $\varepsilon_{avg} = \frac{\varepsilon_A + \varepsilon_B}{2}$ and $\Delta = \frac{\varepsilon_A - \varepsilon_B}{2}$

$\Rightarrow \varepsilon = \varepsilon_{avg} \pm \sqrt{\Delta^2 + 4t^2\cos^2 ka} \Rightarrow$ two bands

lower band (valence band) $\varepsilon_{lower} = \varepsilon_{avg} - \sqrt{\Delta^2 + 4t^2\cos^2 ka}$

upper band (conduction band) $\varepsilon_{upper} = \varepsilon_{avg} + \sqrt{\Delta^2 + 4t^2\cos^2 ka}$

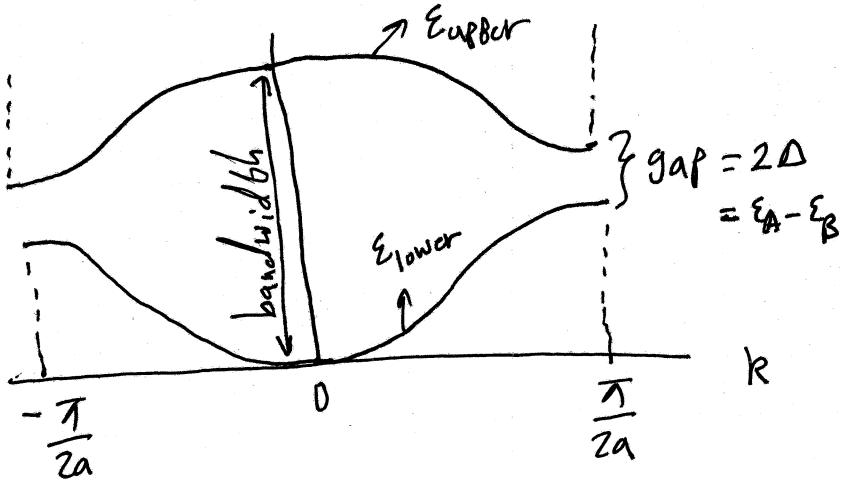
- bandwidth at $k = 0$

bandwidth $= 2\sqrt{\Delta^2 + 4t^2}$

- band gap at $k = \pm \frac{\pi}{2a}$

$\varepsilon_{lower}(\pi/2a) = \varepsilon_{avg} - \Delta$

$\varepsilon_{upper}(\pi/2a) = \varepsilon_{avg} + \Delta$

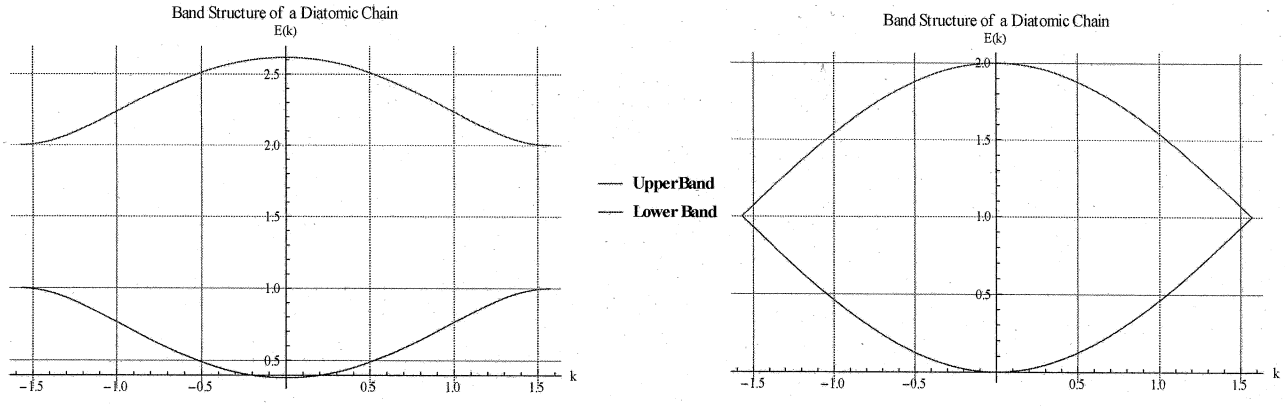


gap $= \varepsilon_{upper} - \varepsilon_{lower} = 2 \cdot \Delta = 2 \cdot \frac{\varepsilon_A - \varepsilon_B}{2} = \varepsilon_A - \varepsilon_B$

Note that if $\varepsilon_A = \varepsilon_B \Rightarrow \varepsilon = \varepsilon_A \pm 2t\cos ka$, and at $k = \pm \pi/2a$, there is no gap and we recover the regular monoatomic chain with no bandgap. The next page is a mathematica code that shows the two cases.

