BULK IMPURITY

$$-\lambda C_n + \epsilon \delta_{n0} C_n + V(C_{n+1} + C_{n-1}) = 0$$

$n=0$: $\quad (-\lambda + \epsilon) C_0 + V(C_1 + C_{-1}) = 0$

$n=1$: $\quad -\lambda C_1 + V(C_2 + C_0) = 0$

$$C_n = A X^{|n|} \Rightarrow -\lambda \cancel{A} X + V \cancel{A}(X^2 + 1) = 0$$

$$\Rightarrow \lambda = V\left(X + \frac{1}{X}\right) \qquad (*)$$

$n=0$: $\quad -\lambda + \epsilon + V(X + X) = 0$

$$-V\left(X + \frac{1}{X}\right) + \epsilon + V(2X) = 0$$

$$-\underbrace{VX} - \frac{V}{X} + \epsilon + \underbrace{2VX} = 0 \Rightarrow VX - \frac{V}{X} + \epsilon = 0$$

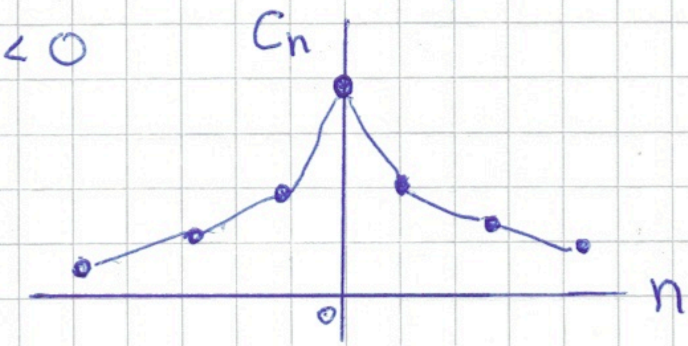
$$X - \frac{1}{X} + \frac{\epsilon}{V} = 0 \quad / \cdot X$$

$$X^2 + \left(\frac{\epsilon}{V}\right) X - 1 = 0$$

$$\Rightarrow X = \frac{-(\epsilon/V) \pm \sqrt{(\epsilon/V)^2 + 4}}{2} = -(\epsilon/2V) \pm \sqrt{(\epsilon/2V)^2 + 1}$$

$$X = \begin{cases} -\left(\frac{\epsilon}{2V}\right) + \sqrt{\left(\frac{\epsilon}{2V}\right)^2 + 1} & \epsilon > 0 \\ -\frac{\epsilon}{2V} - \sqrt{\left(\frac{\epsilon}{2V}\right)^2 + 1} & \epsilon < 0 \end{cases}$$

se cumple $|X| < 1$



Falta normalizar.

$$1 = \sum_{-\infty}^{\infty} |C_n|^2 \rightarrow \text{det. } A$$

$$\frac{\lambda}{V} = \underbrace{x + \frac{1}{x}}_{\frac{x^2+1}{x}} = -\delta + \sqrt{\delta^2+1} + \frac{1}{-\delta+\sqrt{\delta^2+1}}$$

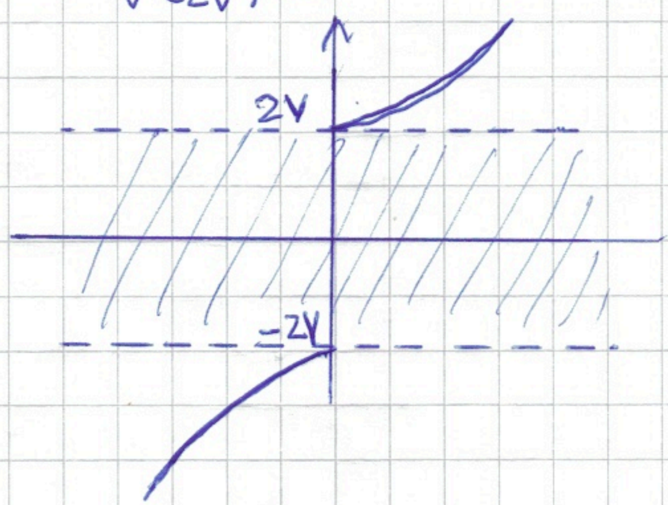
$$\frac{x^2+1}{x} = \frac{\left(-\delta+\sqrt{\delta^2+1}\right)^2+1}{-\delta+\sqrt{\delta^2+1}}$$

