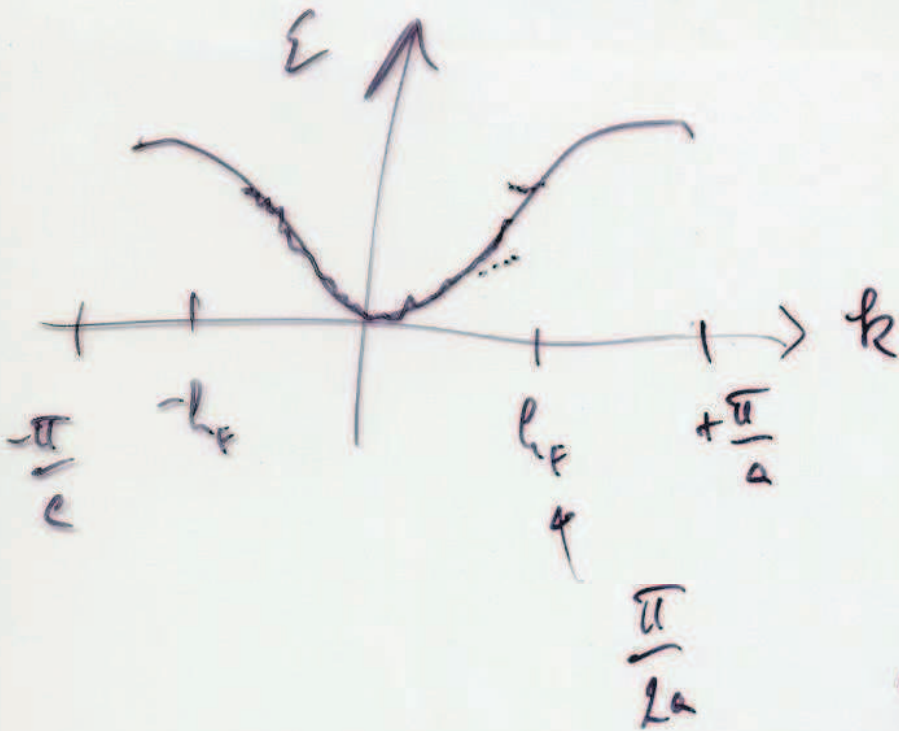
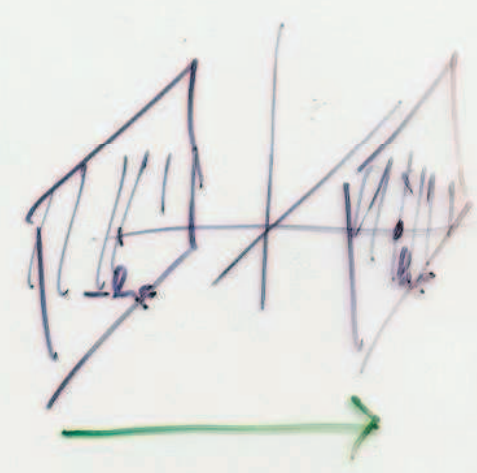
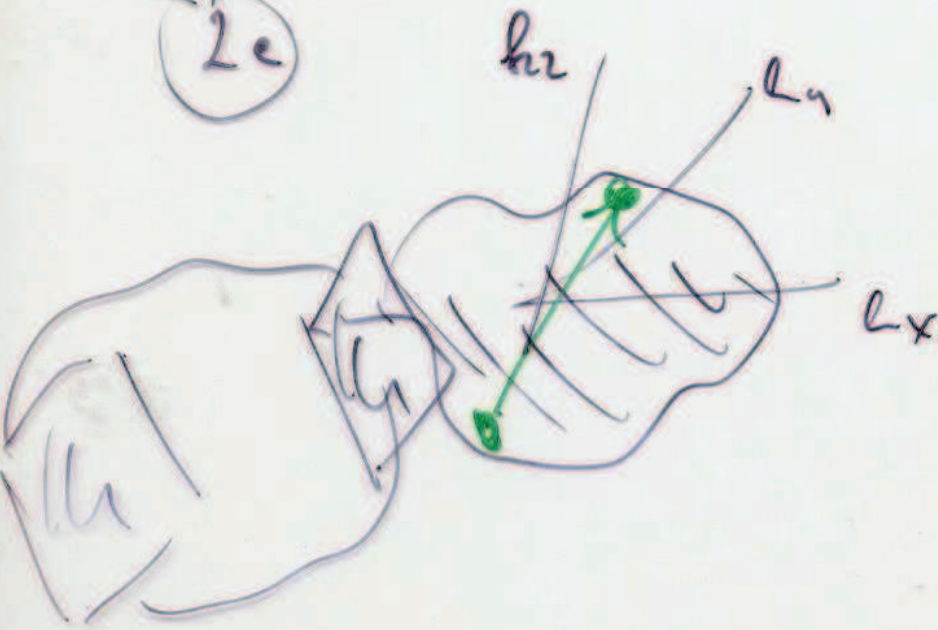
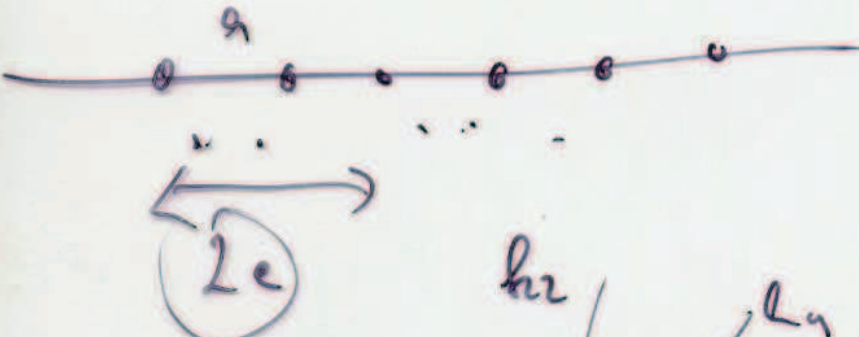
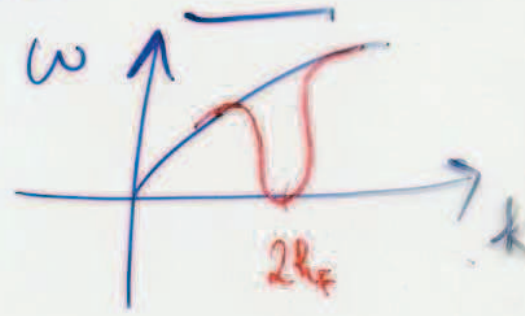