In[54]:=
```
(*Clear all previous definitions*)ClearAll["Global`*"];
```

In[89]:=
```
(*Parameters*)a = 1; (*Lattice constant*)ϵA = 1; (*On-site energy for atom A*)ϵB = 2;
(*On-site energy for atom B*)t = 0.5; (*Hopping integral*)(*Energy dispersion*)
Eplus[k_] := (ϵA + ϵB) / 2 + Sqrt[((ϵA - ϵB) / 2) ^2 + 4 t^2 Cos[k a]^2];
Eminus[k_] := (ϵA + ϵB) / 2 - Sqrt[((ϵA - ϵB) / 2) ^2 + 4 t^2 Cos[k a]^2];

(*Plot*)
Plot[{Eplus[k], Eminus[k]}, {k, -Pi / (2 a), Pi / (2 a)}, PlotRange → All, AxesLabel → {"k", "E(k)"},
 PlotLegends → {"Upper Band", "Lower Band"}, PlotStyle → {Red, Blue}, GridLines → Automatic,
 PlotLabel → "Band Structure of a Diatomic Chain"]
```



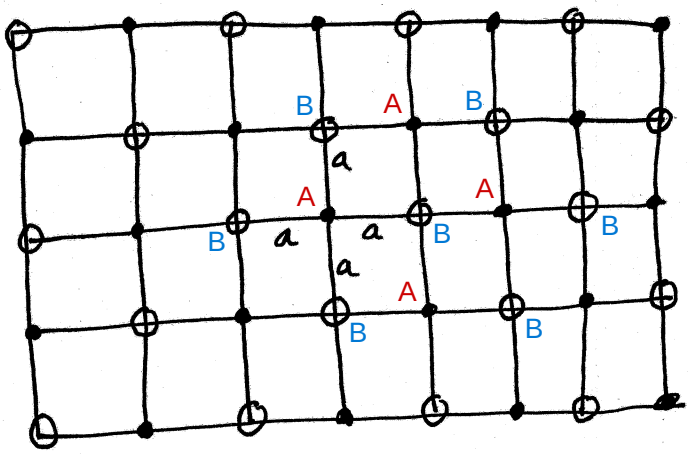
$\epsilon_A \neq \epsilon_B$

$\epsilon_A = \epsilon_B$

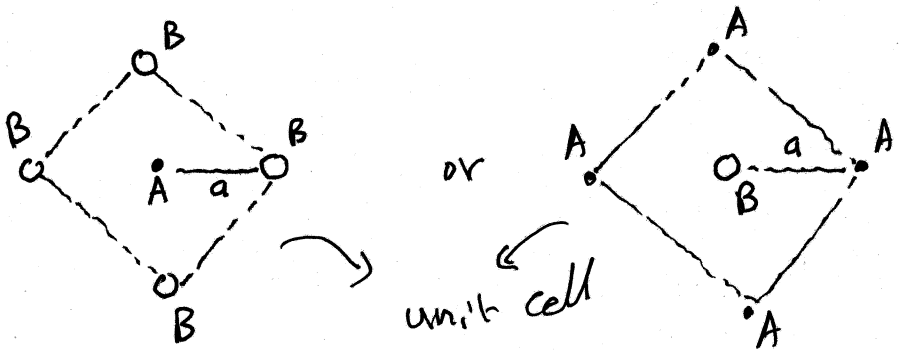
(5)

Diatomic square lattice. The lattice is a square with side length $2a$. each unit cell contains two atoms A and B as shown in figure:

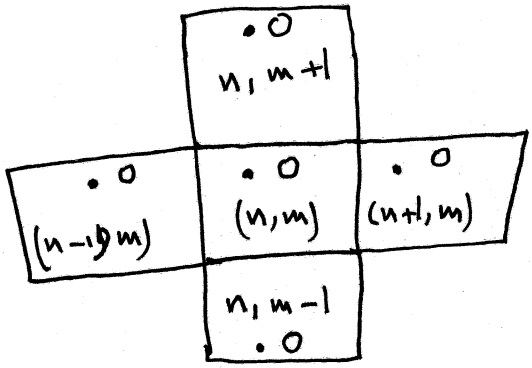
• A , ○ B



each atom is connected to four atoms of the other type, where each unit cell contains only two atoms



on site energies are ε_A and ε_B



let $C^A_{(n,m)} = u_A e^{ik_x an + ik_y am}$, and

$C^B_{(n,m)} = u_B e^{ik_x an + ik_y am}$

n, m are integers

The tight-binding equations are

for atom A

$$\varepsilon_A C^A_{(n,m)} - t\left(C^B_{(n+1,m)} + C^B_{(n-1,m)} + C^B_{(n,m+1)} + C^B_{(n,m-1)}\right) = \varepsilon C^A_{(n,m)}$$