$$\frac{\delta^2+\delta^2+1-2\delta\sqrt{\delta^2+1}+1}{-\delta+\sqrt{\delta^2+1}} = \frac{2\delta^2+2-2\delta\sqrt{\delta^2+1}}{-\delta+\sqrt{\delta^2+1}}$$

$$\frac{2(\delta^2+1)-2\delta\sqrt{\delta^2+1}}{-\delta+\sqrt{\delta^2+1}} = \frac{2\sqrt{\delta^2+1}\,\cancel{\left(-\delta+\sqrt{\delta^2+1}\right)}}{\cancel{-\delta+\sqrt{\delta^2+1}}} = 2\sqrt{\delta^2+1}$$

i.e., $\lambda = 2V\sqrt{\left(\frac{\epsilon}{2V}\right)^2+1}$ $\quad(\epsilon>0)$

and $\lambda = -2V\sqrt{\left(\frac{\epsilon}{2V}\right)+1}$ $\quad(\epsilon<0)$



SURFACE IMPURITY

$$X - o - o - o - o - o - \cdots$$

$$0 \quad 1 \quad 2 \quad 3 \quad 4 \ldots$$

$$-\lambda C_0 + \epsilon C_0 + V C_1 = 0 \qquad (1)$$

$$-\lambda C_n + V(C_{n+1} + C_{n-1}) \qquad (2)$$

$\frac{V}{\epsilon} < 1$

$\epsilon > V$

$$\boxed{C_n = A X^n}$$

$\frac{1-x^2+2}{1-x^2}$

$$\Rightarrow (-\lambda + \epsilon)\cancel{A} + V\cancel{A}X = 0 \Rightarrow -\lambda + \epsilon + VX = 0 \Rightarrow \boxed{\lambda = \epsilon + VX}$$

$$(2): \; -\lambda \cancel{A} X^n + V(\cancel{A}X^{n+1} + \cancel{A}X^{n-1}) \Rightarrow -\lambda X^n + VX^{n+1} + VX^{n-1}$$

$$\Rightarrow \boxed{\lambda = VX + \frac{V}{X}}$$

$$\Rightarrow \epsilon + \cancel{VX} = \cancel{VX} + \frac{V}{X} \Rightarrow \boxed{X = \frac{V}{\epsilon}} \Rightarrow \boxed{\epsilon > V}$$

$$\Rightarrow \lambda = \epsilon + \frac{V^2}{\epsilon} \Rightarrow \boxed{\frac{\lambda}{V} = \frac{\epsilon}{V} + \frac{V}{\epsilon}}$$

$$1 = \sum_n |C_n|^2 = A^2 \sum_n X^{2n} = A^2 + 2A^2 \sum_1^{\infty} (X^2)^n = A^2 + \frac{2A^2}{1-X^2} = A^2\left(1 + \frac{2}{1-X^2}\right)$$

No

$$= A^2\left(\frac{1-X^2+2X^2}{1-X^2}\right) = A^2\left(\frac{1+X^2}{1-X^2}\right) \Rightarrow A^2 = \left(\frac{1+X^2}{1-X^2}\right) \Rightarrow A = \left(\frac{1-X^2}{1+X^2}\right)^{1/2}$$

$$\Rightarrow \boxed{C_n = \left(\frac{1-X^2}{1+X^2}\right)^{1/2} X^n} = \left(\frac{1-(V/\epsilon)^2}{1+(V/\epsilon)^2}\right)^{1/2} \left(\frac{V}{\epsilon}\right)^n \; //$$

