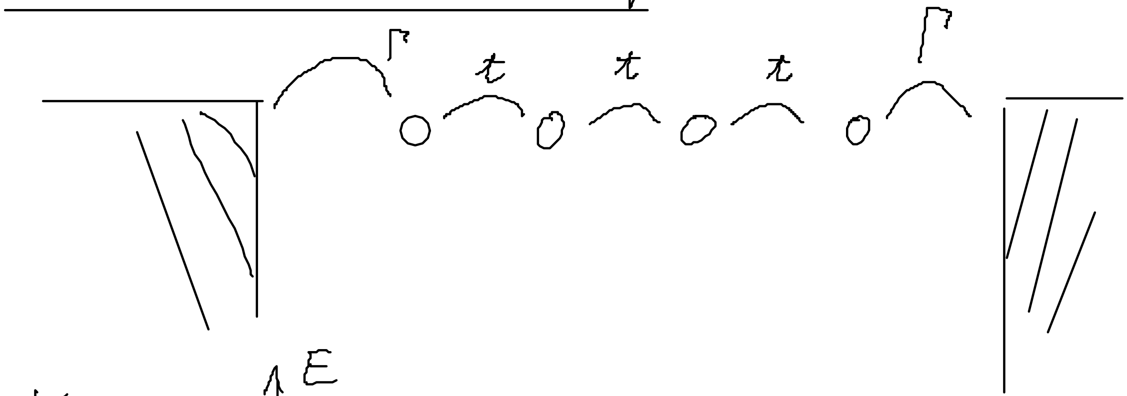
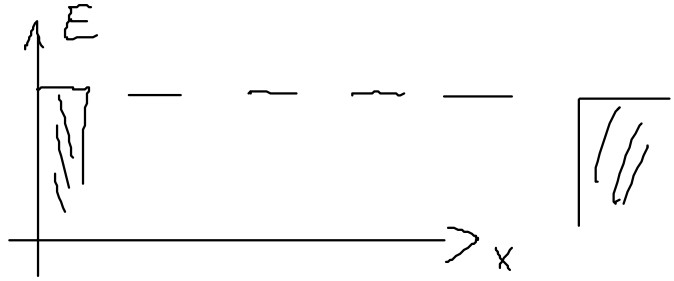
Moleküle als Drähte:

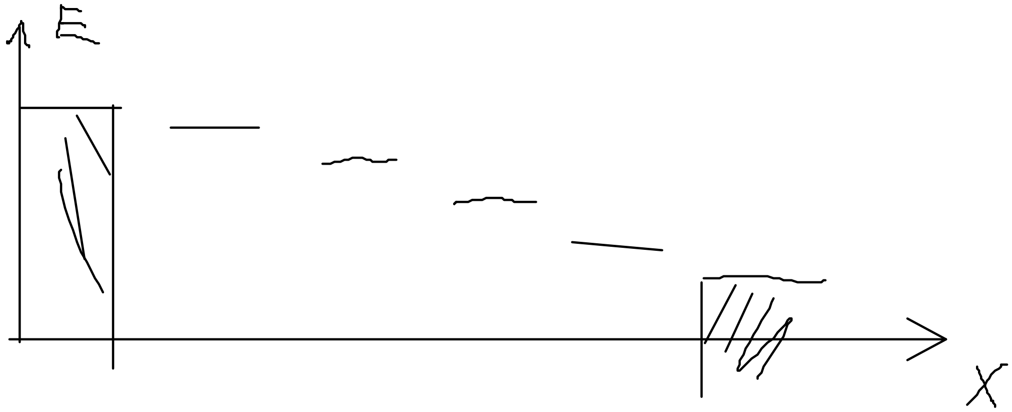
teilweise besetztes Energieniveau nahe der Fermi-Energie



$V = 0$



$V > 0$



$V \neq 0$ Verschiebung der el.-chem. Potentiale in der linken und rechten Elektrode

$\Rightarrow$ Modifikation der Potentiale im Draht

$$I(U) = \int_{-\infty}^{\infty} dE \; T(E,U) \left(f(E-\mu_L) - f(E-\mu_R) \right)$$

Transmission

Fermifunktion links und rechts

T klein

$$\Rightarrow \int_{-\frac{eU}{2}}^{\frac{eU}{2}} dE \; T(E,U)$$

$$T(E,U) = \mathrm{Tr}\left(\Gamma_L \, G^r_{cc} \, \Gamma_R \, G^a_{cc}\right)$$

$$\Gamma_L(E) = \Gamma\left(E - \frac{eU}{2}\right)$$

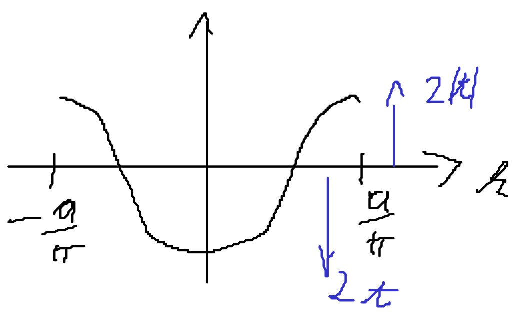
$$\Gamma_R(E) = \Gamma\left(E + \frac{eU}{2}\right)$$

