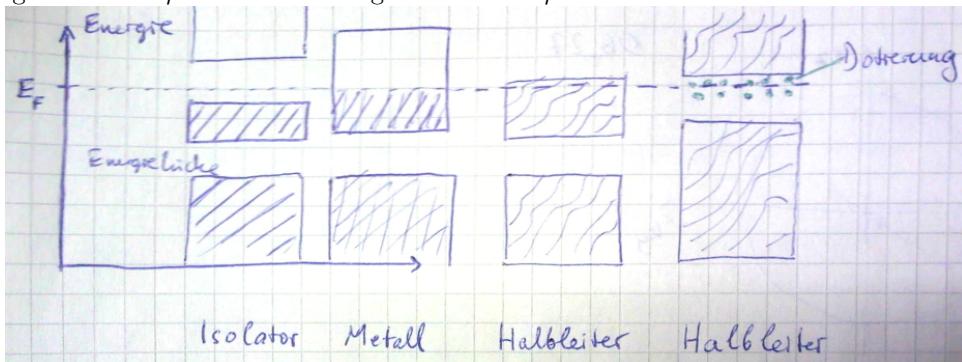


# Chapter 9

## Energiebänder

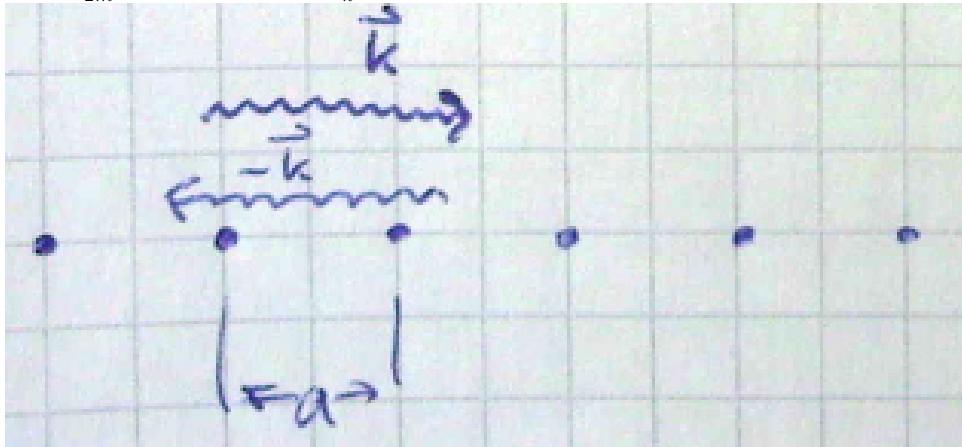
Oder warum unterscheiden wir zwischen Halbleiter, Leiter und Isolatoren.

'gute' Leiter:  $\rho \approx 10^{-10} \Omega \cdot cm$  'gute' Isolator:  $\rho \approx 10^{22} \Omega \cdot cm$



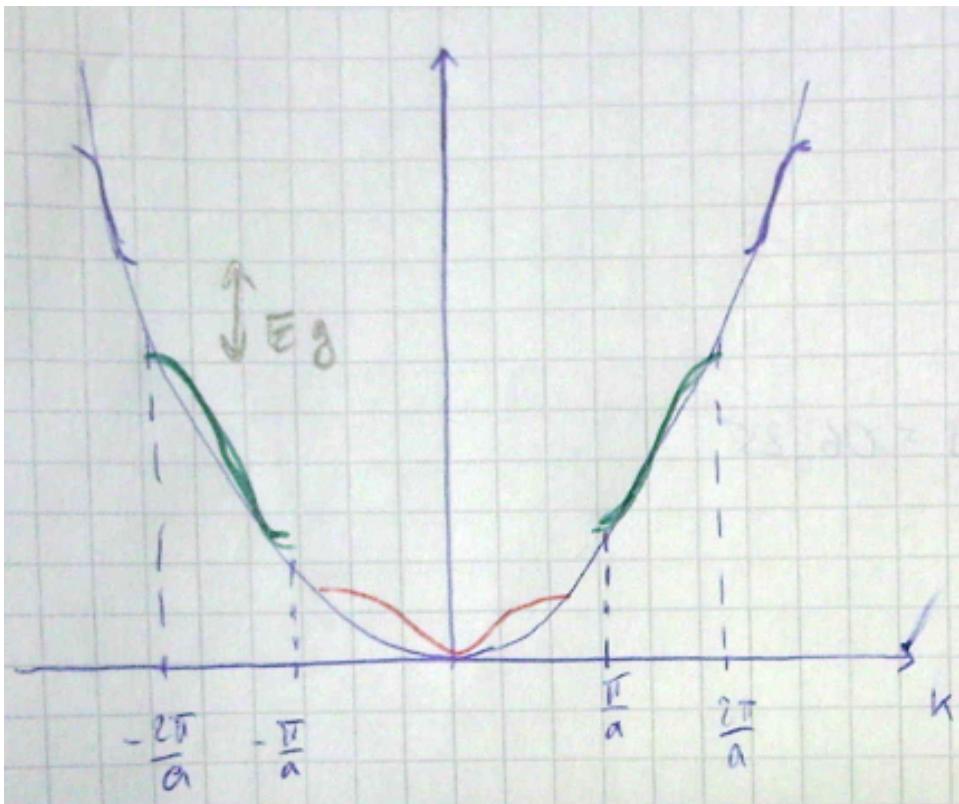
1 Beispiel: Modell des nahezu freien Elektronen

