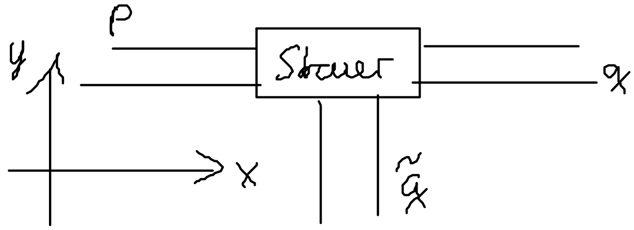
Greensche Funktion

$$G^{r/a} = (E \pm i\eta - H)^{-1}$$
$$G^a = [G^r]^\dagger$$



1dim: $S_{qp} = -\delta_{qp} + i\hbar\sqrt{v_p v_q}\; G^r_{qp}$

2dim: $S_{nm} = -\delta_{nm} + i\hbar\sqrt{v_n v_m} \iint dy_q\, dy_p\, \chi_n(y_q)\, G^r_{qp}(y_q,y_p)\, \chi_m(y_p)$

$$T_{nm} = |S_{nm}|^2 \underset{n \neq m}{=} \hbar^2 v_n v_m \iiiint dy_q\, dy_p\, dy'_q\, dy'_p\, \chi_n(y_q)\, G^r_{qp}(y_q,y_p)\, \chi_m(y_p)$$
$$\cdot\, \chi_n(y'_q)\, G^a_{pq}(y'_p,y'_q)\, \chi_m(y'_p)$$
$$= \hbar^2 \iiiint dy_q\, dy_p\, dy'_q\, dy_{p'}\, \underbrace{\chi_n(y'_q)\, v_n\, \chi_n(y_q)}\, G^r_{qp}(y_q,y_p)$$
$$\cdot\, \underbrace{\chi_m(y_p)\, v_m\, \chi_m(y'_p)}\, G^a_{pq}(y'_p,y'_q)$$

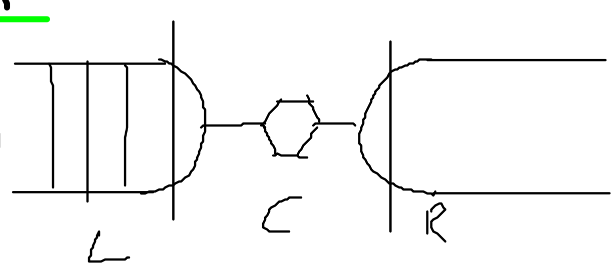
$$T_{qp} = \sum_{n\in q}' \sum_{m \in p} T_{nm} = \iiiint dy_q\, dy_p\, dy'_q\, dy_{p'}\, \Gamma_q(y'_p,y_p)\, G^r_{qp}(y_q,y_p)$$
$$\cdot\, \Gamma_p(y_p,y'_p)\, G^a_{pq}(y'_p,y'_q)$$

$$\boxed{\Gamma_p(y_p,y'_p) = \sum_{m\in p} \chi_m(y_p)\, \hbar\, v_m\, \chi_m(y'_p)}$$

$$\boxed{T_{qp} = \mathrm{Tr}\left[\Gamma_q\, G^r_{qp}\, \Gamma_p\, G^a_{pq}\right]}$$

Tight-Binding-Bild

$$H = \begin{pmatrix} H_{LL} & H_{LC} & 0 \\ H_{CL} & H_{CC} & H_{CR} \\ 0 & H_{RC} & H_{RR} \end{pmatrix}$$



$$(E\mathbb{1} - H)^{-1}\, G = \mathbb{1}$$
$$(E - H_{LL})\, G_{LC} - H_{LC}\, G_{CC} = 0$$
$$-H_{CL}\, G_{LC} + (E - H_{CC})\, G_{CC} - H_{CR}\, G_{RC} = 1$$
$$-H_{RC}\, G_{CR} + (E - H_{RR})\, G_{RC} = 0$$

$$G_{LC} = -(E-H_{LL})^{-1} H_{LC} G_{CC}$$
$$G_{RC} = (E-H_{RR})^{-1} H_{RC} G_{CC}$$
$$\left(-H_{CL}(E-H_{LL})^{-1}H_{LC} + (E-H_{CC}) - H_{CR}(E-H_{RR})^{-1}H_{RC}\right)G_{CC} = 1$$

$$G_{CC} = (E-H_{CC}-\Sigma_L-\Sigma_R)^{-1}$$

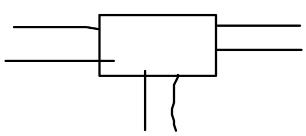
Selbstenergie $\Sigma_X = H_{CX}\, g_{XX}\, H_{XC}$