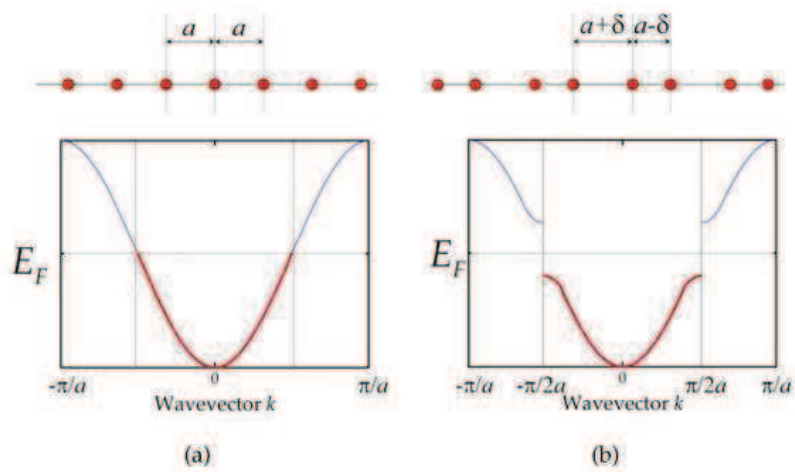
1dim instabilitätsok

$2k_F$

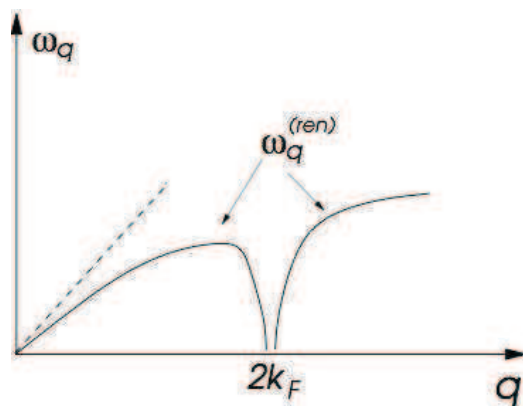


$2k_F = \frac{\pi}{a} \approx \frac{2\pi}{2a}$
 Brillouin \leftrightarrow Kohn





Peierls distortion (https://www.utwente.nl/tmw/pin/onderzoek/physical_properties_of_low-dimensional_systems/physical_properties_of_low-dimensional_systems-8.png)