$$E_x = \frac{\hbar^2 k^2}{2m}; \text{ Wellenfunktion } \psi_{\vec{k}} = e^{i\vec{k}\vec{r}}$$



Laue (Bragg-Reflektion)  $-\vec{k} + \vec{G} = \vec{k}$  mit reziproken Gitter  $\vec{G}$

$$(-\vec{k} + \vec{G})^2 = \vec{k}^2 \Rightarrow 2kG = G^2; \quad k = \frac{G}{2} = \pm \frac{\pi}{2} n_G$$

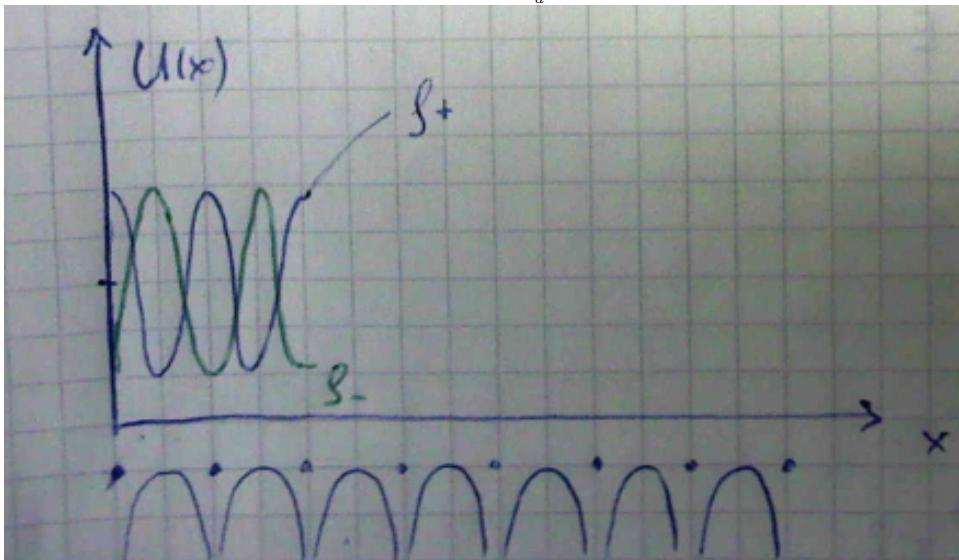


Zwei verschiedene Stehende Wellen:

$$\psi_+ \propto e^{i\frac{\pi x}{a}} + e^{-i\frac{\pi x}{a}} = 2\cos\frac{\pi x}{a}$$

$$\psi_- \propto e^{i\frac{\pi x}{a}} - e^{-i\frac{\pi x}{a}} = 2i\sin\frac{\pi x}{a}$$