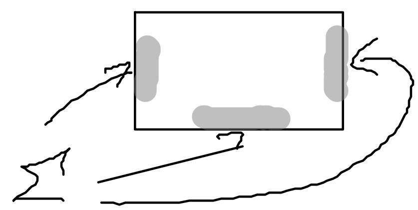
$T_{RL}(E) = Tr\left(\Gamma_R(E)\, G^r_{CC}(E)\, \Gamma_L(E)\, G^a_{CC}(E)\right)$ mit $\boxed{\Gamma = i\left(\Sigma^r_X - \Sigma^a_X\right);\ X=L,R}$

Transmission als „Matrixmultiplikation"

- Γ, G nur im Bereich von C zu bestimmen
- g_{XX} nur für an C koppelnde Atome zu bestimmen

unendliches System $\xrightarrow{\text{ersetzt durch}}$ äquivalenten endl. Leiter





Interpretation Σ

$H_{CC}\,\psi_{\alpha 0} = \varepsilon_{\alpha 0}\,\psi_{\alpha 0}$ $\qquad \boxed{\Sigma = \Sigma_L + \Sigma_R}$

$(H_{CC} + \Sigma^r)\,\psi_\alpha = \varepsilon_\alpha\,\psi_\alpha$

- da $\Sigma^+ \neq \Sigma$ ist $H+\Sigma$ nicht hermitesch $\Rightarrow$ Eigenwert ε_α im allg. komplex

$\varepsilon_\alpha = \varepsilon_{\alpha 0} - \Delta_\alpha + i\frac{\gamma_\alpha}{2}$

- Zeitentwicklung: $\psi_\alpha \propto e^{-i\frac{\varepsilon_\alpha t}{\hbar}} = e^{-\frac{i}{\hbar}(\varepsilon_{\alpha 0}-\Delta_\alpha)t}\, e^{-\frac{\gamma_\alpha}{2\hbar}t}$

  $\rho_\alpha(t) = |\psi_\alpha(t)|^2 \propto e^{-\frac{\gamma_\alpha}{\hbar}t}$

- γ_α: endliche Lebensdauer der Elektronen im Bereich C

  $\tau_\alpha = \frac{\hbar}{\gamma_\alpha} \longrightarrow e^-$ verschwinden in Elektroden

Greensche Funktion für nicht-hermiteschen Hamiltonoperator

$L^+ = \sum_{mn} |m\rangle L^+_{mn} \langle n|$ $\qquad$ mit $L^+ = L$

$L|x^L_n\rangle = x^L_n |x^L_n\rangle$

$\langle x^R_n| L = x^R_n \langle x^R_n| \iff L^+|x^R_n\rangle = (x^R_n)^* |x^R_n\rangle$

- Verknüpfung λ^L_n mit λ^R_n $\qquad \det(A^T) = \det(A) = |A^T| = |A|$

$$|L - \lambda^L \mathbb{1}| = 0$$

$$|L^+ - (\lambda^R)^* \mathbb{1}| = 0 = |L^* - (\lambda^R)^* \mathbb{1}| \Rightarrow |L - \lambda^R \mathbb{1}| = 0$$

- wähle $\lambda^L_n = \lambda^R_n$

$$\langle \lambda^R_n | L | \lambda^L_m \rangle = \lambda^L_m \langle \lambda^R_n | \lambda^L_m \rangle = \lambda^R_n \langle \lambda^R_n | \lambda^L_m \rangle$$

$$0 = (\lambda^L_m - \lambda^R_n) \langle \lambda^R_n | \lambda^L_m \rangle$$

$$\Rightarrow \quad \langle \lambda^R_n | \lambda^L_m \rangle = \delta_{nm}$$

- rechtsseitige und linksseitige EV bilden biorthonormale Basis

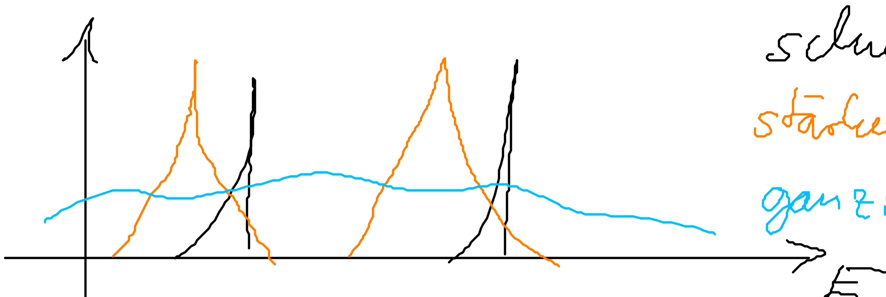
$$(z - L) G = 1 \quad \Rightarrow \quad G = \sum \frac{|\lambda^L_n\rangle\langle \lambda^R_n|}{z - \lambda_n}$$

$$G^{r,a} = \sum_n \frac{\psi_n(\vec{r}) \phi^*_n(\vec{r}\,')}{E - \varepsilon^{r,a}_n} \qquad \varepsilon^{r,a}_n = \varepsilon_{\alpha 0} - \Delta_\alpha \mp \frac{\gamma_\alpha}{2}$$