$$\varepsilon_A u_A e^{ik_x an + ik_y am} - t\left(u_B e^{ik_x a(n+1) + ik_y ma} + u_B e^{ik_x a(n-1) + ik_y ma} + u_B e^{ik_x an + ik_y a(m+1)} + u_B e^{ik_x an + ik_y a(m-1)}\right) = \varepsilon u_A e^{ik_x an + ik_y am}$$

divide by $e^{ik_x an + ik_y am}$, we get

$$\varepsilon_A u_A - t u_B \left(e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a}\right) = \varepsilon u_A$$

$$\Rightarrow \boxed{\varepsilon_A u_A - t u_B (2\cos k_x a + 2\cos k_y a) = \varepsilon u_A} \quad \text{----(1)}$$

similarly for a bom B, we have

$$\varepsilon_B C^{B}_{(n,m)} - t\left(C^{A}_{(n+1,m)} + C^{A}_{(n-1,m)} + C^{A}_{(n,m+1)} + C^{A}_{(n,m-1)}\right) = \varepsilon C^{B}_{(n,m)}$$

$$\varepsilon_B u_B - t u_A \left(e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a}\right) = \varepsilon u_B$$

$$\boxed{\varepsilon_B u_B - t u_A (2\cos k_x a + 2\cos k_y a) = \varepsilon u_B} \quad \text{---- (2)}$$

in matrix form

$$\begin{pmatrix} \varepsilon_A & -2t(\cos k_x a + \cos k_y a) \\ -2t(\cos k_x a + \cos k_y a) & \varepsilon_B \end{pmatrix} \begin{pmatrix} u_A \\ u_B \end{pmatrix} = \varepsilon \begin{pmatrix} u_A \\ u_B \end{pmatrix}$$

$$\Rightarrow \begin{vmatrix} \varepsilon_A - \varepsilon & -2t(\cos k_x a + \cos k_y a) \\ -2t(\cos k_x a + \cos k_y a) & \varepsilon_B - \varepsilon \end{vmatrix} = 0$$

$$\Rightarrow (\varepsilon_A - \varepsilon)(\varepsilon_B - \varepsilon) - 4t^2 [\cos k_x a + \cos k_y a]^2 = 0$$

$$\varepsilon^2 - (\varepsilon_A + \varepsilon_B)\varepsilon + \varepsilon_A \varepsilon_B - 4t^2 [\cos k_x a + \cos k_y a]^2 = 0$$

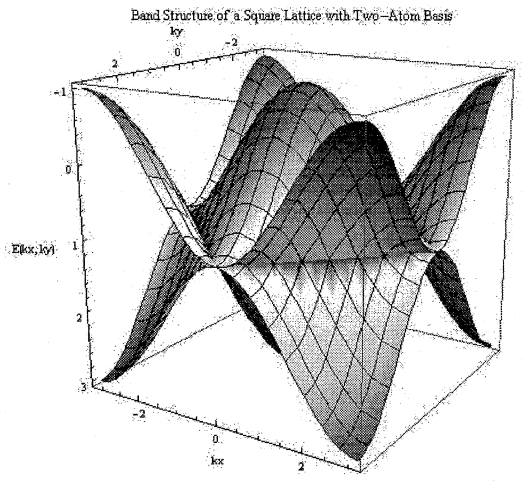
$$\Rightarrow \varepsilon = \frac{\varepsilon_A + \varepsilon_B}{2} \pm \frac{1}{2} \sqrt{(\varepsilon_A + \varepsilon_B)^2 - 4\varepsilon_A \varepsilon_B + 16 t^2 [\cos k_x a + \cos k_y a]^2}$$

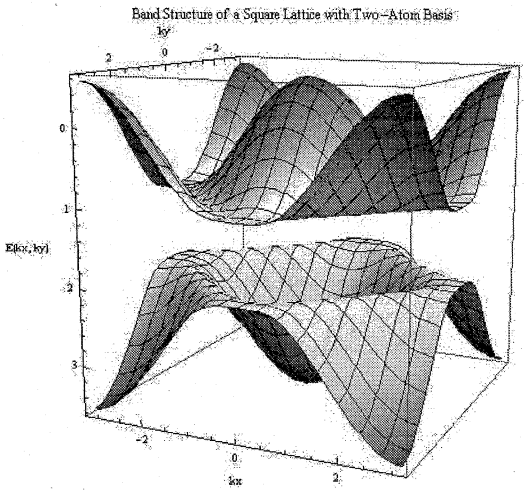
$$= \frac{\varepsilon_A + \varepsilon_B}{2} \pm \sqrt{\left(\frac{\varepsilon_A - \varepsilon_B}{2}\right)^2 + 4t^2 [\cos k_x a + \cos k_y a]^2}$$

let $\varepsilon_{avg} = \frac{\varepsilon_A + \varepsilon_B}{2}$ and $\Delta = \frac{\varepsilon_A - \varepsilon_B}{2}$ $\Rightarrow$

