

Condensed matter physics (phy 771)

HW #6 - solution

Dr. Gassem Alzowbi

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

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

$$\begin{aligned} &= \int d^3r \langle k' | r \rangle U(r) \langle r | k \rangle \\ &= \frac{1}{V} \int d^3r e^{-i\vec{k}' \cdot \vec{r}} \sum_{\vec{k}} U_{\vec{k}} e^{i\vec{k} \cdot \vec{r}} e^{i\vec{k} \cdot \vec{r}} \\ &= \frac{1}{V} \sum_{\vec{k}} U_{\vec{k}} \underbrace{\int d^3r e^{i(\vec{k} + \vec{k} - \vec{k}') \cdot \vec{r}}}_{V \delta_{\vec{k}', \vec{k} + \vec{k}}} \end{aligned}$$

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

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 $\langle k | U | k + k \rangle = U_{k - k - k} = U_{-k}$ where $\text{I see } k' = k, \text{ and } k = k + k$

$$\text{knowing that } \langle k | U | k + k \rangle = \langle k + k | U | k \rangle^* = U_k^* = U_{-k}$$

$$\therefore U_{-k} = U_k^*$$

②

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

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

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

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

$$= \frac{V_0}{a} \left[\int_0^a dx + \int_0^a dx \cos \frac{2\pi}{a}x \right] = \frac{V_0}{a} a = V_0$$

Zero integration over its period $\frac{2\pi}{2\pi/a} = a$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\begin{aligned} \text{now } \underline{\langle k | H | k \rangle} &= \langle k | H_0 + U | k \rangle = \underbrace{\langle k | H_0 | k \rangle}_{\epsilon_k^{(0)}} + \langle k | U | k \rangle \\ &= \epsilon_k^{(0)} \underbrace{\langle k | k \rangle}_1 + \underbrace{\langle k | U | k \rangle}_{V_0} = \epsilon_k^{(0)} + V_0 \end{aligned}$$

similarly

$$\begin{aligned} \underline{\langle k - \pi | H | k - \pi \rangle} &= \langle k - \pi | H_0 + U | k - \pi \rangle \\ &= \langle k - \pi | \underbrace{H_0}_{\epsilon_{k-\pi}^{(0)}} | k - \pi \rangle + \langle k - \pi | U | k - \pi \rangle \\ &= \epsilon_{k-\pi}^{(0)} \underbrace{\langle k - \pi | k - \pi \rangle}_1 + \underbrace{\langle k - \pi | U | k - \pi \rangle}_{V_0} \\ &= \epsilon_{k-\pi}^{(0)} + V_0; \quad \text{but at } k = \pi/2, \text{ we} \\ &= \epsilon_k^{(0)} + V_0, \quad \text{have } \epsilon_k^{(0)} = \epsilon_{k-\pi}^{(0)} \end{aligned}$$

$$\begin{aligned} \text{now } \langle k - \pi | H | k \rangle &= \langle k - \pi | H_0 + U | k \rangle = \underbrace{\langle k - \pi | H_0 | k \rangle}_{\epsilon_k^{(0)} \langle k - \pi | k \rangle} + \langle k - \pi | U | k \rangle \\ &= \epsilon_k^{(0)} \underbrace{\langle k - \pi | k \rangle}_{\text{zero}} + \underbrace{\langle k - \pi | U | k \rangle}_{W_\pi} \end{aligned}$$

$$= W_\pi, \text{ where } \pi = -\frac{2\pi}{a} \quad i \frac{2\pi}{a} x$$

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

$$\begin{aligned}
 W_k &= \frac{V_0}{a} \left[\underbrace{\int_0^a dx e^{i \frac{2\pi}{a} x}}_{\substack{\text{Zero} \\ \text{integrate over} \\ \text{the period}}} + \int_0^a dx \left[\frac{e^{i \frac{2\pi}{a} x} + e^{-i \frac{2\pi}{a} x}}{2} \right] e^{i \frac{2\pi}{a} x} \right] \\
 &= \frac{V_0}{2a} \int_0^a dx \left[e^{i \frac{4\pi}{a} x} + 1 \right] = \frac{V_0}{2a} \left[\int_0^a dx + \int_0^a dx e^{i \frac{4\pi}{a} x} \right] \\
 &= \frac{V_0}{2a} \left[a + \frac{a}{i 4\pi} e^{i \frac{4\pi}{a} x} \Big|_0^a \right] = \frac{V_0}{2a} \left[a + \frac{a}{i 4\pi} (e^{i 4\pi} - 1) \right] = \frac{V_0}{2}
 \end{aligned}$$

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

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

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

$$\Rightarrow \begin{vmatrix} \epsilon_k^{(0)} + V_0 - \epsilon & V_0/2 \\ V_0/2 & \epsilon_k^{(0)} + V_0 - \epsilon \end{vmatrix} = 0 \Rightarrow (\epsilon_k^{(0)} + V_0 - \epsilon)^2 = \frac{V_0^2}{4}$$

$$\Rightarrow \epsilon_k^{(0)} + V_0 - \epsilon = \pm \frac{V_0}{2} \Rightarrow \epsilon = \underbrace{\epsilon_k^{(0)}}_{\text{Zeroth}} + \underbrace{V_0}_{\Delta^{\text{st}}} \pm \underbrace{\frac{V_0}{2}}_{\Delta^{\text{nd}}}$$

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

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

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

③

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

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

$$\begin{aligned} \Rightarrow W(x, y) &= -2U_0 \left[\cos \frac{2\pi}{a}(x+y) + \cos \frac{2\pi}{a}(x-y) \right] \\ &= -2U_0 \left[\frac{e^{i\frac{2\pi}{a}(x+y)} + e^{-i\frac{2\pi}{a}(x+y)}}{2} + \frac{e^{i\frac{2\pi}{a}(x-y)} + e^{-i\frac{2\pi}{a}(x-y)}}{2} \right] \\ &= -U_0 \left[e^{i\frac{2\pi}{a}(x+y)} + e^{-i\frac{2\pi}{a}(x+y)} + e^{i\frac{2\pi}{a}(x-y)} + e^{-i\frac{2\pi}{a}(x-y)} \right] \quad \dots (1) \end{aligned}$$

let us compare this result with

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

$$= \sum_{\vec{k}} U_{\vec{k}} e^{i\kappa_x x + i\kappa_y y}, \text{ we see that the}$$

Fourier components $U_{\vec{k}}$ are the coefficients of the plane waves $e^{i\kappa_x x + i\kappa_y y}$. From (1), we see that $U_{\vec{k}} = -U_0$ and this corresponds to the following reciprocal lattice

vectors

$$e^{i\frac{2\pi}{a}(x+y)} \rightarrow \vec{k}_1 = (\kappa_x, \kappa_y) = \left(\frac{2\pi}{a}, \frac{2\pi}{a}\right)$$

$$e^{-i\frac{2\pi}{a}(x+y)} \rightarrow \vec{k}_2 = (\kappa_x, \kappa_y) = \left(-\frac{2\pi}{a}, -\frac{2\pi}{a}\right)$$

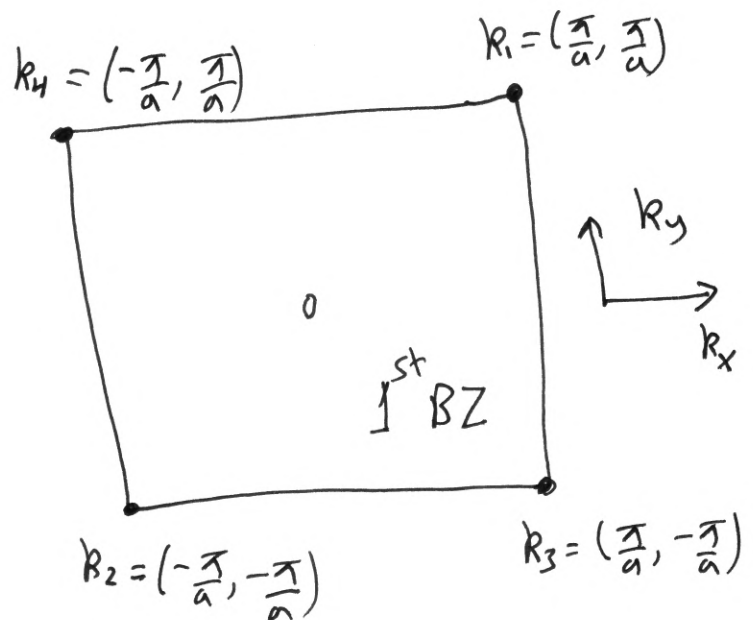
$$e^{i\frac{2\pi}{a}(x-y)} \rightarrow \vec{k}_3 = (k_x, k_y) = \left(\frac{2\pi}{a}, -\frac{2\pi}{a}\right), \text{ and finally}$$

$$e^{-i\frac{2\pi}{a}(x-y)} \rightarrow \vec{k}_4 = (k_x, k_y) = \left(-\frac{2\pi}{a}, \frac{2\pi}{a}\right).$$

$\Rightarrow$ the Fourier components $U_{\vec{k}}$ 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 $U_{\vec{k}} = -U_0$.