DENSIDAD DE ESTADOS

$$\Omega(E) = \frac{1}{N}\sum_{k} \delta(E-E_k) \rightarrow \frac{1}{2\pi}\int_{-\pi}^{\pi} \delta(E-E_k)\,dk$$

$$E_k = 2V\cos(k)$$

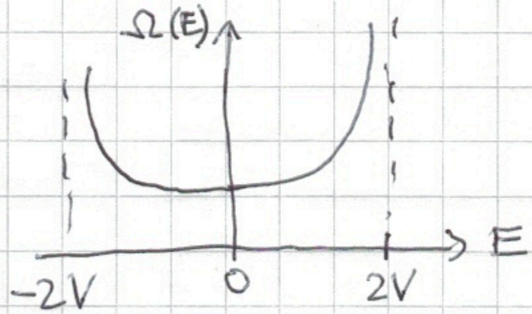
$$\delta(\underbrace{E-E_k}_{f}) = \frac{\delta(k-k^*)}{|f'(k^*)|}$$

$$f(k^*) = 0 = E - E_k = E - 2V\cos(k)$$

$$\Rightarrow k^* = \cos^{-1}(E/2V)$$

$$\Rightarrow f'(k^*) = -2V\sin(k^*) = -2V\sin(\cos^{-1}(E/2V)) = -2V\sqrt{1-(E/2V)^2}$$

$$\therefore \Omega(E) = \frac{(1/2\pi V)}{\sqrt{1-\left(\frac{E}{2V}\right)^2}}$$



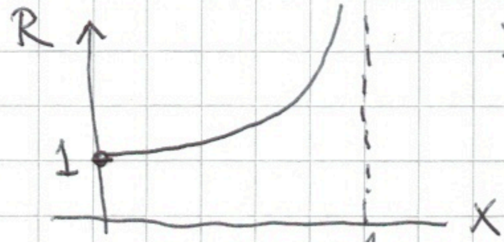
RAZÓN DE PARTICIPACIÓN

$$R \equiv \frac{\left(\sum_n |C_n|^2\right)^2}{\sum_n |C_n|^4}$$

$$C_n = A x^n$$

$$R = \frac{\left(\sum_n \cancel{A^2} x^{2n}\right)^2}{\sum_n \cancel{A^4} x^{4n}} = \frac{\left(\sum_{-\infty}^{\infty} x^{2n}\right)^2}{\sum_{-\infty}^{\infty} x^{4n}} = \frac{\left(1+2\sum_{1}^{\infty} x^{2n}\right)^2}{1+2\sum_{1}^{\infty} x^{4n}} = \frac{\left(1+\frac{2x^2}{1-x^2}\right)^2}{1+\frac{2x^4}{1-x^4}}$$

$$= \frac{\left(\frac{1+x^2}{1-x^2}\right)^2}{\frac{1+x^4}{1-x^4}} = \frac{(1+x^2)^2(1+x^2)}{(1-x^2)(1+x^4)}$$



$$x \equiv V/\epsilon$$

TRANSMISSION COEFFICIENT

$$-\lambda C_n + \epsilon C_n \delta_{n0} + V(C_{n+1} + C_{n-1}) = 0$$

$\underline{n=0}$ $\quad -\lambda C_0 + \epsilon C_0 + V(C_1 + C_{-1}) = 0$

$$C_n = \begin{cases} I e^{ikn} + R e^{-ikn} & n<0 \\ T e^{ikn} & n \geq 0 \end{cases}$$

$$(-\lambda + \epsilon)T + V(Te^{ik} + Ie^{-ik} + Re^{ik}) = 0 \qquad (1)$$

$\underline{n=1}$ $\quad -\lambda C_1 + V(C_2 + C_0) = 0$

$$-\lambda T e^{ik} + VTe^{2ik} + VT = 0 \Rightarrow \boxed{\lambda = 2V\cos(k)} \qquad (2)$$

$\underline{n=-1}$ $\quad -\lambda C_{-1} + V(C_0 + C_{-2}) = 0$

$$-(2V\cos k)(Ie^{-ik} + Re^{ik}) + V(T + Ie^{-2ik} + Re^{2ik}) = 0$$

$$\Rightarrow \boxed{T - I - R = 0} \qquad (3)$$

$$\overset{(1)}{\Rightarrow} \quad T = \frac{2iIV\sin(k)}{\epsilon + 2iV\sin(k)} \Rightarrow t = \left|\frac{T}{I}\right|^2 = \frac{\sin^2(k)}{\left(\frac{\epsilon}{2V}\right)^2 + \sin^2(k)}$$

