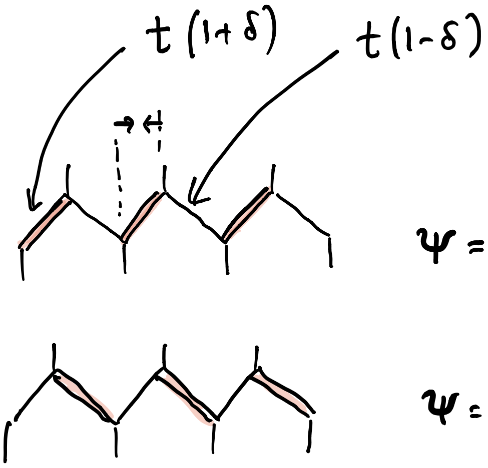
Solitons in Polyacetylene $(CH)_x$

Su, Schrieffer, Heeger, Phys Rev B, 22, 2099 (1980).

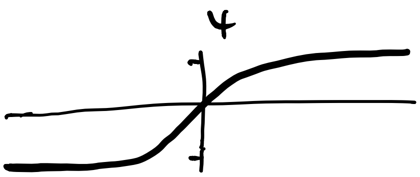
Wu Pei Su Bob Schrieffer Alan Heeger



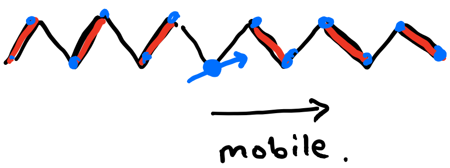
$\psi = -\delta$

$\psi = +\delta$

BROKEN Z_2 SYMMETRY



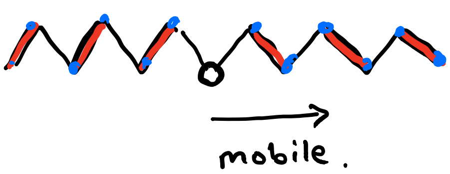
"Soliton"



$q = 0$ $s = 1/2$

Neutral, spin-1/2

"Spinon"



$q_\pm = \pm e$ $s_\pm = 0$

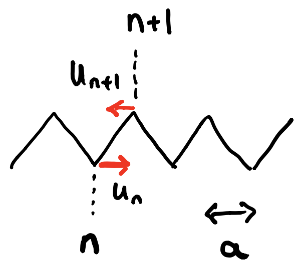
Charged, spinless

"Holon"

The presence of these defects had been infered from NMR measurements

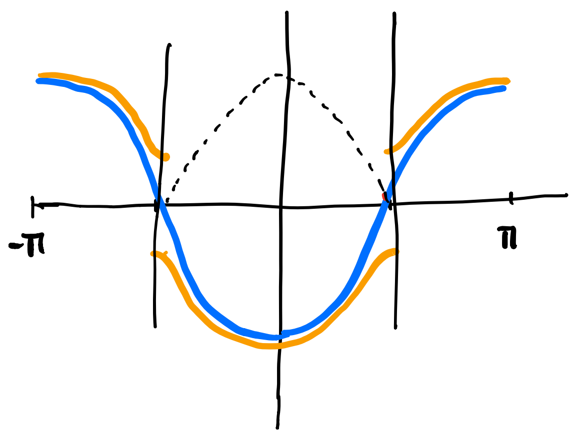
$$\boxed{\begin{aligned} H &= -\sum_n t_{n+1,n}\left(c^{\dagger}_{n+1\sigma} c_{n\sigma} + H.c\right) + \frac{1}{2}K\sum_n \left(u_{n+1}-u_n\right)^2 + \frac{1}{2}\sum_n \frac{p_n^2}{2M} \\ t_{n+1,n} &= t - \alpha\left(u_{n+1}-u_n\right) \qquad [p_n, u_{n'}] = -i\hbar\,\delta_{nn'} \end{aligned}}$$

SSH Model.



Shortening of the bond increases hoping.

We will take $a=1$ initially.



