Experimentelle Techniken zur Herstellung atomarer und molekularer Kontakt

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

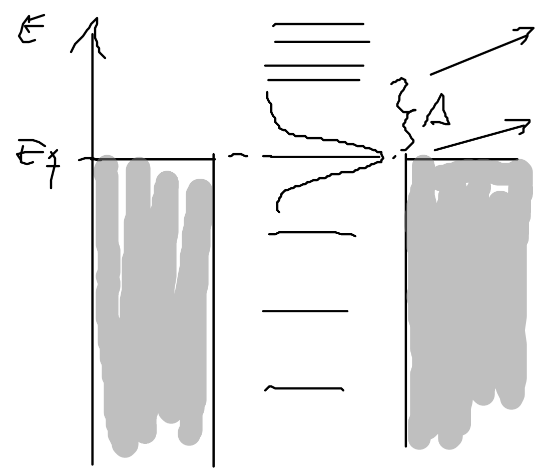
$$G_{CC} = \left(E\,\mathbb{1}_{CC} - H_{CC} - \Sigma_L - \Sigma_R\right)^{-1}$$

$$\Sigma_X = H_{CX}\, g^r_{XX}\, H_{XC} \qquad X = L,R$$

$$g^r_{XX} = \left(E - H_{XX}\right)^{-1}$$

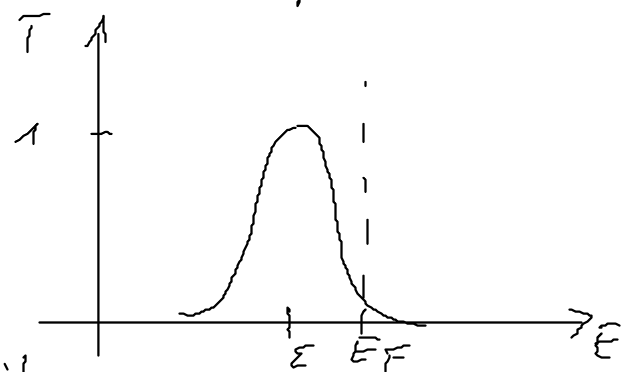
$$\Gamma_X = i\left(\Sigma^r_X - \Sigma^a_X\right) = 2\,\mathrm{Im}\left(\Sigma^a\right)$$

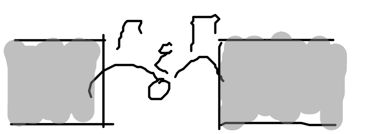
- Typischerweise wird in Modellrechnungen Energieabhängigkeit von Γ_X und Σ_X vernachlässigt.
- WBL: (wide band limit) $\Sigma^a_X = i\frac{\Gamma_X}{2}$; $\Sigma^r_X = -i\frac{\Gamma_X}{2}$



HOMO: highest occupied molecular orbital

LUMO: lowest unoccupied molecular orbital



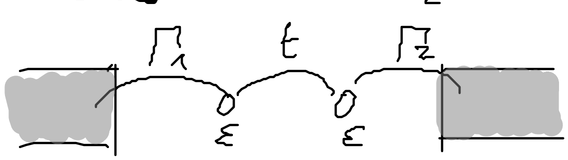


$$H = \varepsilon\,|1\rangle\langle 1|$$

$$T(E) = \Gamma^2\,|G^r_{11}|^2 = \frac{\Gamma^2}{(E-\varepsilon)^2 + \Gamma^2}$$

$$G_{11} = \frac{1}{E - \varepsilon_0 - i\Gamma}$$

Dimer: Pt – H_2 – Pt $\qquad H = \begin{pmatrix} \varepsilon_0 & t \\ t & \varepsilon_0 \end{pmatrix}$



isoliertes System: $E_\pm = \varepsilon_0 \pm t$

$$\Gamma_L = \begin{pmatrix} \Gamma_1 & 0 \\ 0 & 0 \end{pmatrix} \qquad \Gamma_R = \begin{pmatrix} 0 & 0 \\ 0 & \Gamma_2 \end{pmatrix} \qquad \Gamma = \Gamma_1 = \Gamma_2$$