Gruppengeschwindigkeit  $v_G = \frac{\partial E_k}{\partial p} = \frac{\hbar k}{m}|_{k=\pm\frac{\pi}{a}} = ! 0;$



$$\rho_+ = |\psi_+|^2 \propto \cos^2 \frac{\pi x}{a} = \frac{1}{2}(1 + \cos^2 \frac{2\pi x}{a})$$

$$\rho_- = |\psi_-|^2 \propto \sin^2 \frac{\pi x}{a} = \frac{1}{2}(1 - \cos^2 \frac{2\pi x}{a})$$

Wahrscheinlichkeitsdichte  $\psi^* \psi = |\psi|^2$ ;  $\rho_0 = 1e = e^{-ikx} e^{ikx} e$

Erwartungswert der Potentiellen Energie:  $E_{\rho_+} < E_{\text{frei}} < E_{\rho_-}$ ,  $U(x) = U \cos \frac{2\pi x}{4}$ ;

$$E_g = \frac{1}{a} \int dx U(x) [|\psi_-|^2 - |\psi_+|^2] \quad (9.1)$$

$$= \frac{2U}{a} \int_0^a dx \cos \frac{2\pi x}{a} \left[ 1 - \cos \frac{2\pi x}{a} - 1 + \cos \frac{2\pi x}{a} \right] \quad (9.2)$$

$$= \frac{2U}{a} \int_0^a dx \cos^2 \frac{2\pi x}{a} \quad (9.3)$$

$$= \frac{U}{a} \int_0^a dx (1 + \cos \frac{4\pi x}{a}) \quad (9.4)$$

$$= \frac{U}{a} \left( x + \frac{a}{4\pi} \sin \frac{4\pi x}{a} \right) \Big|_0^a \quad (9.5)$$

$$\equiv U = E_B - E_A \quad (9.6)$$

Elektronen in einem periodischen Potential (QM)

$$H\psi(\vec{r}) = \left[ -\frac{\hbar^2}{2m} \nabla + \tilde{V}(\vec{r}) \right] \psi(\vec{r}) = E\psi(\vec{r})$$

Translationsinvariant:  $\tilde{V}(\vec{r}) = \tilde{V}(\vec{r} + \vec{l})$

Entwicklung nach reziproken Gittervektoren  $\vec{G}$  (blochscher Ansatz)

$$\tilde{V}(\vec{r}) = \sum_G \tilde{V}_G \cdot e^{i\vec{G}\vec{r}}$$

$$\psi(\vec{r}) = \sum_k c_k e^{ik\vec{r}}$$

Einsetzen in die SGL:

$$\sum_{\vec{k}} \frac{\hbar^2 k^2}{2m} c_k e^{i\vec{k}\vec{r}} + \sum_{k', \vec{G}} c_{k'} \tilde{V}_G e^{i(k' + \vec{G})\vec{r}} \equiv \sum_k c_k e^{i\vec{k}\vec{r}}$$

Umbenennung (summe über alle  $k'$ ):  $k' + \vec{G} = k \rightarrow$

$$0 = \sum_{\vec{k}} e^{i\vec{k}\vec{r}} \underbrace{\left[ \left( \frac{\hbar^2 k^2}{2m} - E \right) c_k + \sum_G \tilde{V}_G c_{\vec{k}-\vec{G}} \right]}_{=0}$$

$$\left( \frac{\hbar^2 k^2}{2m} - E \right) c_k + \sum_G \tilde{V}_G c_{\vec{k}-\vec{G}} = 0$$