$u_n = (-1)^n u$

STATIC

(BORN-OPPENHEIMER)

Peierl's instability for arbitrarily small coupling α.

$$(u_{n+1}-u_n) = -(-1)^n 2u \Rightarrow t_{n+1,n} = t + (-1)^n 2\alpha u$$

$$\boxed{H^d(u) = -\sum_n \left(t + (-1)^n 2\alpha u\right)\left(c^{\dagger}_{n+1\sigma}c_{n\sigma} + H.c\right) + 2NKu^2}$$

$$c_n = \frac{1}{\sqrt{N}} \sum_{k\in[0,2\pi]} c_k\, e^{ikR_n}$$ Transform to momentum space. $R_n = na \equiv n$.

$$H^d[u] = \sum_{k\in[0,\pi]} \left(c^\dagger_{k+\pi\sigma}, c^\dagger_{k\sigma}\right) \overbrace{\begin{pmatrix} \epsilon_k & -i\Delta_k \\ i\Delta_k & -\epsilon_k \end{pmatrix}}^{\epsilon_k\tau_3 + \Delta_k\tau_2} \begin{pmatrix} c_{k+\pi\sigma} \\ c_{k\sigma} \end{pmatrix} + Nku^2$$

conduction

valence.

$$\boxed{\begin{aligned} \epsilon_k &= 2t\cos k \\ \Delta_k &= 4\alpha u \sin k \end{aligned}}$$

(c.f BCS theory)

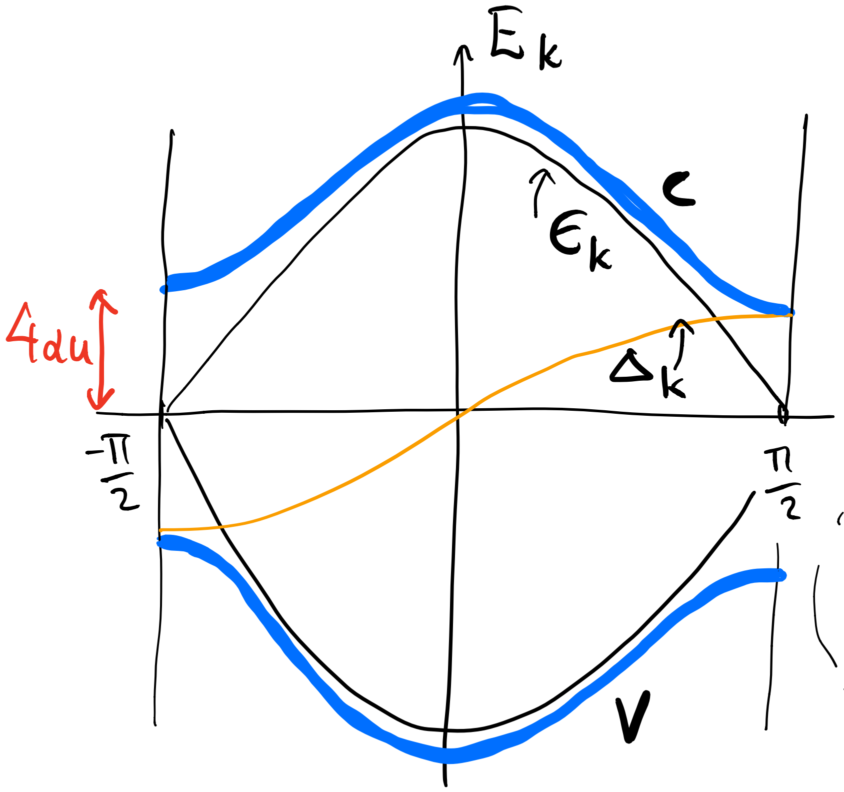
$$\Psi_{k\sigma} = \begin{pmatrix} c_{k+\pi\sigma} \\ c_{k\sigma} \end{pmatrix} = \begin{pmatrix} c^c_{k\sigma} \\ c^v_{k\sigma} \end{pmatrix}$$

