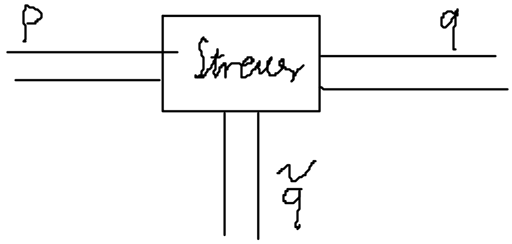
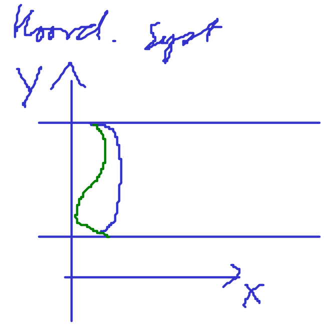
$$G^{r/a} = (E \pm i\eta - H)^{-1}$$





1D

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

2D

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

auslaufende Welle in gleicher Mode wie die angeregte

gesamte auslaufende Welle gesucht, nicht Ortsabhängigkeit

$$T_{nm} = |S_{nm}|^2 = \hbar^2 v_n v_m \iiiint dy_q\, dy_p\, dy'_q\, dy'_p$$

$n \neq m$

χ reell

$$\cdot\, \chi_n(y_q)\, G^r_{qp}(y_q, y_p)\, \chi_m(y_p)$$

gruppenweise $A_{ij} a_j = \lambda_i a_i$

$$\cdot\, \chi_n(y'_q)\, G^a_{pq}(y'_p, y'_q)\, \chi_m(y'_p)$$

$$= \hbar^2 \iiiint dy_q\, dy_p\, dy'_q\, dy'_p\, \underline{\chi_n(y'_q)\, v_n\, \chi_n(y_q)}$$

$$G^r(y_q, y_p)\, \underline{\chi_m(y_p)\, v_m\, \chi_m(y'_p)}\; G^a(y'_p, y'_q)$$

je eine Größe (vgl. Matrixmultipl. mit kontinuierlichen Index)

$$T_{qp} = \sum_{n\in q} \sum_{m \in p} T_{nm} = \iiiint dy_q\, dy_p\, dy'_q\, dy'_p\, \Gamma_q(y'_q, y_q)$$

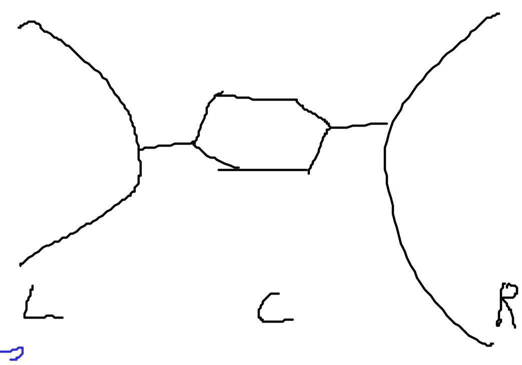
$$G^r_{qp}(y_q, y_p)\, \Gamma_p(y_p, y'_p)\, G^a_{pq}(y'_p, y'_q)$$

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

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

Tight-Binding-Bild mit Greensfunktion

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



kein Überlapp von links und rechts

davon G-Funktion

$$(E\mathbb{1} - H)^{-1}\, G = 1$$

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

$$G_{LC} = (E - H_{LL})^{-1} H_{LC} G_{CC}$$
$$G_{RC} = (E - H_{RR})^{-1} H_{RC} G_{CC}$$

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

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

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

Selbstenergie — Green-Fkt. der Elektrode

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

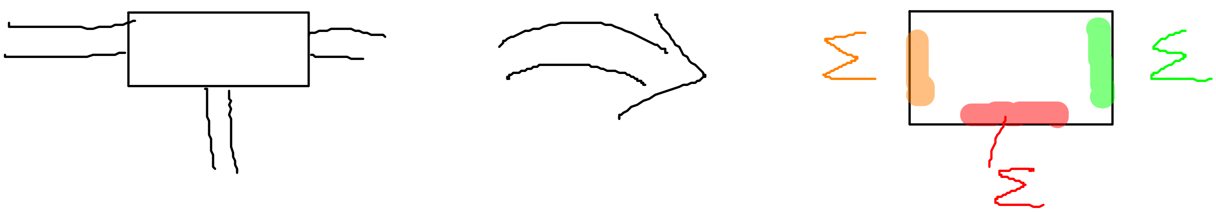
$$\Gamma = i\left[\Sigma^r_X - \Sigma^a_X\right] \qquad X = L, R$$