Now to find the energy gap at $\vec{k}_1 = \left(\frac{\pi}{a}, \frac{\pi}{a}\right)$, we need to couple it to another points that have same energy. Now using

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} (k_x^2 + k_y^2),$$



we see that all points $\vec{k}_1 \rightarrow \vec{k}_4$, have same energy, i.e.

$$E_{\vec{k}_1} = E_{\vec{k}_2} = E_{\vec{k}_3} = E_{\vec{k}_4} = \frac{\hbar^2}{2m} \left(\frac{\pi^2}{a^2} + \frac{\pi^2}{a^2} \right) = \frac{\hbar^2}{2m} \left(\frac{2\pi^2}{a^2} \right) = \frac{\hbar^2 \pi^2}{ma^2}.$$

Now there is another condition, which says that when any two $\vec{k}$ 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 $k_2 \Rightarrow \vec{k}_2 - \vec{k}_1 = \left(-\frac{\pi}{a}, -\frac{\pi}{a}\right) - \left(\frac{\pi}{a}, \frac{\pi}{a}\right) = \left(-\frac{2\pi}{a}, -\frac{2\pi}{a}\right) \checkmark$

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

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

see that coupling k_1 to (k_3 and k_4) results in reciprocal lattice vectors $\left(0, -\frac{2\pi}{a}\right)$, $\left(-\frac{2\pi}{a}, 0\right)$ 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 $\vec{k}_1 = \left(\frac{2\pi}{a}, \frac{2\pi}{a}\right)$ with $\vec{k}_2 = \left(-\frac{2\pi}{a}, -\frac{2\pi}{a}\right)$

- now Schrödinger eqⁿ in reciprocal space reads

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

at κ_1 , it becomes

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

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

but $\sum_{\kappa_1 - \kappa_1} = \sum_{\kappa_2 - \kappa_1} = 0$ as the Fourier components vanish

at $(0,0)$ reciprocal lattice vectors, and

$$\sum_{\kappa_2 - \kappa_1} = \sum_{\kappa_1 - \kappa_2} = -\sum_0 \Rightarrow$$

$$\boxed{\left[\varepsilon_{\kappa_1} - \varepsilon \right] \psi(k - \kappa_1) - \sum_0 \psi(k - \kappa_2) = 0} \quad \text{--- (3)}$$

similarly at κ_2 , we have

$$\left[\underbrace{\frac{\hbar^2}{2m} (k - \kappa_2)^2}_{\epsilon_{\kappa_2}} - \epsilon \right] \psi(k - \kappa_2) + \sum_{\kappa'} U_{\kappa' - \kappa_2} \psi(k - \kappa') = 0$$

$$\left(\epsilon_{\kappa_2} - \epsilon \right) \psi(k - \kappa_2) + \underbrace{U_{\kappa_1 - \kappa_2}}_{-U_0} \psi(k - \kappa_1) + \underbrace{U_{\kappa_2 - \kappa_2}}_{\text{zero}} \psi(k - \kappa_2) = 0$$

$$\boxed{\left(\epsilon_{\kappa_2} - \epsilon \right) \psi(k - \kappa_2) - U_0 \psi(k - \kappa_1) = 0} \quad \text{--- (4)}$$

recall again that $\epsilon_{\kappa_1} = \epsilon_{\kappa_2}$

$$\begin{aligned} \epsilon_{\kappa_1} &= \frac{\hbar^2}{2m} (\kappa_1 - \kappa_1)^2 = \frac{\hbar^2}{2m} \left(\left(\frac{\pi}{a}, \frac{\pi}{a} \right) - \left(\frac{2\pi}{a}, \frac{2\pi}{a} \right) \right)^2 = \frac{\hbar^2}{2m} \left(\left(-\frac{\pi}{a}, -\frac{\pi}{a} \right) \right)^2 = \frac{\hbar^2}{2m} \left(\frac{\pi^2}{a^2} + \frac{\pi^2}{a^2} \right) \\ &= \frac{\hbar^2 2\pi^2}{2ma^2} \\ &= \frac{\hbar^2 \pi^2}{ma^2} \end{aligned}$$

similarly

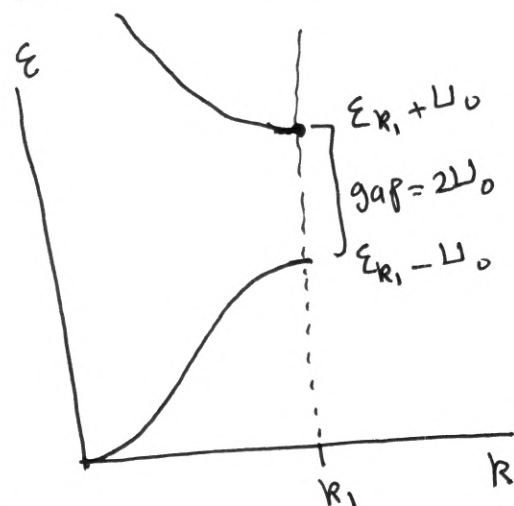
$$\begin{aligned} \epsilon_{\kappa_2} &= \frac{\hbar^2}{2m} (\kappa_2 - \kappa_2)^2 = \frac{\hbar^2}{2m} \left(\left(-\frac{\pi}{a}, -\frac{\pi}{a} \right) - \left(-\frac{2\pi}{a}, -\frac{2\pi}{a} \right) \right)^2 \\ &= \frac{\hbar^2}{2m} \left(\left(\frac{\pi}{a}, \frac{\pi}{a} \right) \right)^2 = \frac{\hbar^2}{2m} \left(\frac{\pi^2}{a^2} + \frac{\pi^2}{a^2} \right) = \frac{\hbar^2 2\pi^2}{2ma^2} = \frac{\hbar^2 \pi^2}{ma^2} \end{aligned}$$

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

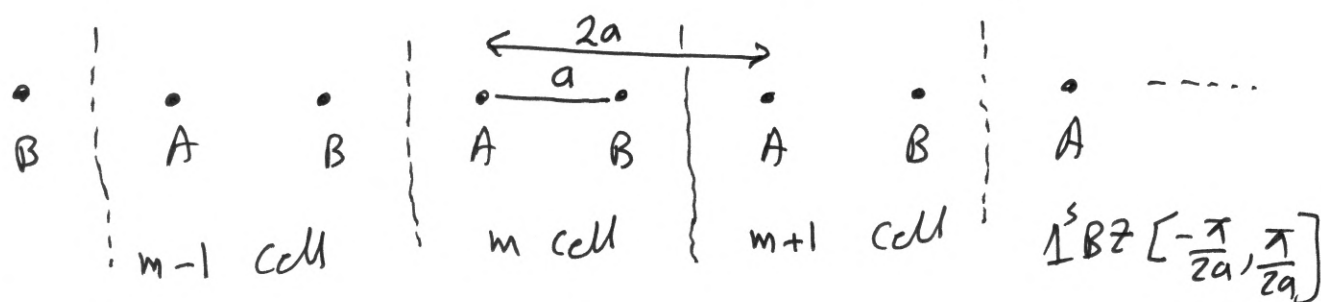
$$\begin{pmatrix} \epsilon_{\kappa_1} - \epsilon & -U_0 \\ -U_0 & \epsilon_{\kappa_1} - \epsilon \end{pmatrix} \begin{pmatrix} \psi(k - \kappa_1) \\ \psi(k - \kappa_2) \end{pmatrix} = 0$$