$$\boxed{\begin{aligned} \psi_n(\vec{r}) &= \langle \vec{r} | \lambda^L_n \rangle \\ \phi_n(\vec{r}) &= \langle \vec{r} | \lambda^R_n \rangle \end{aligned}}$$

$$A(\vec{r}, \vec{r}\,', E) = i(G^r - G^a) = \sum_n \psi_n(\vec{r}) \phi^*_n(\vec{r}\,') \frac{\gamma_\alpha}{(E - \varepsilon_{\alpha 0} + \Delta_\alpha)^2 + \left(\frac{\gamma_\alpha}{2}\right)^2}$$

$$\lim_{\gamma_\alpha \to 0} A = \sum_n \psi_n(\vec{r}) \psi^*_n(\vec{r}\,') \qquad 2\pi\, \delta(E - \varepsilon_{\alpha 0} + \Delta_\alpha)$$



schwache Kopplung γ sehr klein

stärkere Kopplung γ klein

ganz starke Kopplung γ groß

Effekt von Σ:

- Verschiebung der Eigenenergien $\varepsilon_{0\alpha} \to \varepsilon_{0\alpha} + \Delta_\alpha$
- Verbreiterung wegen der endlichen Lebensdauer

Tight-Binding-Hamiltonoperator

$$H = \sum_l |l\rangle \varepsilon_l \langle l| + \sum_{lm} |l\rangle V_{lm} \langle m|$$

$\nearrow$ Onsite Energie $\qquad\qquad \uparrow$ Hüpfelemente

$$\langle l|m\rangle = \delta_{lm} \; ; \; \sum_n |n\rangle\langle n| = 1$$

- Translationsinvarianz: $\varepsilon_l = \varepsilon_0 \; ; \; V_{lm} = V_{0,m-l}$
- Impulszustände $|k\rangle = \frac{1}{\sqrt{N}} \sum_j e^{ikj} |j\rangle \qquad E(k) = \varepsilon_0 + \sum_l V_{0l}\, e^{ikl}$
- Matrixelement im k-Raum:

$$\langle k|H|k'\rangle = \frac{1}{N} \sum_{jlj'l'} \underbrace{\langle j|l\rangle}_{\delta_{jl}} H_{ll'} \underbrace{\langle l'|j'\rangle}_{\delta_{l'j'}} e^{-ikl} e^{ik'l'} \qquad \boxed{\Delta = j' - j}$$

$$= \frac{1}{N} \sum_{jj'} \underbrace{H_{jj'}}_{H_{0,j-j'}} e^{-ikj} e^{ik'j'} = \frac{1}{N} \sum_{j,\Delta} H_{0\Delta}\, e^{ik'\Delta}\, e^{-i(k-k')j}$$

$$= \delta_{kk'} \sum_j H_{0j}\, e^{ikj}$$

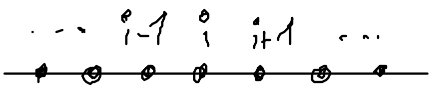
- Schrödingergleichung: $H|\psi\rangle = E|\psi\rangle$

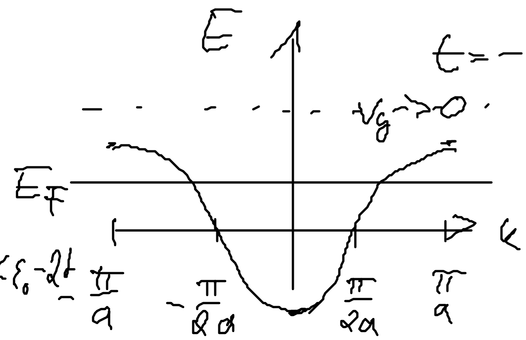
$$\sum_{k'} \langle k|H|k'\rangle\langle k'|\psi\rangle = E\langle k|\psi\rangle$$

$$\left(\sum_j H_{0j} e^{ikj}\right)\langle k|\psi\rangle = E\langle k|\psi\rangle$$

$$E(k) = \sum_j H_{0j} e^{ikj} = \varepsilon_0 + \sum_{l\neq 0} V_{0l}\, e^{ikl}$$

1dim Kette $\quad E(k) = \varepsilon_0 + t\left(e^{ika} + e^{-ika}\right) = \varepsilon_0 + 2t\cos(ka)$





- Dispersionsrelation
- Leitwert

$$\frac{G}{\frac{2e^2}{h}} \propto v_g \cdot \frac{1}{N^{1d}} = \frac{dE}{dk}\frac{1}{\frac{dE}{dk}} = \begin{cases} 1 & \varepsilon_0 + 2t < E < \varepsilon_0 - 2t \\ 0 & \text{sonst} \end{cases}$$