$$\varepsilon = \varepsilon_{avg} \pm \sqrt{\Delta^2 + 4b^2 \left[\cos k_x a + \cos k_y a\right]^2}$$

```
In[96]:= (*Clear all previous definitions*)ClearAll["Global`*"];

(*Parameters*)a = 1; (*Lattice constant*)eA = 1; (*On-site energy for atom A*)eB = 2;
(*On-site energy for atom B*)t = 0.5; (*Hopping integral*)(*Energy dispersion*)
Eplus[kx_, ky_] := (eA + eB) / 2 + Sqrt[((eA - eB) / 2)^2 + 4 t^2 (Cos[kx a] + Cos[ky a])^2];
Eminus[kx_, ky_] := (eA + eB) / 2 - Sqrt[((eA - eB) / 2)^2 + 4 t^2 (Cos[kx a] + Cos[ky a])^2];

(*3D Plot of the bands*)
Plot3D[{Eplus[kx, ky], Eminus[kx, ky]}, {kx, -Pi / a, Pi / a}, {ky, -Pi / a, Pi / a}, PlotRange → All,
 AxesLabel → {"kx", "ky", "E(kx, ky)"}, PlotLabel → "Band Structure of a Square Lattice with Two-Atom Basis",
 ColorFunction → "TemperatureMap", PlotLegends → {"Upper Band", "Lower Band"}, Mesh → Automatic,
 BoxRatios → {1, 1, 1}]
```





$\varepsilon_A = \varepsilon_B$
(No gap)

1st BZ
$k_x \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$
$k_y \left[-\frac{\pi}{a}, \pi/a\right]$

$\varepsilon_A \neq \varepsilon_B$
gap opens

the band gap is the energy difference between the minimum of the upper band and the maximum of the lower band (ε_-):
(ε_+)

upper band minimum occurs when $\cos k_x a + \cos k_y a = 0 \Rightarrow k_x = k_y = \frac{\pi}{2a}$

$$\varepsilon_{upper}^{min} = \varepsilon_{avg} + \frac{|\varepsilon_A - \varepsilon_B|}{2},$$

lower band maximum occurs at the same point $k_x = k_y = \pi/2a$

$$\varepsilon_{lower}^{max} = \varepsilon_{avg} - \frac{|\varepsilon_A - \varepsilon_B|}{2} \Rightarrow \text{gap} = \varepsilon_{upper}^{min} - \varepsilon_{lower}^{max} = |\varepsilon_A - \varepsilon_B|$$

the bandwidth can be calculated for each band separately,

for upper band: $(\mathcal{E}_+) = \mathcal{E}_{avg} + \sqrt{\Delta^2 + 4b^2[\cos k_x a + \cos k_y a]^2}$

Max energy occurs when $\cos k_x a + \cos k_y a = 2$ i.e $k_x = k_y = 0$

$$\Rightarrow \mathcal{E}_+^{max} = \mathcal{E}_{avg} + \sqrt{\Delta^2 + 16t^2}$$

min energy occurs when $\cos k_x a + \cos k_y a = 0 \Rightarrow k_x = k_y = \pi/a$

$$\mathcal{E}_-^{min} = \mathcal{E}_{avg} + |\Delta|$$

$$\Rightarrow \text{bandwidth} = \mathcal{E}_+^{max} - \mathcal{E}_-^{min} = \sqrt{\Delta^2 + 16t^2} - |\Delta|$$

so that if $\mathcal{E}_A = \mathcal{E}_B \Rightarrow \Delta = 0 \Rightarrow$ bandwidth $= 4b$ as obtained in class for monoatomic square lattice

for lower band: $(\mathcal{E}_-) = \mathcal{E}_{avg} - \sqrt{\Delta^2 + 4b^2[\cos k_x a + \cos k_y a]^2}$

we will get same result

$$\text{band width} = \sqrt{\Delta^2 + 16t^2} - |\Delta|$$

(6) Consider a diatomic chain of atoms ABABAB---- . we found in problem (4) that the dispersion relation was

$$\mathcal{E}(k) = \mathcal{E}_{avg} \pm \sqrt{\Delta^2 + 4t^2\cos^2 ka}$$, where $\mathcal{E}_{avg} = \frac{\mathcal{E}_A + \mathcal{E}_B}{2}$, $\Delta = \frac{\mathcal{E}_A - \mathcal{E}_B}{2}$

now the tight-binding density of state is given by

$$D(\mathcal{E}) = \frac{2L}{\pi} \frac{1}{|\nabla_k \mathcal{E}|} = \frac{2L}{\pi} \frac{1}{\left|\frac{d\mathcal{E}}{dk}\right|}$$

$$\frac{D(\mathcal{E})}{L} = \frac{2}{\pi} \frac{1}{|d\mathcal{E}/dk|}$$ density of states per unit length

the $D(\mathcal{E})/L$ can be calculated for each band $\mathcal{E}^+$, $\mathcal{E}^-$