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

$$\begin{aligned} (\epsilon_{\kappa_1} - \epsilon)^2 - U_0^2 &= 0 \Rightarrow \epsilon_{\kappa_1} - \epsilon = \pm U_0 \\ \Rightarrow \epsilon &= \epsilon_{\kappa_1} \pm U_0 \Rightarrow \text{gap} = 2U_0 \end{aligned}$$



④ Diatomic chain $ABABAB \dots$ (Period $2a$)



Let on-site energies be ϵ_A and ϵ_B . Now I need to write the two TB equations for atoms A and B, using

$$\epsilon_0 C_n - t (C_{n-1} + C_{n+1}) = \epsilon C_n, \text{ so}$$

for atom A: $\epsilon_A C_m^A - t (C_m^B + C_{m-1}^B) = \epsilon C_m^A$, where electron on A can hop to atom B on same unit cell and/or to atom B in the previous cell ($m-1$)

for atom B: $\epsilon_B C_m^B - t (C_m^A + C_{m+1}^A) = \epsilon C_m^B$, where electron on atom B can hop to A on same unit cell and/or to A in the next cell ($m+1$)

Let $C_m^A = U_A e^{ik2ma}$ and $C_m^B = U_B e^{ik2ma}$, where the Bloch phase e^{ik2ma} connects unit cells that are spaced by $(2a)$, i.e. it does not connect atoms A-B inside unit cell that are separated by a distance a .

Now substitute C_m^A and C_m^B in the above two TB equations

$$\epsilon_A U_A e^{ik2ma} - t (U_B e^{ik2ma} + U_B e^{ik2(m-1)a}) = \epsilon U_A e^{ik2ma}, \text{ divide by } e^{ik2ma}$$

$$\epsilon_A U_A - t U_B (1 + e^{-ik2a}) = \epsilon U_A \quad \dots (1)$$

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

$$\Rightarrow \boxed{\epsilon_B u_B - t u_A (1 + e^{i2ka}) = \epsilon u_B} \quad \dots (2)$$

in matrix form

$$\begin{pmatrix} \epsilon_A & -t(1 + e^{-i2ka}) \\ -t(1 + e^{i2ka}) & \epsilon_B \end{pmatrix} \begin{pmatrix} u_A \\ u_B \end{pmatrix} = \epsilon \begin{pmatrix} u_A \\ u_B \end{pmatrix}$$

the two equations have non-trivial solution when

$$\begin{vmatrix} \epsilon_A - \epsilon & -t(1 + e^{-i2ka}) \\ -t(1 + e^{i2ka}) & \epsilon_B - \epsilon \end{vmatrix} = 0$$

$$\Rightarrow (\epsilon_A - \epsilon)(\epsilon_B - \epsilon) - t^2 (1 + e^{-i2ka})(1 + e^{i2ka}) = 0$$

$$\hookrightarrow = 1 + e^{i2ka} + e^{-i2ka} + 1 = 2 + 2\cos 2ka$$

$$\Rightarrow \epsilon_A \epsilon_B - \epsilon_A \epsilon - \epsilon_B \epsilon + \epsilon^2 - 4t^2 \cos^2 ka = 0$$

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

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

$$\Rightarrow \epsilon = \frac{(\epsilon_A + \epsilon_B) \pm \sqrt{(\epsilon_A + \epsilon_B)^2 - 4(\epsilon_A \epsilon_B - 4t^2 \cos^2 ka)}}{2}$$

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

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

$$\epsilon = \left(\frac{\epsilon_A + \epsilon_B}{2} \right) \pm \sqrt{\left(\frac{\epsilon_A - \epsilon_B}{2} \right)^2 + 4t^2 \cos^2 ka} \quad \dots (3)$$

let $\epsilon_{avg} = \frac{\epsilon_A + \epsilon_B}{2}$ and $\Delta = \frac{\epsilon_A - \epsilon_B}{2} \Rightarrow$

$$\epsilon = \epsilon_{avg} \pm \sqrt{\Delta^2 + 4t^2 \cos^2 ka} \rightarrow \text{two bands } \epsilon^+, \epsilon^-$$

$$\epsilon^+ = \epsilon_{avg} + \sqrt{\Delta^2 + 4t^2 \cos^2 ka} \quad \text{and} \quad \epsilon^- = \epsilon_{avg} - \sqrt{\Delta^2 + 4t^2 \cos^2 ka}$$

$\Rightarrow$ band gaps at $k = \pm \frac{\pi}{2a}$

$$\epsilon^+\left(\frac{\pi}{2a}\right) = \epsilon_{avg} + \Delta$$

$$\epsilon^-\left(\frac{\pi}{2a}\right) = \epsilon_{avg} - \Delta$$

$$\text{gap} = \epsilon^+ - \epsilon^- = 2\Delta = 2 \frac{\epsilon_A - \epsilon_B}{2}$$

$$= \epsilon_A - \epsilon_B$$

bandwidths can be calculated for each band separately

$$\epsilon^+ \text{ is max at } k=0 \Rightarrow \epsilon_{max}^+ = \epsilon_{avg} + \sqrt{\Delta^2 + 4t^2}$$

$$\epsilon^+ \text{ is min at } k = \frac{\pi}{2a} \Rightarrow \epsilon_{min}^+ = \epsilon_{avg} + |\Delta|$$

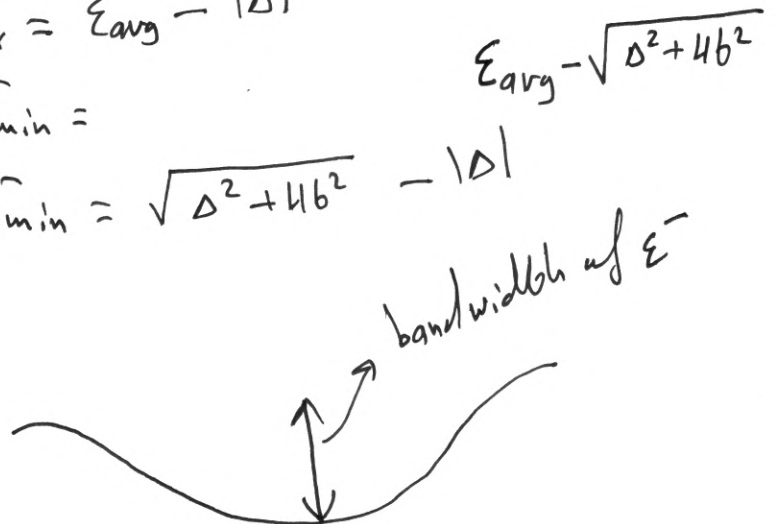
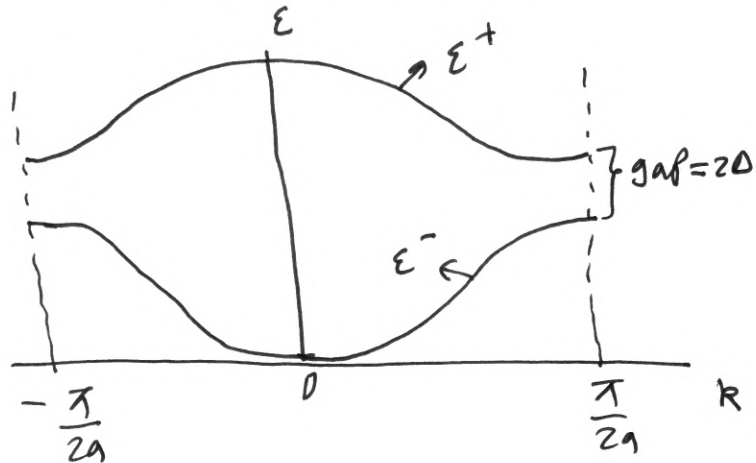
$$\Rightarrow \text{bandwidth of } \epsilon^+ = \epsilon_{max}^+ - \epsilon_{min}^+ = \sqrt{\Delta^2 + 4t^2} - |\Delta|$$

similarly for ϵ^-

$$\epsilon^- \text{ is max at } k = \frac{\pi}{2a} \Rightarrow \epsilon_{max}^- = \epsilon_{avg} - |\Delta|$$

$$\epsilon^- \text{ is min at } k=0 \Rightarrow \epsilon_{min}^- = \epsilon_{avg} - \sqrt{\Delta^2 + 4t^2}$$

$$\Rightarrow \text{bandwidth of } \epsilon^- = \epsilon_{max}^- - \epsilon_{min}^- = \sqrt{\Delta^2 + 4t^2} - |\Delta|$$