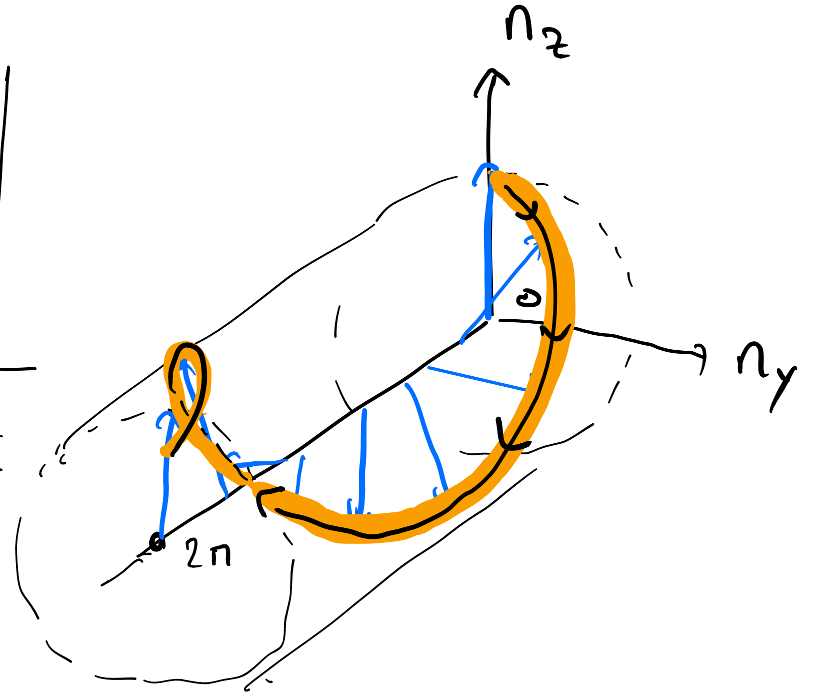
$$H^d[u] = \sum_{k\in[0,\pi]} \Psi^\dagger_k \underline{\mathcal{H}}_k \Psi_k + 2Nku^2$$

$$\mathcal{H}_k = \epsilon_k \tau_3 + \Delta_k \tau_2 \equiv \sqrt{\epsilon_k^2 + \Delta_k^2}\, \underbrace{(\hat{n}_k \cdot \vec{\tau})}_{\pm 1}$$

$$\left(\hat{n}_k = \left(0, \frac{\Delta_k}{\sqrt{\epsilon_k^2+\Delta_k^2}}, \frac{\epsilon_k}{\sqrt{\epsilon_k^2+\Delta_k^2}}\right) \right) \qquad \hat{n}_k^2 = 1$$

$$\boxed{\Rightarrow E_k = \pm\sqrt{\epsilon_k^2 + \Delta_k^2}}$$





$$\left(\epsilon_k \tau_3 + \Delta_k \tau_2\right)\begin{pmatrix} u_k \\ v_k \end{pmatrix} = E_k \begin{pmatrix} u_k \\ v_k \end{pmatrix}$$

$$u_k = \sqrt{\frac{1}{2}\left(1 + \frac{\epsilon_k}{E_k}\right)}$$

$$v_k = i\sqrt{\frac{1}{2}\left(1 - \frac{\epsilon_k}{E_k}\right)}\ \mathrm{sgn}(k)$$

Details.

$$c_n = \frac{1}{\sqrt{N}} \sum_k c_k e^{ikn} \qquad \left(\begin{array}{l} k_m = \frac{2\pi}{N} m \\ c_{n+N} \equiv c_n \end{array} \right)$$

$$c_n^+ = \frac{1}{\sqrt{N}} \sum_{k'} c_{k'}^+ e^{-ik'n}$$

$$H^d = -\sum_{n,k,k'} \frac{1}{N}\Big(t + \overbrace{(-1)^n}^{e^{i\pi n}} 2\alpha u\Big)\left[c_{k'}^+ c_k \, e^{i(k-k')n} e^{-ik'} + h.c \right]$$

$$= -\sum_{k,k'} t \left[c_{k'}^+ c_k \overbrace{\frac{1}{N}\sum_n e^{i(k-k')n}}^{\delta_{k,k'}} e^{-ik'} + h.c \right]$$

$$- \sum_{k,k'} 2\alpha u \left[c_{k'}^+ c_k \underbrace{\frac{1}{N}\sum_n e^{i(k+\pi-k')n}}_{\delta_{k',k+\pi}} e^{-ik'} + h.c \right]$$

$$= -\sum_k t\left(e^{-ik} c_k^+ c_k + h.c\right) + 2\alpha u\left(c_{k+\pi}^+ c_k e^{-ik} + h.c\right)$$