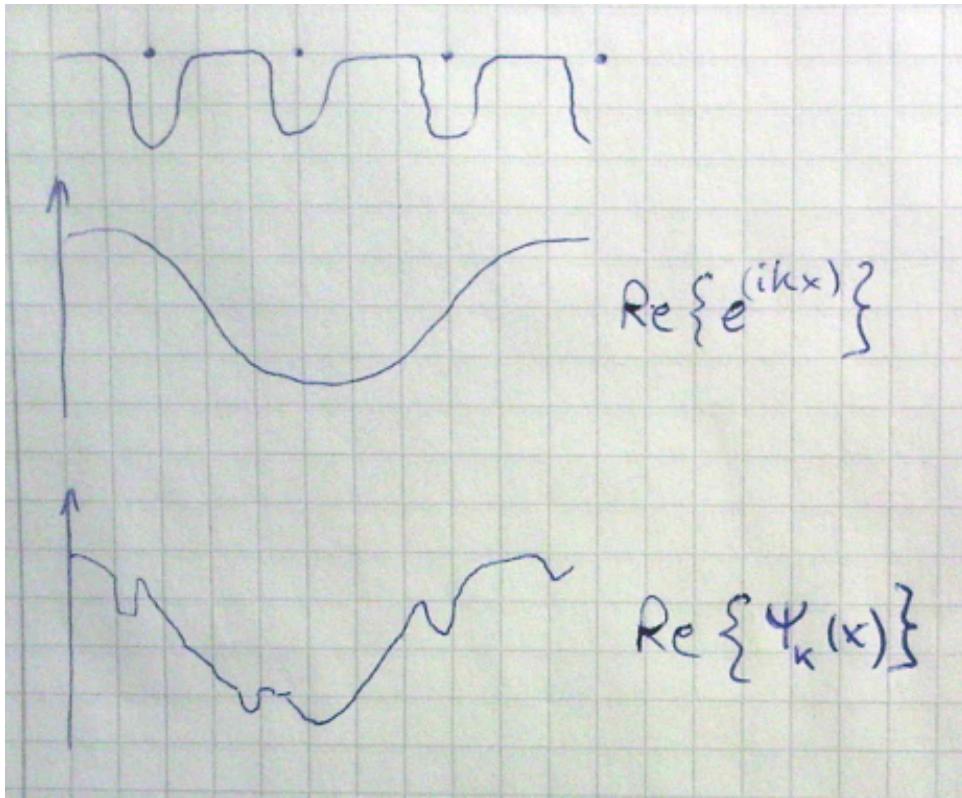
Dieser Satz algebraischer Gleichungen ist die Darstellung der Schrödigner Gleichung im  $\vec{k}$ -Raum  $\Rightarrow E_k$ -Energie Eigenwert.

$$\psi_k(\vec{r}) = \sum_{\vec{G}} c_{\vec{k}-\vec{G}} e^{i(\vec{k}-\vec{G})\vec{r}} \quad (9.7)$$

$$= \underbrace{e^{i\vec{k}\vec{r}}}_{\text{ebene Welle}} \underbrace{\sum_{\vec{G}} c_{\vec{k}-\vec{G}} e^{-i\vec{G}\vec{r}}}_{U_k(\vec{r})} \quad (9.8)$$

$$= U_k(\vec{r}) e^{i\vec{k}\vec{r}} \quad (9.9)$$

Bloch Theorem: Die Eigenfunktionen der SG. für ein periodisches Potential sind das Produkt aus einer ebenen Welle und einer Funktion  $U_k(\vec{r})$  mit der Periodizität des Gitters.



$$\psi_k(\vec{r} + \vec{R}) = \underbrace{U_k(\vec{r} + \vec{R}) e^{i\vec{k}\vec{r}}}_{\psi_{\vec{r}}} e^{i\vec{k}\vec{R}} \quad (9.10)$$

$$\psi_{k+G}(\vec{r}) \sum_G c_{k+g'-G} e^{i(\vec{k}+G'-G)\vec{r}}$$

Umbenennung  $G'' = G - G'$

$$\Rightarrow e^{i\vec{k}\vec{r}} \sum_{G''} \underbrace{c_{\vec{k}-\vec{G}''} e^{-i\vec{G}''\vec{r}}}_{U_{\vec{k}}(\vec{r})}$$