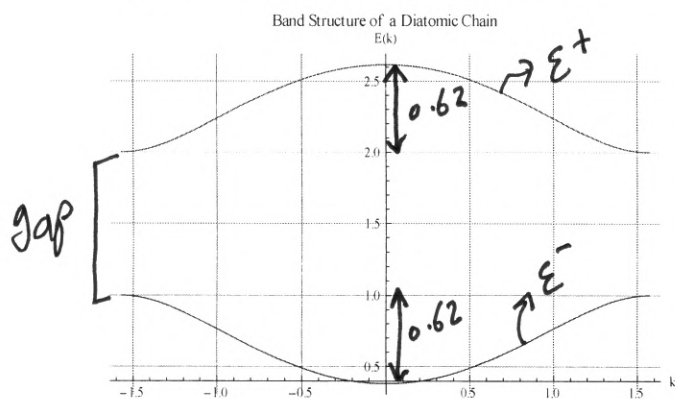


```
in[54]:= (*Clear all previous definitions*)ClearAll["Global`*"];
```

```
in[69]:= (*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*)
```

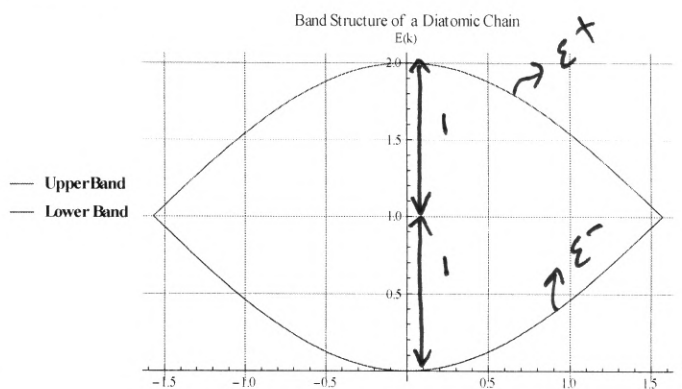
```
Plot[{Eplus[k], Eminus[k]}, {k, -Pi / (2 a), Pi / (2 a)}, PlotRange → All, AxesLabel → {"k", "E(k)"},  
PlotLegends → {"Upper Band", "Lower Band"}, PlotStyle → {Red, Blue}, GridLines → Automatic,  
PlotLabel → "Band Structure of a Diatomic Chain"]
```



$$\epsilon_A \neq \epsilon_B$$

$$\text{gap} = |\epsilon_A - \epsilon_B| = 1$$

$$\begin{aligned} \text{bandwidth of } \epsilon^+ &= \sqrt{\Delta^2 + 4b^2} - |\Delta| \\ &= \sqrt{\left(\frac{\epsilon_A - \epsilon_B}{2}\right)^2 + 4b^2} - |\Delta| \\ &= \sqrt{\left(\frac{\epsilon_A - \epsilon_B}{2}\right)^2 + 4t^2} - \frac{|\epsilon_A - \epsilon_B|}{2} \\ &= \sqrt{\frac{(1-2)^2}{4} + 4 \times \left(\frac{1}{2}\right)^2} - \frac{1}{2} \\ &= 0.62 \\ &= \text{bandwidth of } \epsilon^- \end{aligned}$$



$$\epsilon_A = \epsilon_B$$

$$\Rightarrow \Delta = 0$$

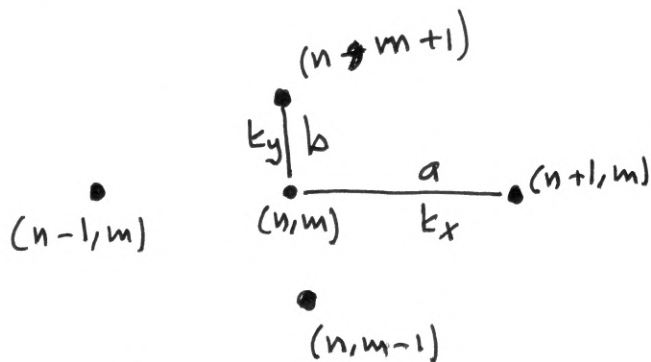
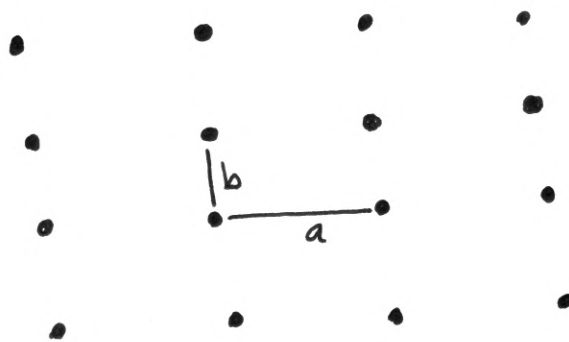
$$\begin{aligned} \text{bandwidth of } \epsilon^+ &= 2t = 2 \times \frac{1}{2} = 1 \\ \text{bandwidth of } \epsilon^- &= 2b = 2 \times \frac{1}{2} = 1 \\ \text{total bandwidth} &= 1 + 1 = 2 \end{aligned}$$

⑤

2D rectangular lattice

let on-site energy be ϵ_0 .

the tight-binding equation is



$$\epsilon_0 c(n, m) - t_x (c(n+1, m) + c(n-1, m)) - t_y (c(n, m+1) + c(n, m-1)) = \epsilon c(n, m) \quad \text{--- (1)}$$

let $c(n, m) = u e^{i k_x n a + i k_y m b}$, substitute in (1), to get

$$\begin{aligned} \epsilon_0 u e^{i k_x n a + i k_y m b} - t_x (u e^{i k_x (n+1) a + i k_y m b} + u e^{i k_x (n-1) a + i k_y m b}) \\ - t_y (u e^{i k_x n a + i k_y (m+1) b} + u e^{i k_x n a + i k_y (m-1) b}) \\ = \epsilon u e^{i k_x n a + i k_y m b} \quad \text{--- (2)} \end{aligned}$$

divide by

$$u e^{i k_x n a + i k_y m b}, \text{ to get}$$

$$\epsilon_0 - t_x \left(e^{i k_x a} + e^{-i k_x a} \right) - t_y \left(e^{i k_y b} + e^{-i k_y b} \right) = \epsilon \quad \text{--- (3)}$$

$$\epsilon_0 - 2 t_x \cos k_x a - 2 t_y \cos k_y b = \epsilon$$

$$\epsilon = \epsilon_0 - 2b_x \cos k_x a - 2b_y \cos k_y b \quad \text{--- (1) only on } \epsilon \text{ band}$$

$\epsilon^{\max}$ occurs when $\cos k_x a = \cos k_y b = -1$

$$\Rightarrow \epsilon^{\max} = \epsilon_0 + 2b_x + 2b_y = \epsilon_0 + 2(b_x + b_y) \quad , \text{ and}$$