- for the upper band $\mathcal{E}^+(k) = \mathcal{E}_{avg} + \sqrt{\Delta^2 + 4t^2\cos^2 ka}$

$$\frac{d\mathcal{E}}{dk} = \frac{1}{2}\left(\Delta^2 + 4t^2\cos^2 ka\right)^{-1/2} \left(2 \cdot 4t^2 \cos ka\,(-\sin ka) \cdot a\right)$$

$$= \frac{-4at^2 \sin ka \cos ka}{\sqrt{\Delta^2 + 4t^2\cos^2 ka}}$$

$$\Rightarrow \frac{D(\mathcal{E})}{L} = \frac{2}{\pi} \frac{1}{|d\mathcal{E}/dk|} = \frac{2}{\pi} \frac{\sqrt{\Delta^2 + 4t^2\cos^2 ka}}{4at^2 |\sin ka \cos ka|}$$

$$= \frac{1}{2\pi at^2} \frac{\sqrt{\Delta^2 + 4t^2\cos^2 ka}}{|\sin ka \cos ka|} \quad \text{---- (1)}$$

from $\mathcal{E} = \mathcal{E}_{avg} + \sqrt{\Delta^2 + 4t^2\cos^2 ka} \Rightarrow \mathcal{E} - \mathcal{E}_{avg} = \sqrt{\Delta^2 + 4t^2\cos^2 ka}$

square $\Rightarrow (\mathcal{E} - \mathcal{E}_{avg})^2 = \Delta^2 + 4t^2\cos^2 ka \Rightarrow \cos^2 ka = \dfrac{(\mathcal{E} - \mathcal{E}_{avg})^2 - \Delta^2}{4t^2}$

and using $\sin^2 ka = 1 - \cos^2 ka$, we have

$$\sin^2 ka = 1 - \frac{(\mathcal{E} - \mathcal{E}_{avg})^2 - \Delta^2}{4t^2}, \text{ substitute in (1)}$$

$$\frac{D(\mathcal{E})}{L} = \frac{1}{2\pi ab^2} \frac{\sqrt{\Delta^2 + (\mathcal{E} - \mathcal{E}_{avg})^2 - \Delta^2}}{\sqrt{1 - \dfrac{((\mathcal{E} - \mathcal{E}_{avg})^2 - \Delta^2)}{4b^2}} \sqrt{\dfrac{(\mathcal{E} - \mathcal{E}_{avg})^2 - \Delta^2}{4b^2}}}$$

$$= \frac{2}{\pi a} \frac{(\mathcal{E} - \mathcal{E}_{avg})}{\sqrt{4t^2 - ((\mathcal{E} - \mathcal{E}_{avg})^2 - \Delta^2)} \sqrt{(\mathcal{E} - \mathcal{E}_{avg})^2 - \Delta^2}} \quad \text{--- (2)}$$

Now let us find the energy range of this upper band

$$\mathcal{E}^+ = \mathcal{E}_{avg} + \sqrt{\Delta^2 + 4b^2\cos^2 ka}$$

minimum of the upper band occurs when $\sqrt{\Delta^2 + 4b^2\cos^2 ka}$ is minimized which happens when $\cos^2 ka = 0$, i.e

$$k = \pm \pi/2a$$

$$\Rightarrow \mathcal{E}^+_{min} = \mathcal{E}_{avg} + \sqrt{\Delta^2} = \mathcal{E}_{avg} + |\Delta|$$

maximum of the upper band occurs when $\sqrt{\Delta^2 + 4b^2\cos^2 ka}$ is maximized which happens when $\cos^2 ka = 1$, i.e at $k = 0, \pm \frac{\pi}{a}$

$$\Rightarrow \mathcal{E}^+_{max} = \mathcal{E}_{avg} + \sqrt{\Delta^2 + 4b^2}$$

$\therefore$ upper band $\mathcal{E} = \mathcal{E}_{avg} + \sqrt{\Delta^2 + 4b^2\cos^2 ka}$, where