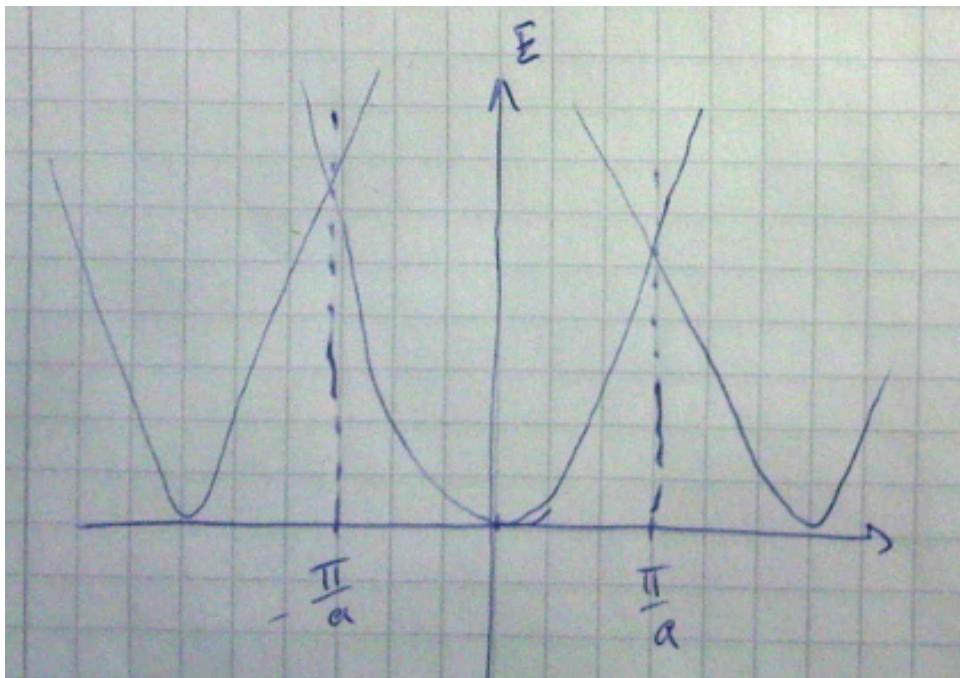
$$\Rightarrow \psi_{\vec{k}+\vec{a}}(\vec{r}) = \psi_k(\vec{r})$$

$$H\psi_{k+G}(\vec{r}) = E_{\vec{k}+\vec{G}'} \psi_{\vec{k}+\vec{G}'}(\vec{r})$$

$$H\psi_k(\vec{r}) = E_{\vec{k}+\vec{G}'} \psi_{\vec{k}}(\vec{r})$$

$$\Rightarrow E_{k+G'} = E_k$$

Lösung der SG. an der Grenze der Brillouin Zone.



$$(E - \frac{\hbar^2}{2m}|k - G|^2)c_{k-G} = \sum_G \tilde{V}_{G'} c_{k-G-G'}$$

$$c_{k-G} = \frac{\sum_G \tilde{V}_{G'} c_{k-G-G'}}{E - \frac{\hbar^2}{2m}|k - G|^2} \quad (9.11)$$

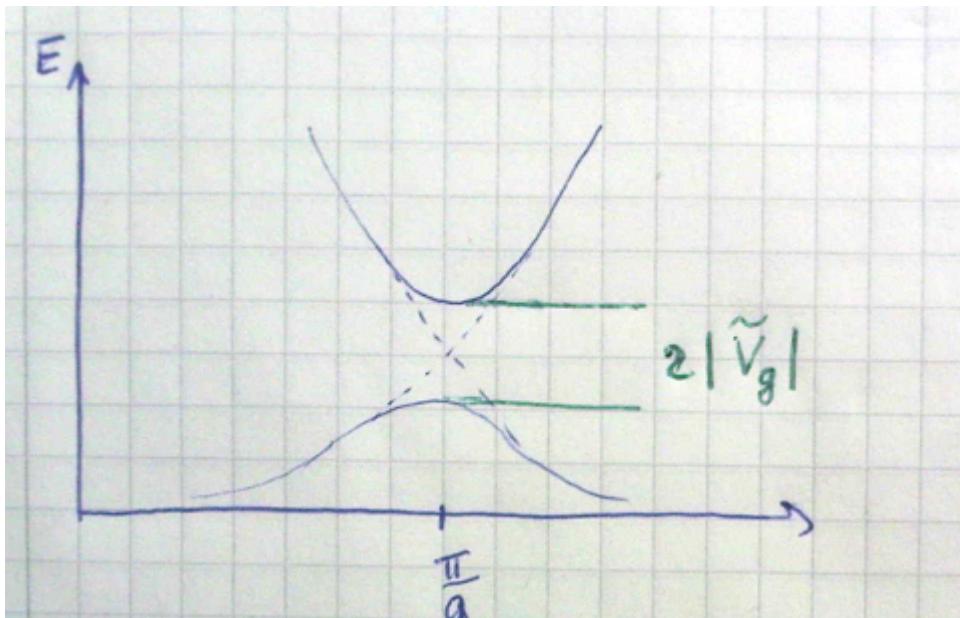
$$= \frac{\sum_{G''} V_{G''-G} c_{k-G''}}{\frac{\hbar^2}{2m}(k^2 - |k - G|^2)} \quad (9.12)$$