$\epsilon^{\min}$ occurs when $\cos k_x a = \cos k_y b = 1$

$$\Rightarrow \epsilon^{\min} = \epsilon_0 - 2b_x - 2b_y = \epsilon_0 - 2(b_x + b_y)$$

$$\text{bandwidth} = \epsilon^{\max} - \epsilon^{\min} = 4(b_x + b_y) \quad \text{--- (5)}$$

now the critical point occur when $\nabla \epsilon = 0$

$$\nabla \epsilon = \left(\frac{\partial \epsilon}{\partial k_x}, \frac{\partial \epsilon}{\partial k_y} \right) = 0$$

$$\Rightarrow (2b_x a \sin k_x a, 2b_y b \sin k_y b) = 0$$

$$\Rightarrow \sin k_x a = 0 \Rightarrow k_x a = 0, \pi \Rightarrow k_x = 0, \pi/a \quad , \text{ and}$$

$$\sin k_y b = 0 \Rightarrow k_y b = 0, \pi \Rightarrow k_y = 0, \pi/b$$

$\Rightarrow$ critical points are

$$(0, 0) \quad , \quad (0, \frac{\pi}{b}) \quad , \quad (\frac{\pi}{a}, 0) \quad , \quad (\frac{\pi}{a}, \frac{\pi}{b})$$

$\downarrow$
P

$\downarrow$
X

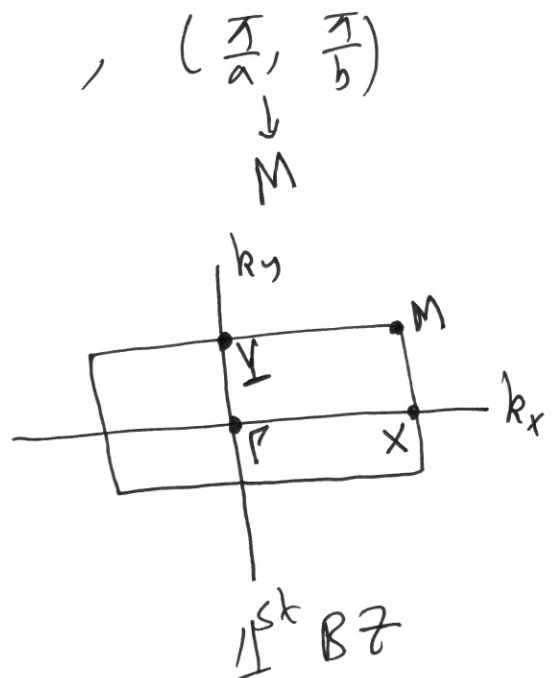
$\downarrow$
Y

$\downarrow$
M

with 1st BZ bounded by

$$k_x \left(-\frac{\pi}{a}, \frac{\pi}{a} \right)$$

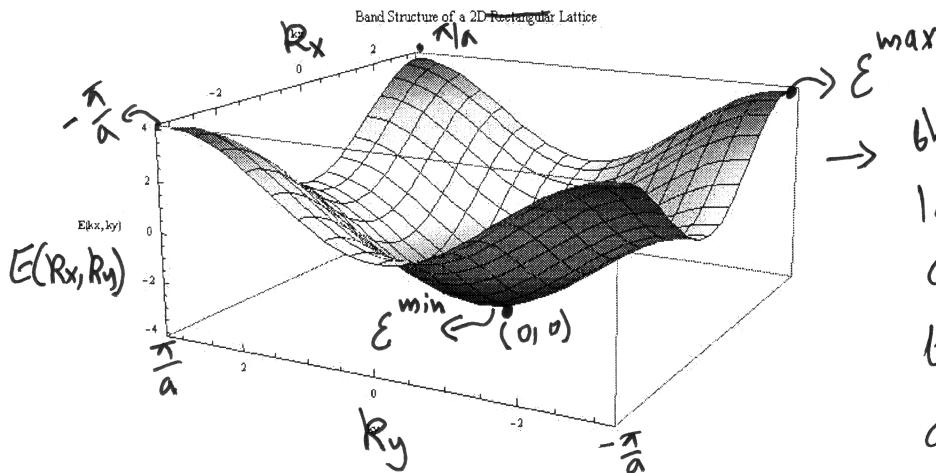
$$k_y \left(-\frac{\pi}{b}, \frac{\pi}{b} \right)$$



```
(*Parameters*) a = 1; (*Lattice constant in x-direction*) b = 1; (*Lattice constant in y-direction*)
E0 = 0; (*On-site energy*) tx = 1; (*Hopping integral in x-direction*) ty = 1; (*Hopping integral in y-direction*)
(*Energy dispersion-renamed from E to Energy*) Energy[kx_, ky_] := E0 - 2 tx Cos[kx a] - 2 ty Cos[ky b];
```

```
(*Plot*)
```

```
Plot3D[Energy[kx, ky], {kx, -Pi/a, Pi/a}, {ky, -Pi/b, Pi/b}, PlotRange -> All,
  AxesLabel -> {"kx", "ky", "E(kx, ky)"}, PlotLabel -> "Band Structure of a 2D Rectangular Lattice",
  ColorFunction -> "TemperatureMap"]
```



→ this is a square monoatomic lattice which is a special case of rectangular lattice that occurs when $a=b$ and $t_x=t_y=t$

$$\Rightarrow E(k_x, k_y) = E_0 - 2t \cos k_x a - 2t \cos k_y a$$

$$= E_0 - 2t (\cos k_x a + \cos k_y a)$$

$E^{\max}$ occurs when $\cos k_x a + \cos k_y a = -2$, which happens when $\cos k_x a = \cos k_y a = -1 \Rightarrow k_x a = \pi$ and $k_y a = \pi$

$$\Rightarrow (k_x, k_y) = (\pi/a, \pi/a)$$

$$\Rightarrow E^{\max} = E_0 + 4t$$

$E^{\min}$ occurs when $\cos k_x a + \cos k_y a = 2$, which happens when $\cos k_x a = \cos k_y a = 1 \Rightarrow k_x a = 0$ and $k_y a = 0$

$$\Rightarrow (k_x, k_y) = (0, 0)$$

$$\Rightarrow E^{\min} = E_0 - 4t$$

$$\text{bandwidth} = E^{\max} - E^{\min}$$

$$= 8t \text{ as obtained before in class}$$

critical points occur when $\vec{\nabla} \varepsilon = 0$

$$\Rightarrow \left(\frac{\partial \varepsilon}{\partial k_x}, \frac{\partial \varepsilon}{\partial k_y} \right) = 0 \Rightarrow$$

$$\frac{\partial \varepsilon}{\partial k_x} = 2ba \sin k_x a = 0 \Rightarrow k_x a = 0, \pi \Rightarrow k_x = 0, \pi/a$$

$$\frac{\partial \varepsilon}{\partial k_y} = 2ba \sin k_y a = 0 \Rightarrow k_y a = 0, \pi \Rightarrow k_y = 0, \pi/a$$

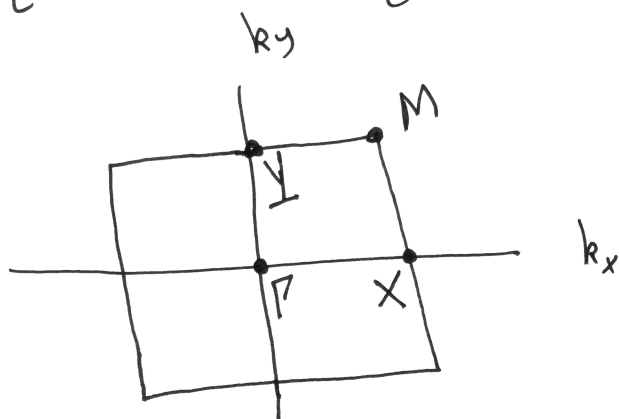
$\Rightarrow$ critical points are

$$(0, 0), \quad (\pi/a, \pi/a), \quad (\pi/a, 0), \quad (0, \pi/a)$$

Γ
 $\Downarrow$
 $\varepsilon_{\min}$

M
 $\Downarrow$
 $\varepsilon_{\max}$

X Y
└──────────────────┘
Saddle points
(Van Hove singularity)