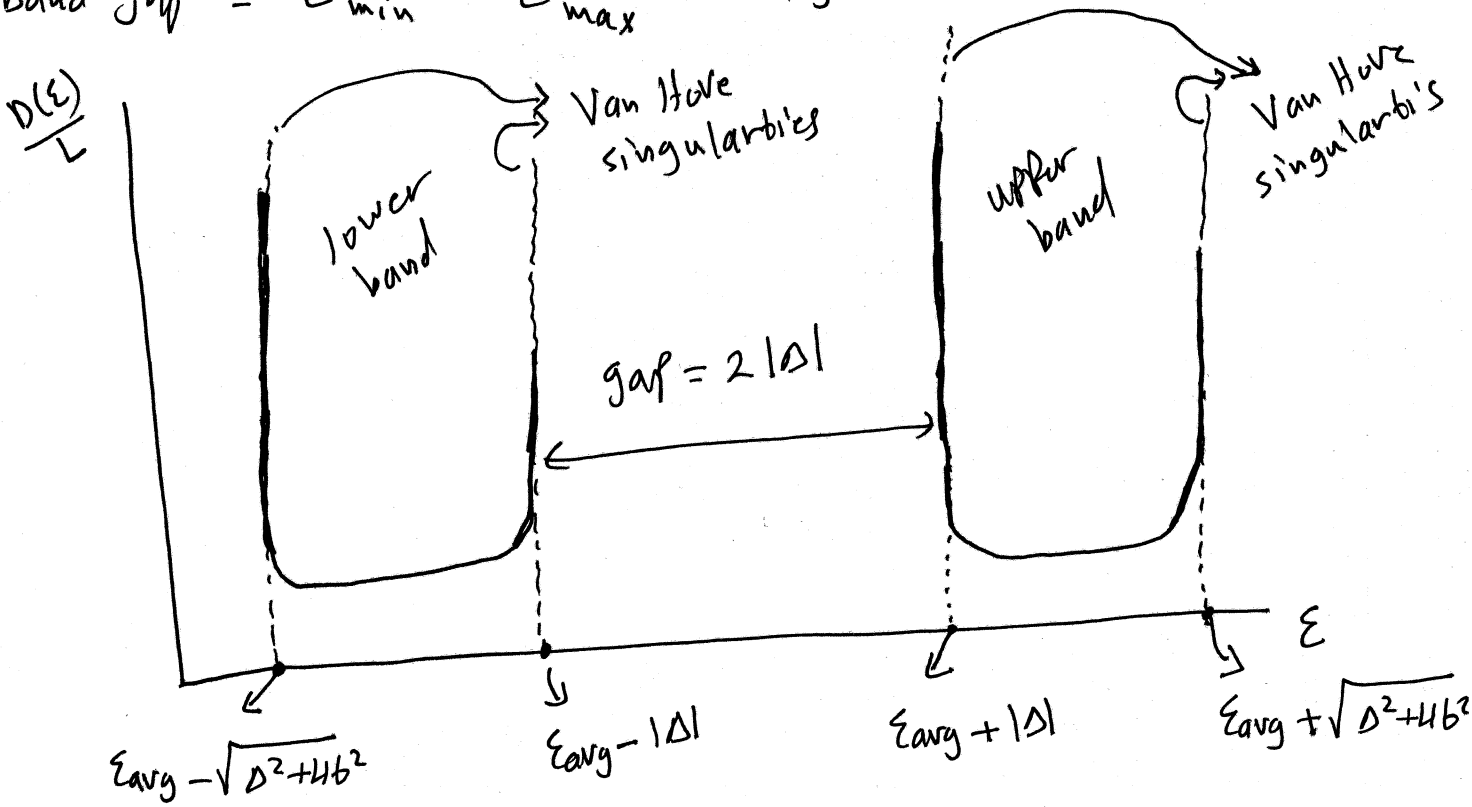
$$\mathcal{E}_{avg} + |\Delta| \leq \mathcal{E}^+ \leq \mathcal{E}_{avg} + \sqrt{\Delta^2 + 4b^2}$$