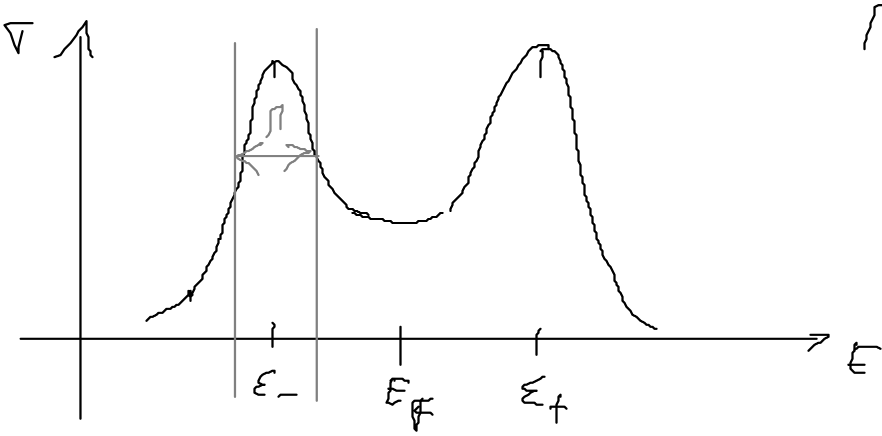
$$T(E) = \mathrm{Tr}\left(\Gamma_L\, G^r_{CC}\, \Gamma_R\, G^a_{CC}\right) = \Gamma^2\,|G^r_{12}|^2$$

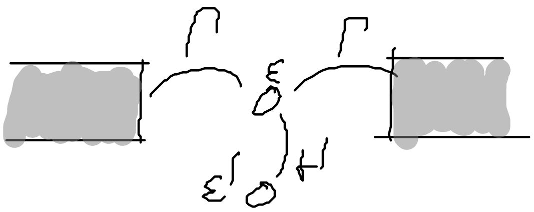
$$G^r = \begin{pmatrix} E-\varepsilon_0 + i\frac{\Gamma}{2} & -t \\ -t & E-\varepsilon_0 + i\frac{\Gamma}{2} \end{pmatrix}^{-1}$$

$$G^r_{12} = \frac{t}{\left(E-\varepsilon_0 + i\frac{\Gamma}{2}\right)^2 - t^2} = \frac{t}{\underbrace{\left(E-\varepsilon_0 - t + i\frac{\Gamma}{2}\right)}_{E-\varepsilon_+}\underbrace{\left(E-\varepsilon_0 + t - i\frac{\Gamma}{2}\right)}_{E-\varepsilon_-}}$$

$$\boxed{T(E) = \frac{t^2\Gamma^2}{\left((E-\varepsilon_+)^2 + \frac{\Gamma^2}{4}\right)\left((E-\varepsilon_-)^2 + \frac{\Gamma^2}{4}\right)}}$$

$\Gamma \ll t$: Summe aus zwei Lorentzkurven

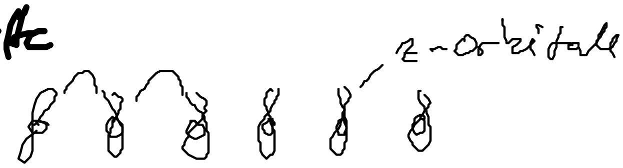


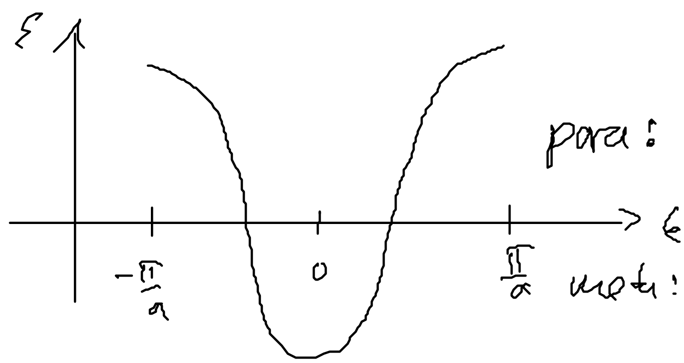


$$T(E) = \frac{\Gamma^2}{\left|E-\varepsilon + i\Gamma - \frac{t'}{E-\varepsilon'}\right|^2} = \frac{\Gamma^2}{\Gamma^2 + \left(E-\varepsilon - \frac{t'}{E-\varepsilon'}\right)^2}$$

$$E_{T=1} = \frac{\varepsilon+\varepsilon'}{2} \pm \sqrt{\left(\frac{\varepsilon-\varepsilon'}{2}\right)^2 + t'^2} \qquad E_{T=0} = \varepsilon'$$

Kette





$$k_F = \frac{\pi}{2a}$$

para: $T \propto |t_1 + t_2|^2 = t \cdot \left|e^{i\frac{\pi}{2a}3a} + e^{i\frac{\pi}{2a}3a}\right|^2 = 4t^2$

meta: $T \propto \left||t_1| e^{i\frac{\pi}{2a}4a} + |t_2| e^{i\frac{\pi}{2a}2a}\right|^2 = |t_2|^2 \left|\frac{|t_1|}{|t_2|} e^{i\pi} + 1\right|^2 \approx 0$

für $|t_1| \approx |t_2|$