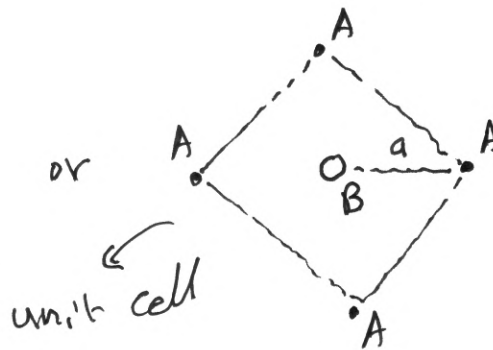
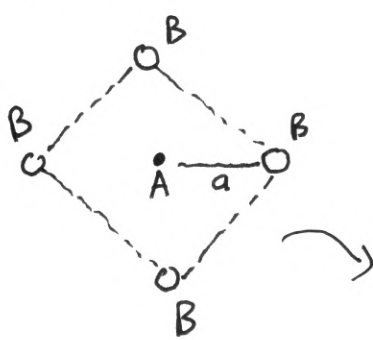
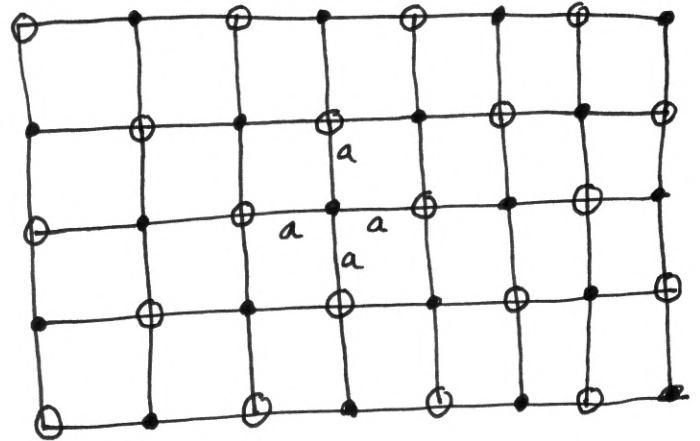
$\downarrow$
DOS diverges

⑥

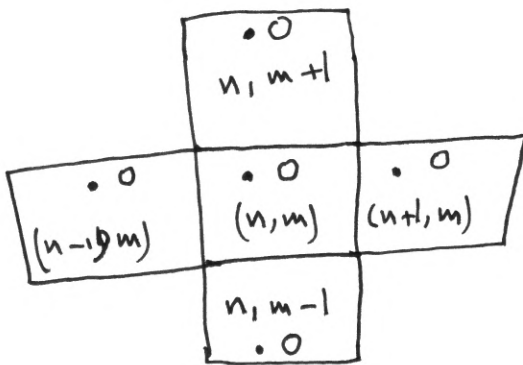
Diatomic square lattice - The lattice is a square with side length $2a$. each unit cell contains two atoms A and B as shown in figure:

• 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 $C_{(n,m)}^A = U_A e^{ik_x a n + i k_y a m}$, and
 $C_{(n,m)}^B = U_B e^{ik_x a n + i k_y a m}$
 n, m are integers

The tight-binding equations are

for atom A

$$\epsilon_A C_{(n,m)}^A - t (C_{(n+1,m)}^B + C_{(n-1,m)}^B + C_{(n,m+1)}^B + C_{(n,m-1)}^B) = \epsilon C_{(n,m)}^A$$

$$\epsilon_A U_A e^{ik_x a n + i k_y a m} - t (U_B e^{ik_x a (n+1) + i k_y a m} + U_B e^{ik_x a (n-1) + i k_y a m} + U_B e^{ik_x a n + i k_y a (m+1)} + U_B e^{ik_x a n + i k_y a (m-1)}) = \epsilon U_A e^{ik_x a n + i k_y a m}$$

divide by $e^{ik_x a n + i k_y a m}$, we get

$$\epsilon_A u_A - t u_B (e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a}) = \epsilon u_A$$

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

similarly for atom B, we have

$$\epsilon_B C^B(n, m) - t (C^A(n+1, m) + C^A(n-1, m) + C^A(n, m+1) + C^A(n, m-1)) = \epsilon C^B(n, m)$$

$$\epsilon_B u_B - t u_A (e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a}) = \epsilon u_B$$

$$\boxed{\epsilon_B u_B - t u_A (2 \cos k_x a + 2 \cos k_y a) = \epsilon u_B} \text{----- (2)}$$

in matrix form

$$\begin{pmatrix} \epsilon_A & -2t(\cos k_x a + \cos k_y a) \\ -2t(\cos k_x a + \cos k_y a) & \epsilon_B \end{pmatrix} \begin{pmatrix} u_A \\ u_B \end{pmatrix} = \epsilon \begin{pmatrix} u_A \\ u_B \end{pmatrix}$$

$$\Rightarrow \begin{vmatrix} \epsilon_A - \epsilon & -2t(\cos k_x a + \cos k_y a) \\ -2t(\cos k_x a + \cos k_y a) & \epsilon_B - \epsilon \end{vmatrix} = 0$$

$$\Rightarrow (\epsilon_A - \epsilon)(\epsilon_B - \epsilon) - 4t^2 [\cos k_x a + \cos k_y a]^2 = 0$$

$$\epsilon^2 - (\epsilon_A + \epsilon_B)\epsilon + \epsilon_A \epsilon_B - 4t^2 [\cos k_x a + \cos k_y a]^2 = 0$$

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

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

$$\text{let } \epsilon_{\text{avg}} = \frac{\epsilon_A + \epsilon_B}{2} \quad \text{and} \quad \Delta = \frac{\epsilon_A - \epsilon_B}{2} \Rightarrow$$

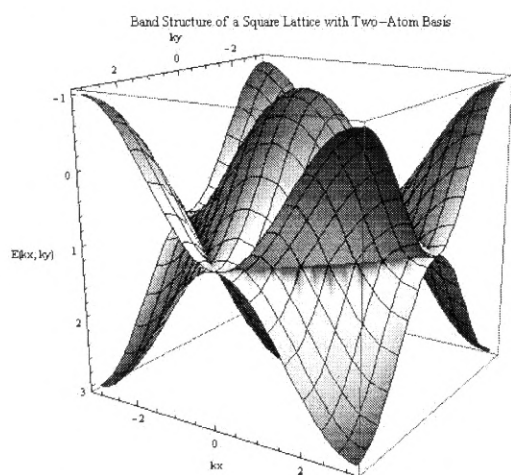
$$\epsilon = \epsilon_{\text{avg}} \pm \sqrt{\Delta^2 + 4t^2 [\cos k_x a + \cos k_y a]^2}$$

`in[92] = (*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];`

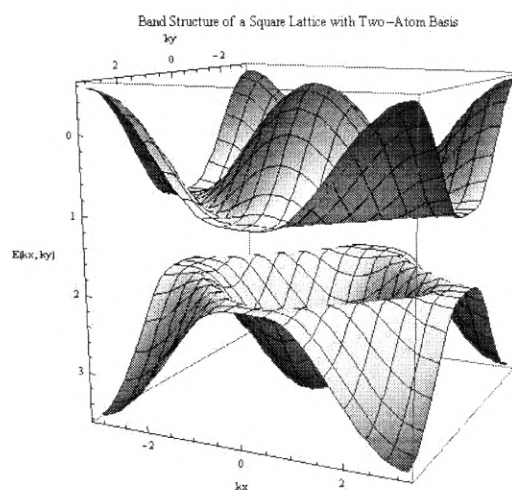
`(*3D Plot of the bands*)`

`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}]`



$\epsilon_A = \epsilon_B$
(No gap)

$\int_{BZ}$
 $k_x \in [-\frac{\pi}{a}, \frac{\pi}{a}]$
 $k_y \in [-\frac{\pi}{a}, \frac{\pi}{a}]$



$\epsilon_A \neq \epsilon_B$
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 $\cos k_x a + \cos k_y a = 0 \Rightarrow k_x = k_y = \frac{\pi}{2a}$

$$\epsilon_{\text{upper}}^{\text{min}} = \epsilon_{\text{avg}} + \frac{|\epsilon_A - \epsilon_B|}{2},$$