similar calculations for the lower band $\mathcal{E}^-$ results in

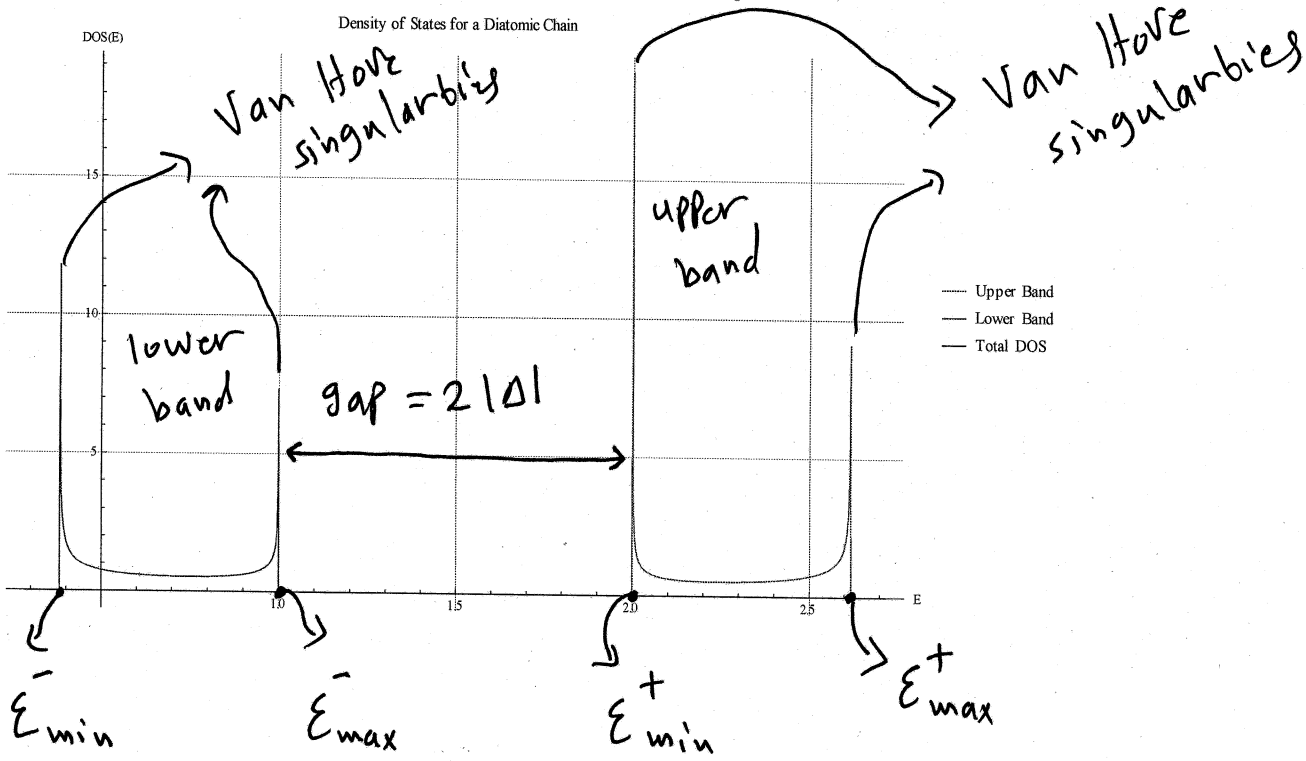
$$\mathcal{E}^- = \mathcal{E}_{avg} - \sqrt{\Delta^2 + 4b^2\cos^2 ka}, \text{ where}$$

$$\mathcal{E}_{avg} - \sqrt{\Delta^2 + 4b^2} \leq \mathcal{E}^- \leq \mathcal{E}_{avg} - |\Delta|$$

$$\text{band gap} = \mathcal{E}^+_{min} - \mathcal{E}^-_{max} = \mathcal{E}_{avg} + |\Delta| - (\mathcal{E}_{avg} - |\Delta|) = 2|\Delta|$$



```
(*Clear all previous definitions*)ClearAll["Global`*"];
(*Parameters*)a = 1; (*Lattice constant*)eA = 1; (*On-site energy for atom A*)eB = 2;
(*On-site energy for atom B*)t = 0.5; (*Hopping integral*)avg = (eA + eB) / 2;
delta = (eA - eB) / 2;

(*Energy range for the bands*)
lowerBandMin = avg - Sqrt[delta^2 + 4 t^2];
lowerBandMax = avg - Abs[delta];
upperBandMin = avg + Abs[delta];
upperBandMax = avg + Sqrt[delta^2 + 4 t^2];

(*DOS for Upper Band*)
DOSUpper[E_?NumericQ] :=
  Piecewise[{{1 / (Pi a) * (E - avg) / (Sqrt[(E - avg)^2 - delta^2] * Sqrt[4 t^2 + delta^2 - (E - avg)^2]),
     upperBandMin ≤ E ≤ upperBandMax}}, 0];

(*DOS for Lower Band*)
DOSLower[E_?NumericQ] :=
  Piecewise[{{1 / (Pi a) * (avg - E) / (Sqrt[(avg - E)^2 - delta^2] * Sqrt[4 t^2 + delta^2 - (avg - E)^2]),
     lowerBandMin ≤ E ≤ lowerBandMax}}, 0];

(*Total DOS*)
(*DOS[E_?NumericQ]:=DOSUpper[E]+DOSLower[E];*)

(*Plot the DOS*)
Plot[{DOSUpper[E], DOSLower[E], (*DOS[E]*)}, {E, lowerBandMin - 0.1, upperBandMax + 0.1}, PlotRange → All,
 AxesLabel → {"E", "DOS(E)"}, PlotLegends → {"Upper Band", "Lower Band", "Total DOS"},
 PlotStyle → {Red, Blue, Black}, GridLines → Automatic, Exclusions → None,
 PlotLabel → "Density of States for a Diatomic Chain"]
```



see that if $\varepsilon_A = \varepsilon_B \Rightarrow \varepsilon_{avg} = \frac{\varepsilon_A + \varepsilon_B}{2} = \varepsilon_A = \varepsilon_B$, and $\Delta = \frac{\varepsilon_A - \varepsilon_B}{2} = \text{zero} \Rightarrow$ no band gap, so for the upper band, we have

$$\frac{D(\varepsilon)}{L} = \frac{2}{\pi a} \frac{\varepsilon - \varepsilon_A}{\sqrt{4b^2 - (\varepsilon - \varepsilon_A)^2}\sqrt{(\varepsilon - \varepsilon_A)^2}} = \frac{2}{\pi a} \frac{1}{\sqrt{4b^2 - (\varepsilon - \varepsilon_A)^2}}$$