Red binaria

$$i\dot{C}_n^1 + G\, C_n^2 + K\, C_{n-1}^2 = 0$$

$$i\dot{C}_n^2 + G\, C_n^1 + K\, C_{n+1}^1 = 0$$

$$\left.\begin{array}{l} C_n^1 = \epsilon_1\, e^{i(kn-\omega t)} \\ C_n^2 = \epsilon_2\, e^{i(kn-\omega t)} \end{array}\right\} \begin{array}{l} \omega\epsilon_1 + G\,\epsilon_2 + K\epsilon_2\, e^{-ik} = 0 \\ \omega\,\epsilon_2 + G\epsilon_1 + K\,\epsilon_1 e^{ik} = 0 \end{array}$$

$$\Rightarrow \cancel{\omega C_n^1 + G C_n^2 + K C_{n-1}^2}$$

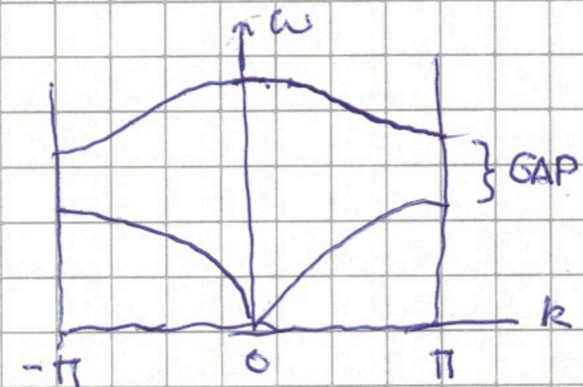
$$\Rightarrow \quad \omega\epsilon_1 + (G + Ke^{-ik})\,\epsilon_2 = 0$$

$$(G + Ke^{ik})\,\epsilon_1 + \omega\,\epsilon_2 = 0$$

$$\Rightarrow \quad 0 = \begin{vmatrix} \omega & G+Ke^{-ik} \\ G+Ke^{ik} & \omega \end{vmatrix} = \omega^2 - |G + Ke^{ik}|^2$$

$$= G^2 + K^2 + 2GK\cos(k)$$

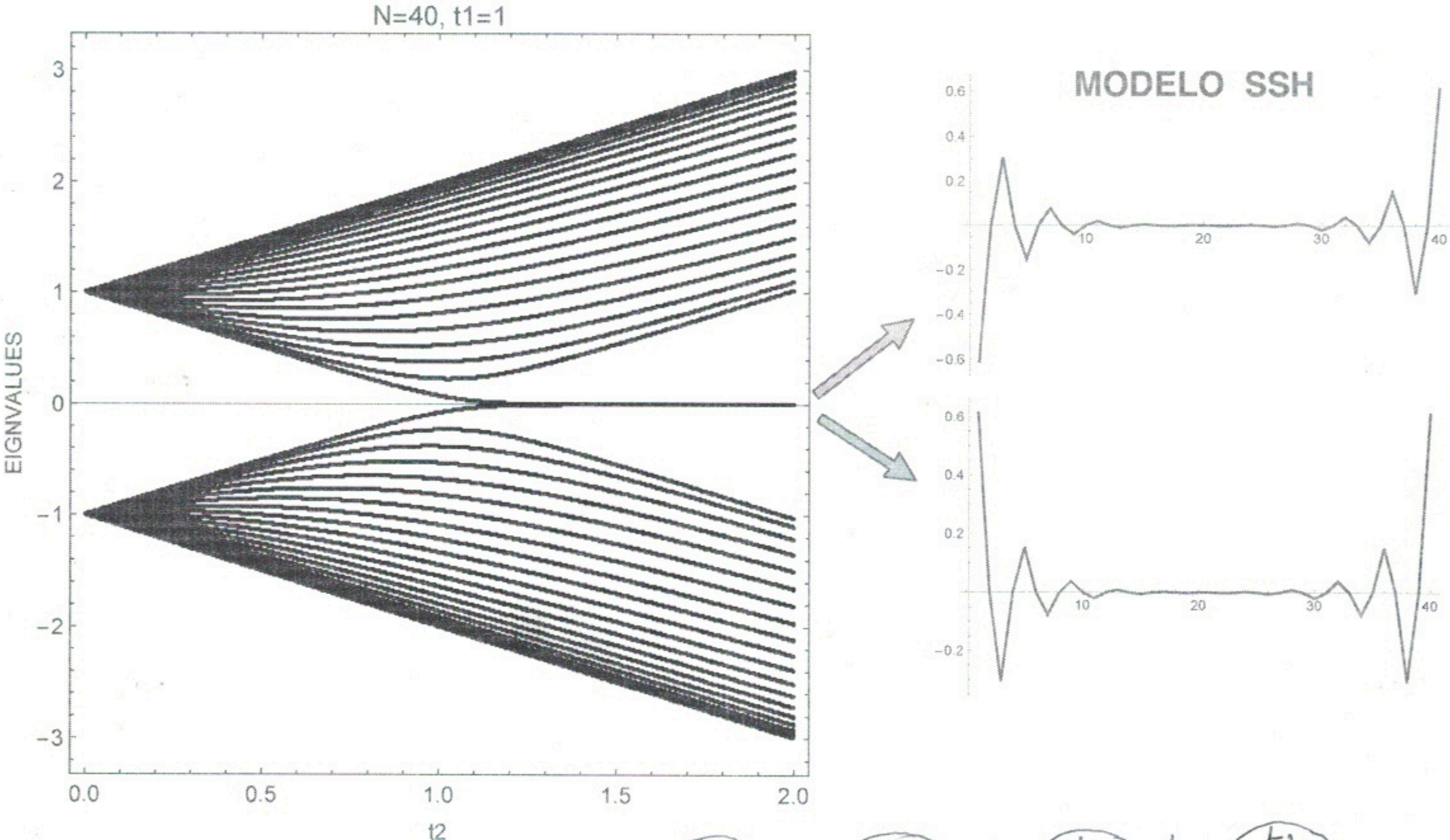
$$\omega = (G^2 + K^2 + 2GK\cos(k))^{1/2}$$

