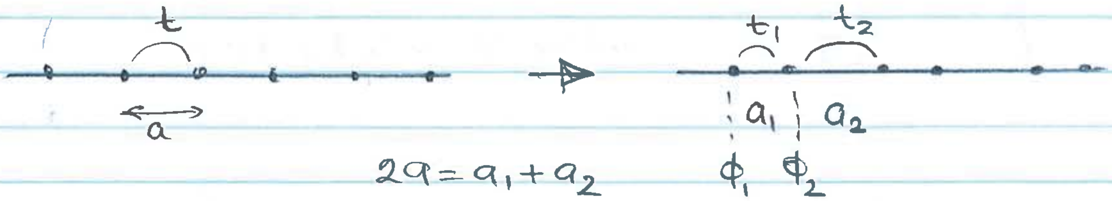
Peierl's transition : dimerization of a 1-D chain
metal - to - insulator transition



$$2a = a_1 + a_2$$

$$\langle \phi_1(r) | H | \phi_1(r) \rangle = E_0 \qquad \langle \phi_1(r) | H | \phi_1(r-a_1-a_2) \rangle = 0$$

$$\langle \phi_2(r-a_1) | H | \phi_2(r-a_1) \rangle = E_0 \qquad \langle \phi_2(r-a_1) | H | \phi_2(r+a_2) \rangle = 0$$

$$\langle \phi_1(r) | H | \phi_2(r-a_1) \rangle = t_1$$

$$\langle \phi_1(r) | H | \phi_2(r+a_2) \rangle = t_2 \qquad t \equiv \frac{t_1+t_2}{2} \; ; \; \Delta t = t_2 - t_1 \rightarrow \begin{array}{l} t_1 = t + \frac{1}{2}\Delta t \\ t_2 = t - \frac{1}{2}\Delta t \end{array}$$

$$\psi_1^k(r) = \frac{1}{\sqrt{N}} \sum_{R_1} e^{ikR_1} \phi_1(r-R_1)$$

$$\psi_2^k(r) = \frac{1}{\sqrt{N}} \sum_{R_2} e^{ikR_2} \phi_2(r-R_2)$$

$$\langle \psi_1^k(r) | H | \psi_1^k(r) \rangle = E_0$$

$$\langle \psi_2^k(r) | H | \psi_2^k(r) \rangle = E_0$$

$$\langle \psi_1^k(r) | H | \psi_2^k(r) \rangle = \sum_R e^{ikR} \langle \phi_1(R) | H | \phi_2(r-R) \rangle$$

$$= (R=a_1)\; e^{ika_1} \cdot t_1 + (R=-a_2)\; e^{-ika_2} \cdot t_2$$

$$a_1 \approx a_2 = a \qquad \approx t_1 e^{ika} + t_2 e^{-ika}$$

$$= t(e^{ika} + e^{-ika}) + \tfrac{1}{2}\Delta t\,(e^{ika} - e^{-ika})$$

$$= 2t\cos(ka) + i\Delta t \sin(ka).$$

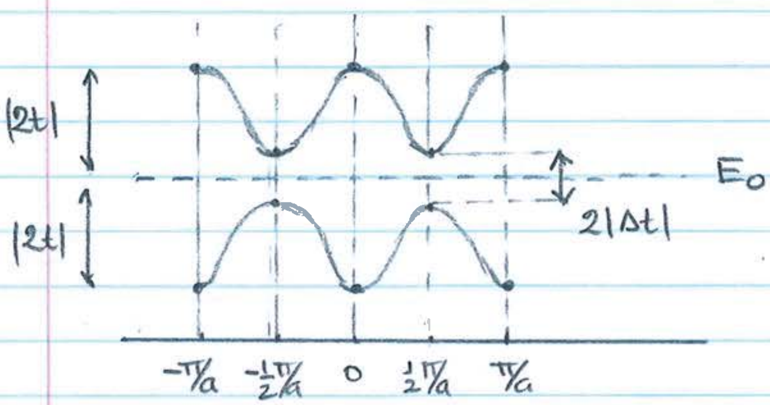
$$\langle \psi_2^k(r) | H | \psi_1^k(r) \rangle = 2t\cos(ka) - i\Delta t \sin(ka)$$

$$H_{\varphi_1^k,\varphi_2^k} = \begin{bmatrix} E_0 & 2t\cos(ka) + i\Delta t\sin(ka) \\ 2t\cos(ka) - i\Delta t\sin(ka) & E_0 \end{bmatrix}$$

$$k=0: \quad H = \begin{bmatrix} E_0 & 2t \\ 2t & E_0 \end{bmatrix} \longrightarrow E_\pm = E_0 \pm |2t|$$

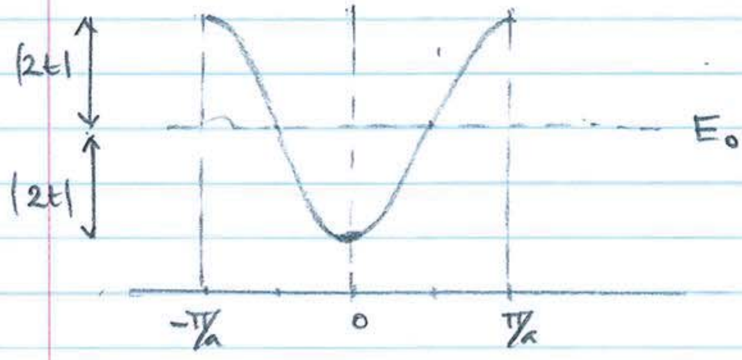
$$k=\frac{\pi}{a}: \quad H = \begin{bmatrix} E_0 & -2t \\ -2t & E_0 \end{bmatrix} \longrightarrow E_\pm = E_0 \pm |2t|$$

$$k=\frac{\pi}{2a}: \quad H = \begin{bmatrix} E_0 & i\Delta t \\ -i\Delta t & E_0 \end{bmatrix} \longrightarrow E_\pm = E_0 \pm |\Delta t|$$



Insulator for half-filling

Intensity of "fold-back" bands is proportional to $|\Delta t|$.



Metal for half-filling