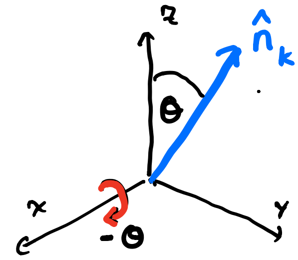
$$= \sum_k \left(-2t\cos k \, c_k^+ c_k + 2\alpha u\left(c_{k+\pi}^+ c_k e^{-ik} + h.c\right)\right)$$

$$= \sum_{k\in[0,\pi]} \Big(-2t\cos k \, c_k^+ c_k + 2t\cos k \, c_{k+\pi}^+ c_{k+\pi}$$
$$+ 2\alpha u \Big[\left(c_{k+\pi}^+ c_k - c_k^+ c_{k+\pi}\right) e^{-ik} + \left(c_k^+ c_{k+\pi} - c_{k+\pi}^+ c_k\right) e^{ik} \Big] \Big)$$

$$= \sum_{k\in[0,\pi]} \left(c_{k+\pi}^+ , c_k^+\right) \begin{bmatrix} \overbrace{2t\cos k}^{\epsilon_k} & -4\alpha u i \sin k \\ \underbrace{4\alpha u i \sin k}_{i\Delta_k} & -2t\cos k \end{bmatrix} \begin{pmatrix} c_{k+\pi\sigma} \\ c_{k\sigma} \end{pmatrix}$$

$$\boxed{\begin{aligned}\mathcal{H} &= \epsilon_k \tau_3 + \Delta_k \tau_2 \\ &= E_k\left(\cos\theta\, \tau_3 + \sin\theta\, \tau_1\right)\end{aligned}}$$

$$= E_k\, \hat{n}_k \cdot \vec{\tau}$$



$$\boxed{\begin{aligned}U_x(-\theta) &= e^{i\theta/2\, \tau_1} \\ &= \cos\frac{\theta}{2} + i\sin\frac{\theta}{2}\,\tau_1\end{aligned}}$$

$$\cos\theta_k = \frac{\epsilon_k}{E_k}$$

$$\mathcal{H} = U\, \epsilon_k \tau_3\, U^\dagger$$

$$\begin{pmatrix} u_k \\ v_k \end{pmatrix} = U \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\theta/2 \\ i\sin\theta/2 \end{pmatrix}$$

$$2\cos^2\theta/2 - 1 = \cos\theta = \frac{\epsilon}{E} \Rightarrow \cos\theta/2 = u_k = \sqrt{\frac{1}{2}\left(1 + \frac{\epsilon_k}{E_k}\right)}$$

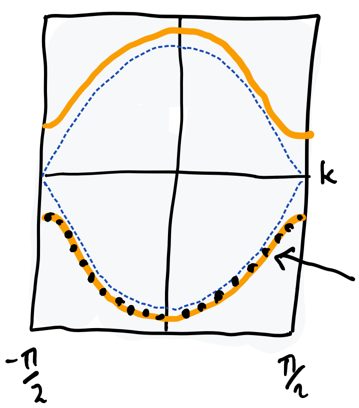
$$1 - 2\sin^2\theta/2 = \frac{\epsilon}{E} \Rightarrow \sin\theta/2 = v_k = \sqrt{\frac{1}{2}\left(1 - \frac{\epsilon_k}{E_k}\right)}\ \text{sign}(k)$$

$$(v_k \sim \Delta_k)$$

$$N\int \frac{dk}{2\pi}$$

$$\uparrow$$

$$E_g = -2\sum_k E_k + 2NKu^2$$



$$\boxed{\frac{E_g}{N} = -2\int_{-\pi/2}^{\pi/2} \frac{dk}{2\pi}\sqrt{\epsilon_k^2 + \Delta_k^2} + 2Ku^2}$$

Approximate $\pm\epsilon_k = \pm v_F\left(k - \frac{\pi}{2}\right)$ $\quad \Delta_k^2 \sim \Delta^2 = (4\alpha u)^2$