$\frac{D(\varepsilon)}{L}$ is singular at $4b^2 = (\varepsilon - \varepsilon_A)^2 \Rightarrow \varepsilon = \varepsilon_A + 2b$

similarly for the lower band

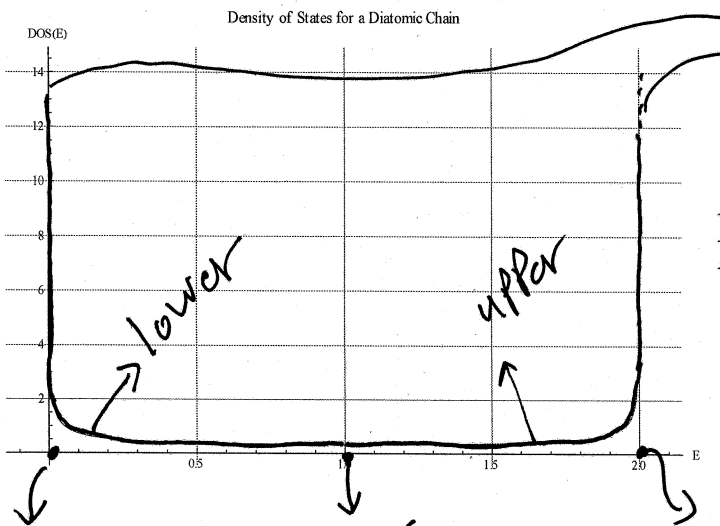
$$\frac{D(\varepsilon)}{L} = \frac{2}{\pi a} \frac{(\varepsilon_{avg} - \varepsilon)}{\sqrt{(\varepsilon_{avg} - \varepsilon)^2 - \Delta^2}\sqrt{4b^2 + \Delta^2 - (\varepsilon_{avg} - \varepsilon)^2}}$$

$$= \frac{2}{\pi a} \frac{(\varepsilon_A - \varepsilon)}{(\varepsilon_A - \varepsilon)\sqrt{4b^2 - (\varepsilon_A - \varepsilon)^2}} = \frac{2}{\pi a} \frac{1}{\sqrt{4b^2 - (\varepsilon_A - \varepsilon)^2}}$$

$\frac{D(\varepsilon)}{L}$ is singular when $4b^2 = (\varepsilon_A - \varepsilon)^2 \Rightarrow \varepsilon = \varepsilon_A - 2b$

```
(*Clear all previous definitions*)ClearAll["Global`*"];

In[1]:= (*Parameters*)a = 1; (*Lattice constant*)eA = 1; (*On-site energy for atom A*)eB = 1;
(*On-site energy for atom B*)t = 0.5; (*Hopping integral*)avg = (eA + eB) / 2;
delta = (eA - eB) / 2;

(*Energy range for the bands*)
lowerBandMin = avg - Sqrt[delta^2 + 4 t^2];
lowerBandMax = avg - Abs[delta];
upperBandMin = avg + Abs[delta];
upperBandMax = avg + Sqrt[delta^2 + 4 t^2];

(*DOS for Upper Band*)
DOSUpper[E_?NumericQ] :=
  Piecewise[{{1 / (Pi a) * (E - avg) / (Sqrt[(E - avg)^2 - delta^2] * Sqrt[4 t^2 + delta^2 - (E - avg)^2]),
     upperBandMin ≤ E ≤ upperBandMax}}, 0];

(*DOS for Lower Band*)
DOSLower[E_?NumericQ] :=
  Piecewise[{{1 / (Pi a) * (avg - E) / (Sqrt[(avg - E)^2 - delta^2] * Sqrt[4 t^2 + delta^2 - (avg - E)^2]),
     lowerBandMin ≤ E ≤ lowerBandMax}}, 0];

(*Total DOS*)
(*DOS[E_?NumericQ]:=DOSUpper[E]+DOSLower[E];*)

(*Plot the DOS*)
Plot[{DOSUpper[E], DOSLower[E], (*DOS[E]*)}, {E, lowerBandMin - 0.1, upperBandMax + 0.1}, PlotRange → All,
 AxesLabel → {"E", "DOS(E)"}, PlotLegends → {"Upper Band", "Lower Band", "Total DOS"},
 PlotStyle → {Red, Blue, Black}, GridLines → Automatic, Exclusions → None,
 PlotLabel → "Density of States for a Diatomic Chain"]
```

Out[9]=



Van Hove singularities

No gap

$\varepsilon = \varepsilon_A - 2b$

$\varepsilon_A = \varepsilon_B$

$\varepsilon = \varepsilon_A + 2b$