Kohn anomaly (<http://www.itp.phys.ethz.ch/education/fs14/sst/slides/Peierls.pdf>)

Konjugált polimerek kvantunkémiai leírása

- Born-Oppenheimer (adiabatikus) közelítés

$$\Psi(\{\xi\}_{el}, \{R\}_{nuc}) = \Psi_{el}(\{\xi\}, \{R\}) \times \Psi_{nuc}(\{R\})$$

- σ - π szeparáció

$$\Psi_{el}(\{\xi_{\pi}, \xi_{\sigma}\}) = \Psi_{\pi}(\{\xi_{\pi}\}) \times \Psi_{\sigma}(\{\xi_{\sigma}\})$$

További közelítések \rightarrow „egyszerű” modellek (π)

- Hückel - modell

egyelektron kép,
nincs explicit σ - π kölcsönhatás

- Hubbard - modell

azonos atomon lévő π elektron
párok σ -tartását figyelembe veszi

- Pariser-Parr Pople
PPP - modell

bármely két atomon lévő π elektron
párok σ -tartását figyelembe veszi

(Össz-egyelektron módszerek σ és π !)
szemiklasszikus (NDO, MNDO ...)
ab initio , DFT

HÜCKEL - MODELL

- független elektronok (1 Slater-determináns)

$$\Psi_{\pi}(\{\xi_{\pi}\}) = \Psi(\xi_1 \dots \xi_N) = \hat{A}(\psi_1(1) \dots \psi_N(N))$$

$$(\psi_i = \phi_i(\vec{r}) \cdot \gamma_i(s) \quad \text{spin-orbital})$$

- LCAO-MO

$$\phi_i(\vec{r}) = \sum_j C_j^{(i)} \cdot \chi_j(\vec{r})$$

MO ← AO

$$\chi_j(\vec{r}) = \chi_{p_z}(\vec{r} - \vec{r}_j)$$

Másodkvantált formalizmusban:

$$\hat{H} = \sum_{m,n} \sum_s h_{mn} a_{ms}^+ a_{ns} =$$

$$= \sum_m \alpha_m \sum_s a_{ms}^+ a_{ms} + \sum_{m,n} \beta_{mn} \sum_s a_{ms}^+ a_{ns}$$

előző szomszédok

$$\Rightarrow \hat{H} = \sum_m \alpha_m \sum_s a_{ms}^+ a_{ms} + \sum_i \beta_i \sum_s (a_{i_1s}^+ a_{i_2s} + a_{i_2s}^+ a_{i_1s})$$

atomok kötések

$i: i_1 \leftrightarrow i_2$

$\beta: rezonancia hopping$

Spec. azonos atomok

$$\hat{H} = \alpha \sum_m \sum_s a_{ms}^+ a_{ms} + \beta \sum_i \sum_s (a_{i_1s}^+ a_{i_2s} + a_{i_2s}^+ a_{i_1s})$$

TOPOLOGIA

HUBBARD - MODELL

$$\hat{H} = \sum_{mn,s} h_{mn} a_{ms}^\dagger a_{ns} + \sum_n \gamma_n \hat{N}_{n\uparrow} \hat{N}_{n\downarrow}$$

$$(\hat{N}_{n\uparrow} \equiv a_{n\uparrow}^\dagger a_{n\uparrow})$$

spec. arwms atomok

$$\hat{H} = \sum_{n,s} \epsilon_{ns} a_{ns}^\dagger a_{ns} + \beta \sum_{i,s} (a_{i2s}^\dagger a_{i1s} + a_{i1s}^\dagger a_{i2s}) + U \sum_n \hat{N}_{n\uparrow} \hat{N}_{n\downarrow}$$

PPP - modell

$$\hat{H} = \sum_{mn,s} h_{mn} a_{ms}^\dagger a_{ns} + \frac{1}{2} \sum_{mn} \sum_{s_1 s_2} \gamma_{mn} \hat{N}_{ms_1} \hat{N}_{ns_2} - \frac{1}{2} \sum_{ns} \gamma_{nn} \hat{N}_{ns}$$

$$\gamma_{mn} = \begin{cases} \frac{1}{R_{mn} + 2/(\gamma_{nn} + \gamma_{mm})} \\ \frac{1}{\sqrt{R_{mn}^2 + 4/(\gamma_{nn} + \gamma_{mm})^2}} \end{cases}$$

Mataga - Nishimoto

Ohno