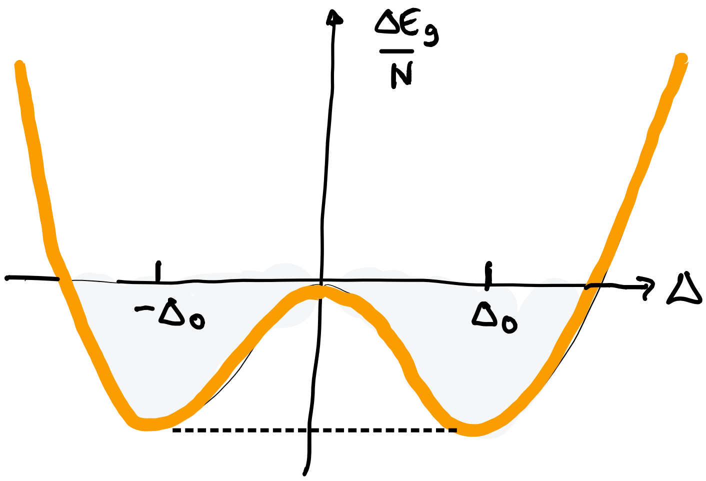
$$\boxed{\frac{E_g}{2} = -2\int_{-\Lambda}^{\Lambda} \frac{dk}{2\pi}\sqrt{(v_F k)^2 + \Delta_0^2} + 2Ku^2}$$

$$\boxed{\begin{aligned} \frac{\Delta E_g}{N} &= -\frac{\Delta^2}{\pi v_F} \ln\left(\frac{\Delta_0 \sqrt{e}}{|\Delta|}\right) \\ \Delta_0 &= 2(v_F \Lambda)\, e^{-1/2\lambda} \end{aligned}}$$

$$\frac{1}{\lambda} = \frac{k \pi v_F}{4\alpha^2}$$

$\left(\begin{array}{l} \text{c.f } \quad v_F \Lambda \equiv \omega_D \\ \text{in BCS} \end{array} \right)$

$$\frac{1}{N}\frac{\partial \Delta E_g}{\partial \Delta} = -\frac{2\Delta}{\pi v_F} \ln\left(\frac{\Delta_0}{\Delta}\right) = 0 \Rightarrow \Delta = \Delta_0$$



$$\frac{\Delta E_g^{(0)}}{N} = -\frac{\Delta_0^2}{2\pi v_F}$$

$$= -\frac{\Delta^2}{2} \rho$$

$$\rho = \frac{1}{\pi v_F}. = \text{DOS.}$$

More details

Substituting $\Delta \sinh\theta = v_F k \Rightarrow dk = \dfrac{\Delta \cosh\theta \, d\theta}{v_F}$

$$\Rightarrow \sqrt{(v_F k)^2 + \Delta^2} = \Delta \cosh\theta$$

$$\Rightarrow \theta_{max} = \sinh^{-1}\left(\frac{v_F \Lambda}{\Delta}\right)$$

$$\frac{E_g^{(2)}}{N} = -\frac{\Delta^2}{\pi v_F} \int_{-\theta_{max}}^{\theta_{max}} d\theta \, \cosh^2\theta = -\frac{\Delta^2}{\pi v_F}\left[\frac{\theta}{2} + \frac{1}{2}\sinh\theta\cosh\theta\right]_{-\theta_m}^{\theta_m}$$

$$= \frac{-\Delta^2}{\pi v_F}\left[\theta_m + \sinh\theta_m \cosh\theta_m\right]$$

$$\frac{E_g}{N} = -\frac{\Delta^2}{\pi v_F}\left[\sinh^{-1}\left(\frac{v_F \Lambda}{\Delta}\right) + \left(\frac{v_F \Lambda}{\Delta}\right)\sqrt{1 + \left(\frac{v_F \Lambda}{\Delta}\right)^2}\right]$$

$$\sinh x \sim \frac{e^x}{2} = y \Rightarrow x = \ln 2y = \sinh^{-1} y.$$

$$\frac{E_g}{N} = \frac{-\Delta^2}{\pi v_F}\left[\ln\frac{2 v_F \Lambda}{\Delta} + \left(\frac{v_F \Lambda}{\Delta}\right)^2\left[1 + \frac{1}{2}\left(\frac{\Delta}{v_F \Lambda}\right)^2 + \ldots\right]\right] + 2ku^2$$

$$= \underbrace{-\frac{v_F \Lambda^2}{\pi}}_{E_g^{(0)}/N} - \frac{\Delta^2}{\pi v_F} \ln\left[\frac{2 v_F \Lambda \sqrt{e}}{\Delta}\right] + \underbrace{2ku^2}_{\frac{2k}{(4\alpha)^2}\Delta^2 = \frac{\Delta^2}{2g}}$$