Transmission als Matrixmultiplikation

T, G nur im Bereich von C zu bestimmen

γ_{XX} nur für an C koppelnde Atome zu bestimmen

unendliche System — äquiv. endl. Leiter



Interpretation Σ

$$H_{CC}\,\Psi_{\alpha 0} = \varepsilon_{\alpha 0}\,\Psi_{\alpha 0}$$

$$\underbrace{(H_{CC} + \Sigma^{r})}_{\text{nicht hermitesch wegen } \Sigma^{+} \neq \Sigma}\,\Psi_\alpha = \varepsilon_\alpha\,\Psi_\alpha$$

$\Sigma = \Sigma_L + \Sigma_R$

$\Rightarrow$ ε_α auch komplex

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

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

zeitl. Zerfall der WF

$$P_\alpha(t) = |\Psi_\alpha(t)|^2 \propto e^{-\frac{\gamma_\alpha}{2}t}$$

Zerfall $\hat{=}$ Elektron geht in die Elektroden und "zerfällt" somit für die Mitte C

γ_α : endl. Lebensdauer der Elektronen im Bereich C

$\tau_\alpha = \frac{\hbar}{\gamma_\alpha} \longrightarrow$ e^- verschwindet in Elektrode

Greensche Funktion für nicht-hermiteschen "Hamiltonian"

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

$$L\,|\lambda_n^L\rangle = \lambda_n^L\,|\lambda_n^L\rangle$$

$$\langle\lambda_n^R|\,L = \lambda_n^R\,\langle\lambda_n^R| \iff L^+\,|\lambda_n^R\rangle = \lambda_n^{R*}\,|\lambda_n^R\rangle$$

Verknüpfung λ_n^L, λ_n^R

$$|L-\lambda^L 1| = 0$$

$$\underbrace{|L^+-\lambda^{R*}1|}_{\det(\,)} = 0 \qquad |A^T| = |A|$$

$$= |L^*-\lambda^{R*}1| \implies |L-\lambda^R 1| = 0$$

Eigenwerte gleich aber EVe nicht

Wähle $\lambda_n^L = \lambda_n^R = \lambda_n$

$$\langle\lambda_n^R|\,L\,|\lambda_m^L\rangle = \lambda_m^L\,\langle\lambda_n^R|\lambda_m^L\rangle = \lambda_n^R\,\langle\lambda_n^R|\lambda_m^L\rangle$$

$$\implies 0 = (\lambda_m^L-\lambda_n^R)\,\langle\lambda_n^R|\lambda_m^L\rangle$$

$$\langle\lambda_n^R|\lambda_m^L\rangle = \delta_{nm}$$

Rechtsseitige und linksseitige EV bilden biorthonormale Basis

$$(z-L)\,G = 1$$

$$G = \sum_n \frac{|\lambda_n^L\rangle\langle\lambda_n^R|}{z-\lambda_n} \qquad \psi_n(\vec r) = \langle\vec r|\lambda_n^L\rangle$$

$$\phi(\vec r) = \langle\vec r|\lambda_n^R\rangle$$

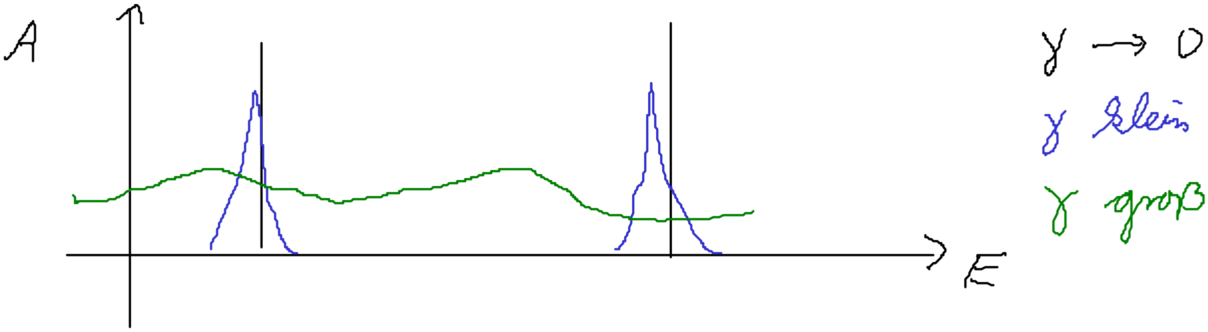
$$G^{r/a} = \sum_n \frac{\psi_n(\vec r)\,\phi_n^*(\vec r\,')}{(E-\varepsilon_n)^{?*}}$$