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

$$\epsilon_{\text{lower}}^{\text{max}} = \epsilon_{\text{avg}} - \frac{|\epsilon_A - \epsilon_B|}{2} \Rightarrow \text{gap} = \epsilon_{\text{upper}}^{\text{min}} - \epsilon_{\text{lower}}^{\text{max}} = |\epsilon_A - \epsilon_B|$$

the bandwidth can be calculated for each band separately
for upper band (ϵ^+)

$$\epsilon^+ = \epsilon_{avg} + \sqrt{\Delta^2 + 4b^2 [\cos k_x a + \cos k_y a]^2}$$

ϵ^+ max occurs when $\cos k_x a + \cos k_y a = 2$ i.e. $k_x = k_y = 0$

$$\Rightarrow \epsilon_{max}^+ = \epsilon_{avg} + \sqrt{\Delta^2 + 16t^2}$$

ϵ^+ min occurs when $\cos k_x a + \cos k_y a = 0 \Rightarrow$ i.e. $k_x = k_y = \frac{\pi}{2a}$

$$\Rightarrow \epsilon_{min}^+ = \epsilon_{avg} + |\Delta|$$

$$\Rightarrow \text{bandwidth of } \epsilon^+ = \sqrt{\Delta^2 + 16t^2} - |\Delta| \quad \leftarrow \text{Same bandwidth}$$

for lower band (ϵ^-) ; $\epsilon^- = \epsilon_{avg} - \sqrt{\Delta^2 + 4b^2 [\cos k_x a + \cos k_y a]^2}$

ϵ_{max}^- occurs when $\cos k_x a + \cos k_y a = 0 \Rightarrow k_x = k_y = \pi/2a$

$$\Rightarrow \epsilon_{max}^- = \epsilon_{avg} - |\Delta|$$

ϵ_{min}^- occurs when $\cos k_x a + \cos k_y a = 2 \Rightarrow k_x = k_y = 0$

$$\Rightarrow \epsilon_{min}^- = \epsilon_{avg} - \sqrt{\Delta^2 + 16t^2}$$

$$\Rightarrow \text{bandwidth of } \epsilon^- = \epsilon_{max}^- - \epsilon_{min}^- = \sqrt{\Delta^2 + 16t^2} - |\Delta|$$

- now when $\epsilon_A = \epsilon_B \Rightarrow \Delta = 0$ and the two bands merge with
total bandwidth $= 2(\sqrt{\Delta^2 + 16t^2} - |\Delta|)$; set $\Delta = 0$
 $= 8t$, as expected for monoatomic square lattice.

⑦ consider a diatomic chain of atoms ABABAB..... we found in problem (4) that the dispersion relation was

$$\epsilon(k) = \epsilon_{\text{avg}} \pm \sqrt{\Delta^2 + 4t^2 \cos^2 ka}, \text{ where } \epsilon_{\text{avg}} = \frac{\epsilon_A + \epsilon_B}{2}, \Delta = \frac{\epsilon_A - \epsilon_B}{2}$$

now the tight-binding density of state is given by

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

$$\frac{D(\epsilon)}{L} = \frac{2}{\pi} \frac{1}{\left| d\epsilon/dk \right|} \quad \text{density of states per unit length}$$

the $D(\epsilon)/L$ can be calculated for each band ϵ^+, ϵ^-

- for the upper band $\epsilon^+(k) = \epsilon_{\text{avg}} + \sqrt{\Delta^2 + 4t^2 \cos^2 ka}$

$$\begin{aligned} \frac{d\epsilon}{dk} &= \frac{1}{2} (\Delta^2 + 4t^2 \cos^2 ka)^{-1/2} (2 \cdot 4t^2 \cos ka (-\sin ka) \cdot a) \\ &= \frac{-4at^2 \sin ka \cos ka}{\sqrt{\Delta^2 + 4t^2 \cos^2 ka}} \end{aligned}$$

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

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

from $\epsilon = \epsilon_{avg} + \sqrt{\Delta^2 + 4t^2 \cos^2 ka} \Rightarrow \epsilon - \epsilon_{avg} = \sqrt{\Delta^2 + 4t^2 \cos^2 ka}$
 square $\Rightarrow (\epsilon - \epsilon_{avg})^2 = \Delta^2 + 4t^2 \cos^2 ka \Rightarrow \cos^2 ka = \frac{(\epsilon - \epsilon_{avg})^2 - \Delta^2}{4t^2}$
 and using $\sin^2 ka = 1 - \cos^2 ka$, we have

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

$$\begin{aligned} \frac{D(\epsilon)}{L} &= \frac{1}{2\pi ab^2} \frac{\sqrt{\Delta^2 + (\epsilon - \epsilon_{avg})^2 - \Delta^2}}{\sqrt{1 - \frac{(\epsilon - \epsilon_{avg})^2 - \Delta^2}{4b^2}} \sqrt{\frac{(\epsilon - \epsilon_{avg})^2 - \Delta^2}{4b^2}}} \\ &= \frac{2}{\pi a} \frac{(\epsilon - \epsilon_{avg})}{\sqrt{4t^2 - ((\epsilon - \epsilon_{avg})^2 - \Delta^2)} \sqrt{(\epsilon - \epsilon_{avg})^2 - \Delta^2}} \quad \dots (2) \end{aligned}$$

now let us find the energy range of this upper band

$$\epsilon^+ = \epsilon_{avg} + \sqrt{\Delta^2 + 4b^2 \cos^2 ka}$$

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

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

$$\Rightarrow \epsilon_{min}^+ = \epsilon_{avg} + \sqrt{\Delta^2} = \epsilon_{avg} + |\Delta|$$

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 $k = 0, \pm \frac{\pi}{a}$

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

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

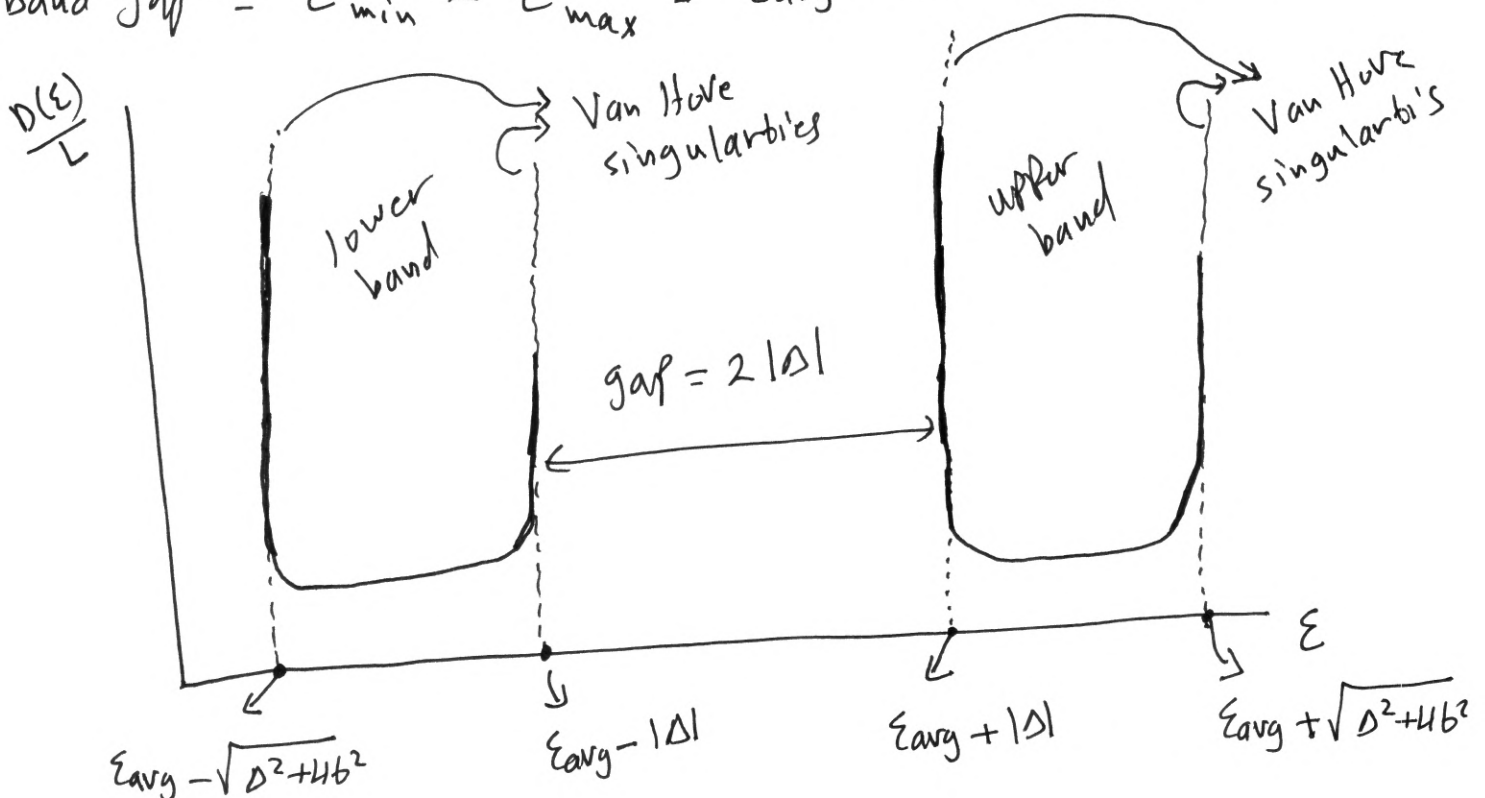
$$\mathcal{E}_{\text{avg}} + |\Delta| \leq \mathcal{E}^+ \leq \mathcal{E}_{\text{avg}} + \sqrt{\Delta^2 + 4b^2}$$