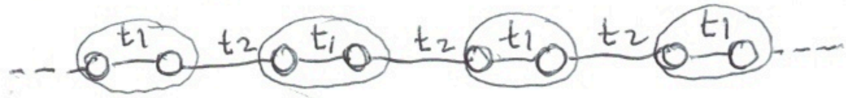


$$-\lambda C_n + V_{n,n+1} C_{n+1} + V_{n,n-1} C_{n-1} = 0$$

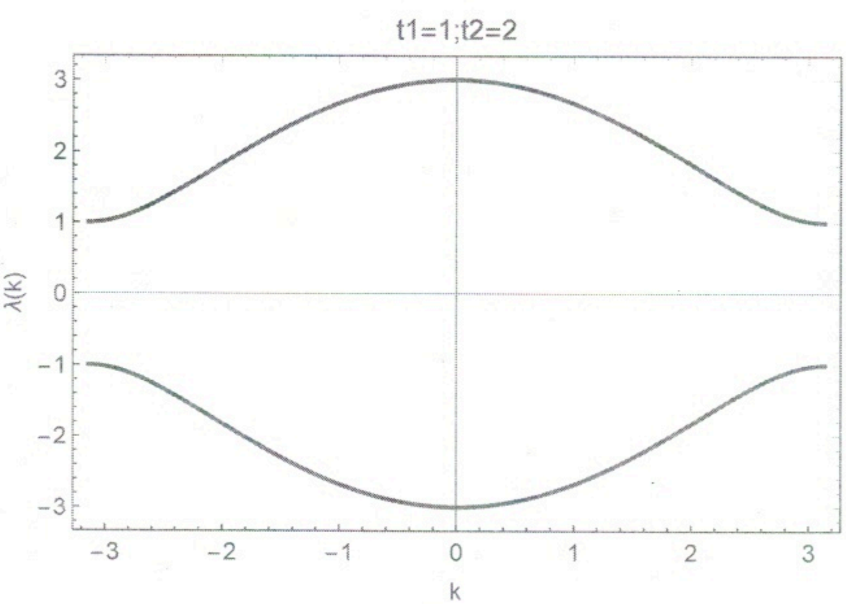
$$V_{n,n+1} = t_1 \text{ for } n \text{ odd}$$