$$\varepsilon_n^{r/a} = \varepsilon_{\alpha 0} - \Delta_\alpha \mp \frac{\gamma_\alpha}{2}$$

$$A(\vec r,\vec r\,',E) = i\,(G^r - G^a)$$

$$? \to = \sum_n \psi_n(\vec r)\,\phi_n^*(\vec r\,')\,\frac{\gamma_\alpha}{(E-\varepsilon_{\alpha 0}+\Delta_\alpha)^2+\left(\frac{\gamma_\alpha}{2}\right)^2}$$

$$\xrightarrow[\gamma_\alpha\to 0]{} \sum \psi_n(\vec r)\,\phi_n^*(\vec r\,')\,2\pi\,\delta(E-\varepsilon_{\alpha 0}+\Delta_\alpha)$$



Zwei Effekte:

- Verschiebung der Eigenenergien
- Verbreiterung durch endl. Lebensdauer

TB - Hamiltonian

$$H = \sum_\ell |\ell\rangle \varepsilon_\ell \langle \ell| + \sum |\ell\rangle V_{\ell m} \langle m|$$

Onsite - Energie Hüpfelemente

$\langle \ell | m\rangle = \delta_{\ell m}$ $\quad 1 = \sum_n |n\rangle\langle n|$

Translationsinvarianz $\varepsilon_\ell = \varepsilon_0$, $V_{\ell m} = V_{0,m-\ell}$

$$|k\rangle = \frac{1}{\sqrt{N}} \sum_j e^{ikj} |j\rangle$$ (lokaler Zustand am Gitterplatz j)

$$E(k) = \varepsilon_0 + \sum_\ell V_{0\ell}\, e^{ik\ell}$$

$$\langle k|H|k'\rangle = \frac{1}{N} \sum_{j\ell\ell'j'} \langle j|n\rangle H_{\ell\ell'} \langle \ell|j'\rangle e^{-ik\ell} e^{ik'\ell'}$$

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

j fest, j' liefert alle Beiträge
$\Rightarrow$ j gibt das N-fache

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

$$= \delta_{kk'} \sum_j H_{0j}\, e^{ik'j} \quad \Rightarrow \quad H_{kk'} \text{ diagonal}$$

$$H|\psi\rangle = E|\psi\rangle$$

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

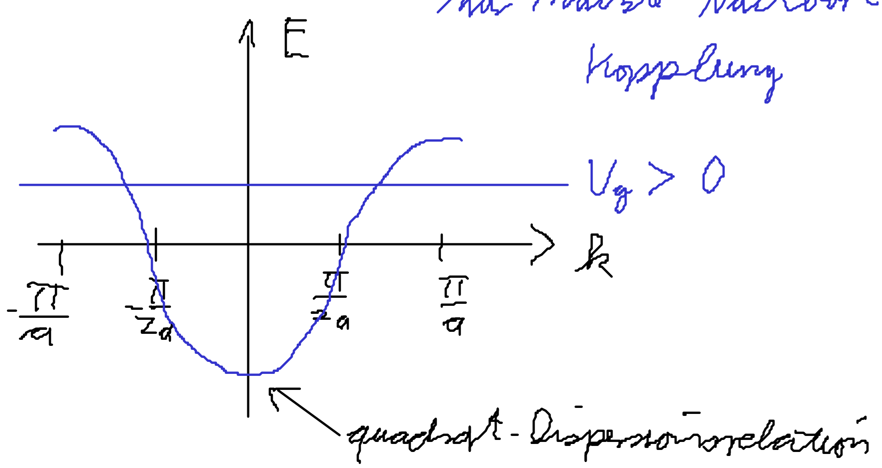
$$\left(\sum_j H_{0j}\, e^{ikj}\right)\langle k|\psi\rangle = E\,\langle k|\psi\rangle$$

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

1D – Kette

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

(nur nächste Nachbar-Kopplung



$$G \propto V_g \frac{1}{N^{1D}} = \frac{dE}{dk}\,\frac{1}{\frac{dE}{dk}} = \begin{cases} 1 & \varepsilon_0 + 2t < E < \varepsilon_0 - 2t \\ 0 & \text{sonst} \end{cases}$$