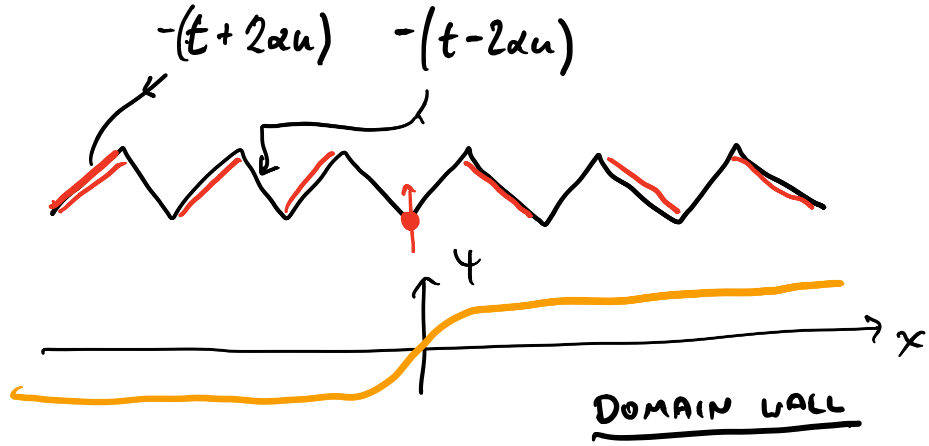
$$\frac{1}{g} = \frac{k}{4\alpha^2}$$

$$\frac{1}{\lambda} = \frac{\pi v_F}{g} = \frac{1}{g\rho} = \frac{k \pi v_F}{4\alpha^2}$$

$$\frac{\Delta E_g}{N} = -\frac{\Delta^2}{\pi v_F}\left[\ln\left(\frac{2 v_F \Lambda \sqrt{e}}{\Delta}\right) - \frac{1}{2\lambda}\right]$$

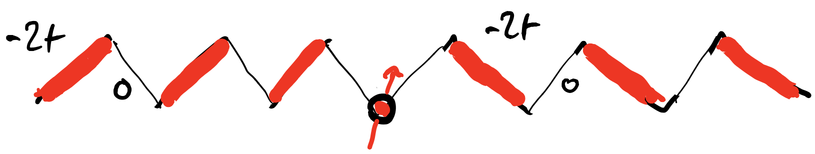
$$= -\frac{\Delta^2}{\pi v_F}\left[\ln\left(\frac{2 v_F \Lambda \sqrt{e}\, e^{-1/2\lambda}}{|\Delta|}\right)\right]$$