$$V_{n,n+1} = t_2 \text{ for } n \text{ even}$$

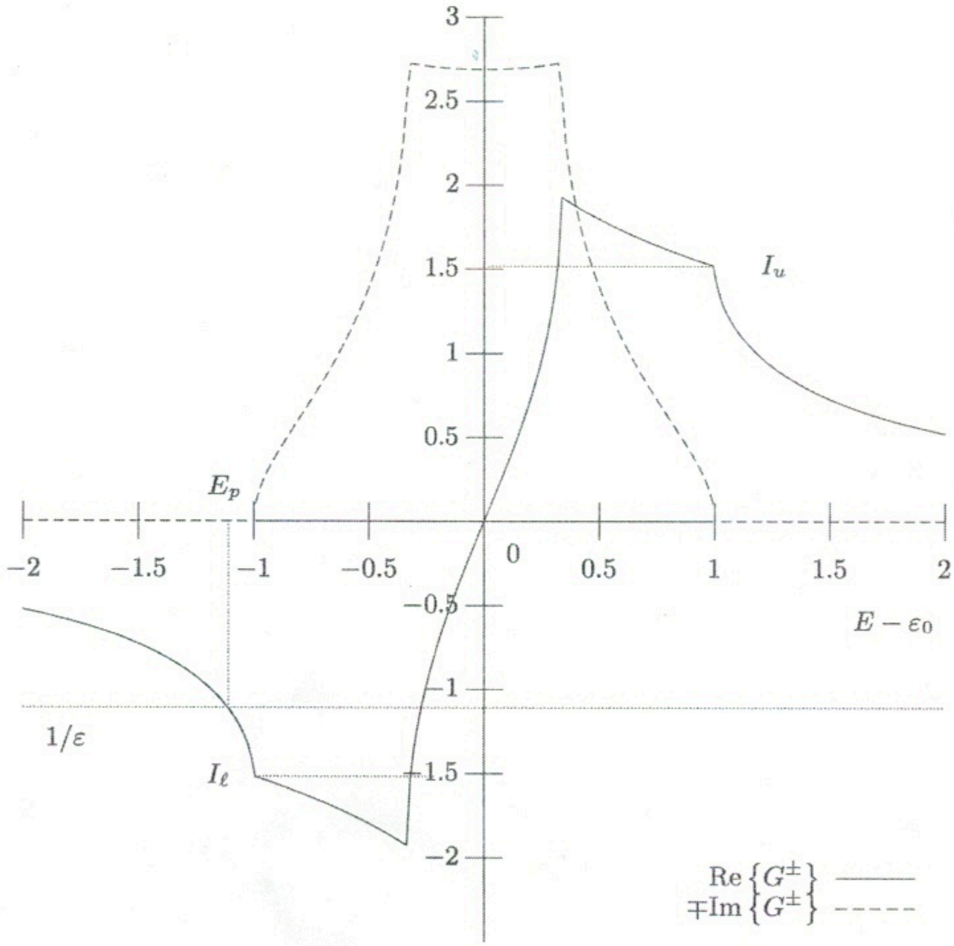




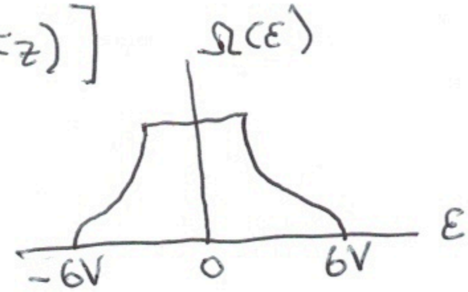
$$\lambda(k) = \pm(t_1^2 + t_2^2 + 2t_1 t_2 \cos(k))^{1/2}$$



3D CUBIC LATTICE



$$\varepsilon(\vec{K}) = 2V\left[\cos(K_x) + \cos(K_y) + \cos(K_z)\right]$$



$$\Omega(E) = \frac{1}{(2\pi)^3}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \delta(E-\varepsilon(\vec{K}))\, d^3K$$

Numérico.

$$\Omega(E) = \frac{1}{\sqrt{2\pi\sigma^2}}\int_{PZB} e^{-\frac{(E-\varepsilon(\vec{K}))^2}{2\sigma^2}}\, d^3K$$

otro numérico.. $\Omega(\varepsilon) = \frac{1}{N}\sum_{n}^{N}\frac{1}{\sqrt{2\pi\sigma^2}}\, e^{-\frac{(\varepsilon-\varepsilon_n)^2}{2\sigma^2}}$