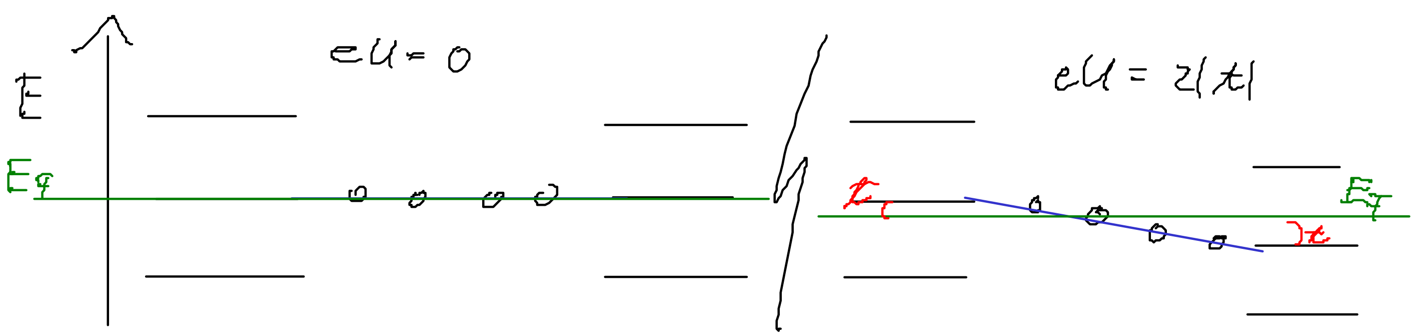
Verschiebung in Elektroden

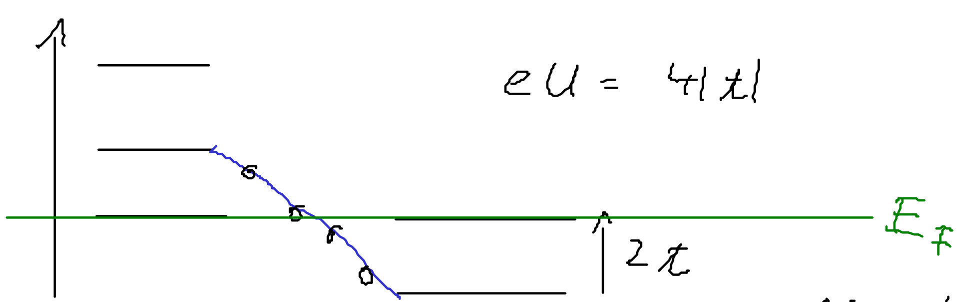
$$G^r_{cc} = \left(E - H_{cc}(U) - \Sigma_L\left(E - \frac{eU}{2}\right) - \Sigma_R\left(E + \frac{eU}{2}\right)\right)^{-1}$$

Potentialverlauf im Draht

1D - Draht







für eU > 4|t|
bricht Strom zusammen

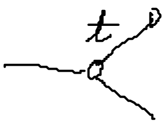
Graphen

(2 primitive Einheitsvektoren)

$$\psi_k(\vec r) = \sum_{\ell \text{ alle Zellen}} \underbrace{e^{i \vec k \vec R_\ell}}_{\text{Bloch Theorem}} \big(b_1 \underbrace{\phi(\vec r - \vec A)}_{\phi_A(\vec r - \vec R_\ell)} + b_2 \underbrace{\phi(\vec r - \vec B)}_{\phi_B(\vec r - \vec R_\ell)} \big)$$

Wellenfunktion von Teilchen A und B in der Einheitszelle ℓ

$$\phi_{A,B} = p_z(\vec r - \vec r_{A/B})$$



Hüpfen von B nach A

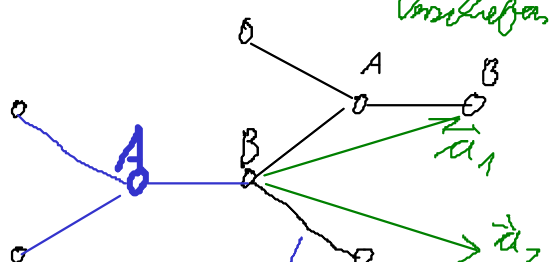
$$\begin{pmatrix} E(\vec k) & -t\alpha(\vec k) \\ -t\alpha(\vec k) & E(\vec k) \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = 0$$

mit tight-binding Hamilton

Eigenenergie

$$\alpha(\vec k) = 1 + e^{-i\vec k \vec a_1} + e^{-i \vec k \vec a_2}$$

Verschieben + Koppeln



$\Rightarrow$ Hüpfterm

Kopplung

$\alpha(\vec k) = 0$ liefert $\vec K$ und $\vec K'$

$$E(\vec k) = \pm \hbar v \, |\delta k| \qquad \vec k - \vec k' = \delta k$$

$$|s = \pm 1\rangle = \frac{1}{\sqrt 2} \begin{pmatrix} s\, e^{-i\theta_k/2} \\ s\, e^{i\theta_k/2} \end{pmatrix}$$

"Spin"-Darstellung wegen 2 Untergittern

$$H = \hbar v_F \, |\delta k| \, \sigma_z \qquad \frac{\delta k_x}{\delta k_y} = \tan \theta_k$$