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

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

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

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



```

(*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];

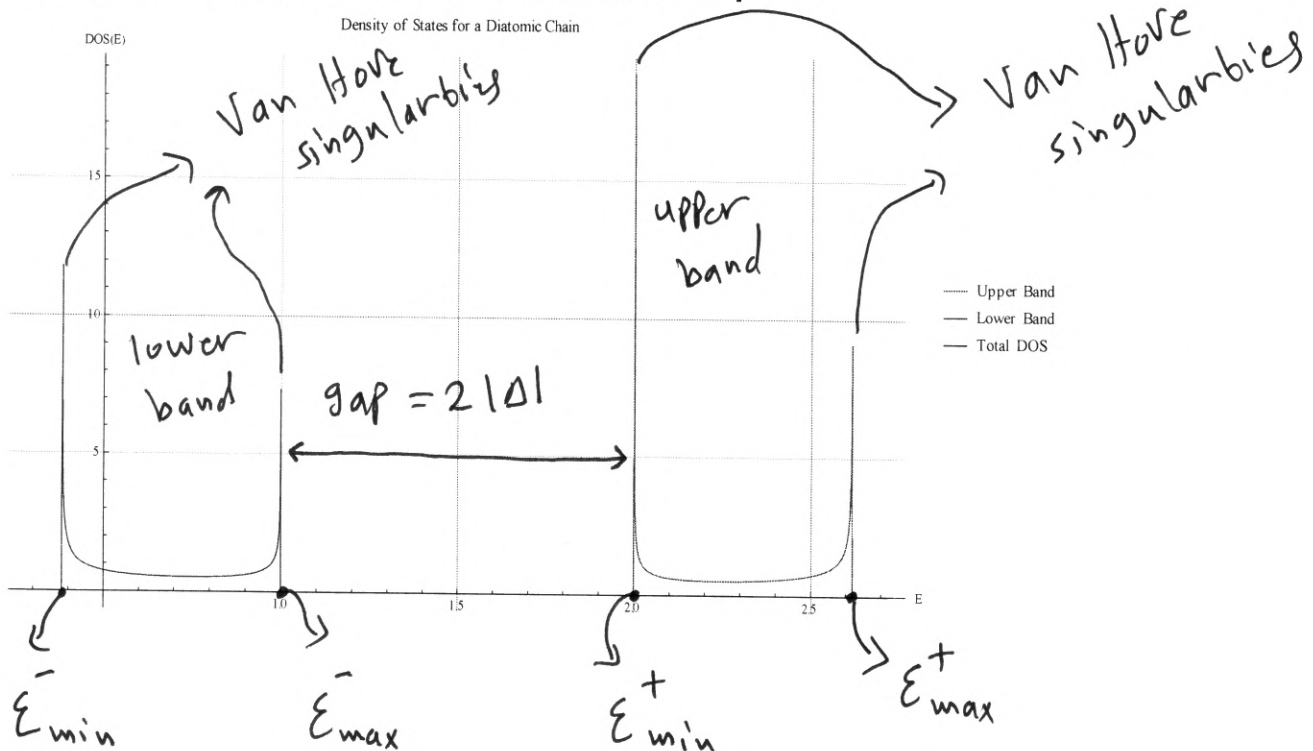
(*DOS for Upper Band*)
DOSUpper[E_?NumericQ] :=
  Piecewise[{{1 / (Pi a) * (E - avg) / (Sqrt[(E - avg)^2 - delta^2] * Sqrt[4 t^2 + delta^2 - (E - avg)^2]),
    upperBandMin <= E <= upperBandMax}}, 0];

(*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 $\epsilon_A = \epsilon_B \Rightarrow \epsilon_{avg} = \frac{\epsilon_A + \epsilon_B}{2} = \epsilon_A = \epsilon_B$, and
 $\Delta = \frac{\epsilon_A - \epsilon_B}{2} = \text{zero} \Rightarrow$ no band gap, so for the

upper band, we have

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

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

similarly for the lower band

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

$$= \frac{2}{\pi a} \frac{(\cancel{\epsilon_A} - \epsilon)}{(\cancel{\epsilon_A} - \epsilon) \sqrt{4b^2 - (\epsilon_A - \epsilon)^2}} = \frac{2}{\pi a} \frac{1}{\sqrt{4b^2 - (\epsilon_A - \epsilon)^2}}$$

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

```

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

(*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];

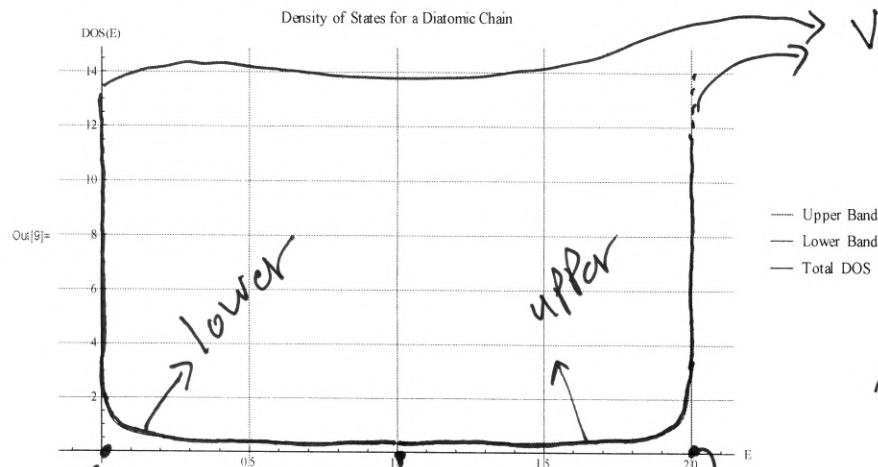
(*DOS for Upper Band*)
DOSUpper[E_?NumericQ] :=
  Piecewise[{{1 / (Pi a) * (E - avg) / (Sqrt[(E - avg)^2 - delta^2] * Sqrt[4 t^2 + delta^2 - (E - avg)^2]),
    upperBandMin ≤ E ≤ upperBandMax}}, 0];

(*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"]

```



Van Hove singularities

No gap

$$E = \epsilon_A - 2t$$

$$\epsilon_A = \epsilon_B$$

$$E = \epsilon_A + 2t$$