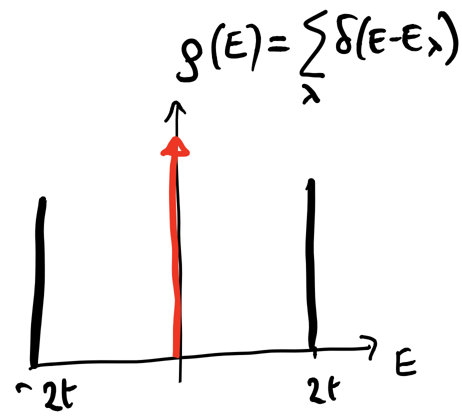
Soliton



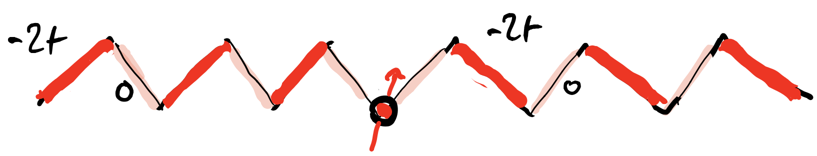
$$u_n = (-1)^n \psi_n$$

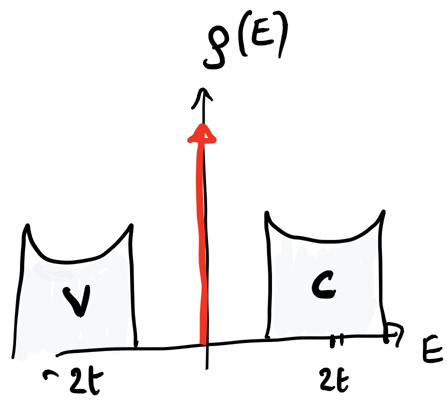
Let $2\alpha u = t$, then

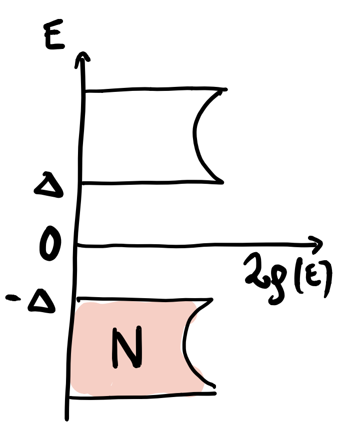




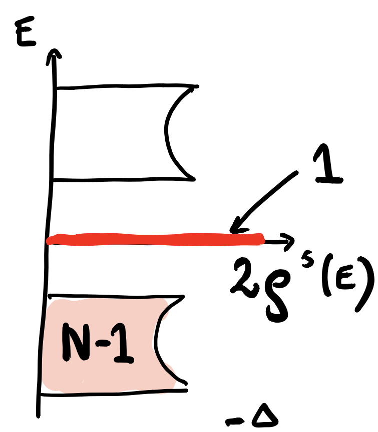
Now adiabatically reduce $|2\alpha u| < t$







No Soliton



Soliton $\displaystyle\int_{-\infty}^{-\Delta} \Delta\rho(E)\,dE = -\frac{1}{2}$

$\Delta\rho(E)$ = change in d.o.s in valence/conduction band

$$\rho^s(E) - \rho(E) = \delta(E) + \Delta\rho(E)$$

$$\int_{-\infty}^{-\Delta} + \int_{\Delta}^{\infty} \Delta\rho(E)\, dE + 1 = 0$$

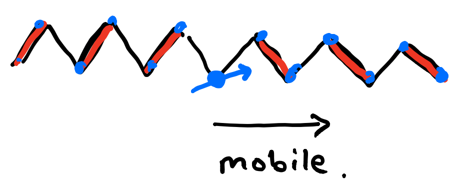
no change in # states.

$$\Rightarrow \int_{-\infty}^{-\Delta_g} \Delta\rho(E)\, dE = -\frac{1}{2}$$

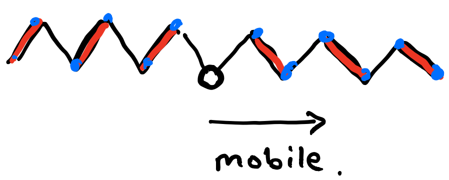
Deficit of ½ state/spin in valence band.

$$\boxed{\Delta \#\ \text{valence } e^- = 2\int_{-\infty}^{-\Delta_g} \Delta\rho(E)\, dE = -1}$$

One e^- remove from valence band

S_0 

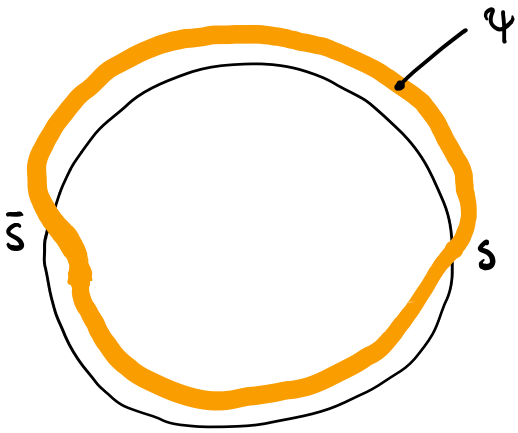
$q = 0 \quad s = 1/2$ "spinon"

$S_\pm$ 

$q_\pm = \pm e \quad s_\pm = 0$ "holon/doublon"

- What about Kramer's theorem? Creating a neutral soliton does not change the electron count, so how can one have a half integer spin?

In practice, in a system with periodic B.C's, solitons are created in pairs, having total spin $S=0$ or 1.



$(\psi_n = (-1)^n u_n.)$

In a finite chain with ends, the compensating spin is at the chain ends.

- Charge + neutral solitons have the same energy, usually less than $\Delta_g/2$.

- Addition of an electron creates a spinon & a holon.

FRACTIONALIZATION.