Umbenennung:  $G = G'' - G$  Nullstellen:  $k^2 = |\vec{k} - \vec{G}|^2$  Abkürzungen  $g = \frac{2\pi}{a}$ ;  $G = 0, G = g; \lambda_k = \frac{\hbar^2 k^2}{2m}$   
Zwei Komponenten Näherung

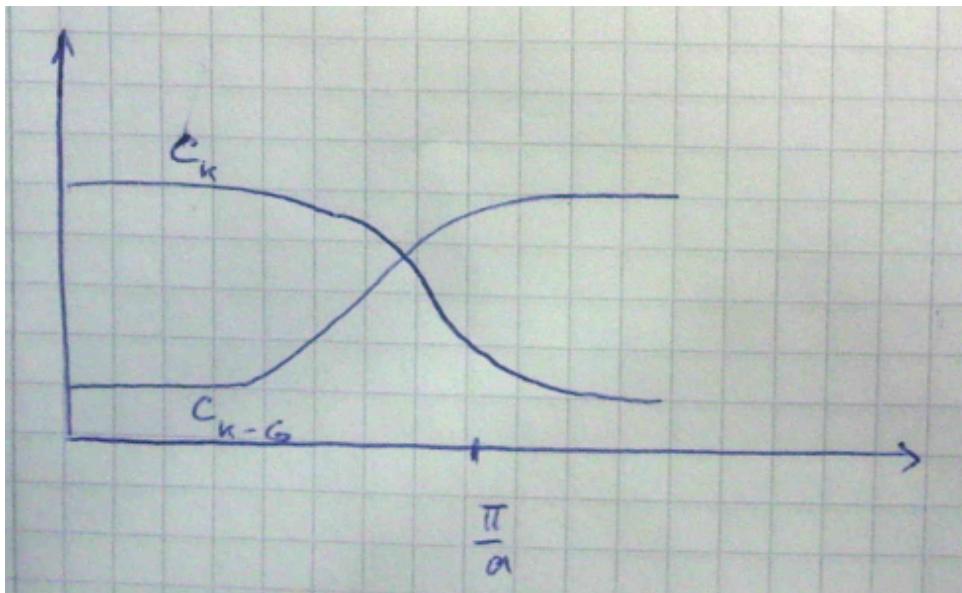
Erste Bedingung:  $\rightarrow (\lambda_k - E)c_k + \tilde{V}_g c_{k-g} = 0$  zweite Bedingung:  $\rightarrow (\lambda_{k-g} - E)c_{k-g} + \tilde{V}_g c_k = 0$

Daraus resultieren Energieniveaus:  $E_{\pm} = \frac{1}{2}(\lambda_{k-g} + \lambda_k \pm \sqrt{(\lambda_{k-g} - \lambda_k)^2 + \tilde{V}_g^2})$  und  $k = \frac{g}{2} \rightarrow \lambda_{k-g} = \lambda_k$   
An der Grenze der Brillouin Zone

$$E_{\pm} = E_{\frac{g}{2}} \pm |\tilde{V}_g|$$

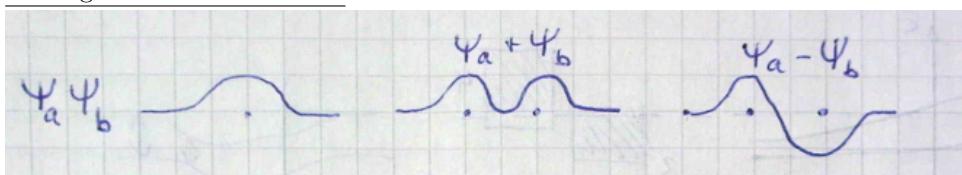


$$\frac{c_{k-G}}{c_k} = \frac{E-\lambda}{\tilde{V}_g}$$

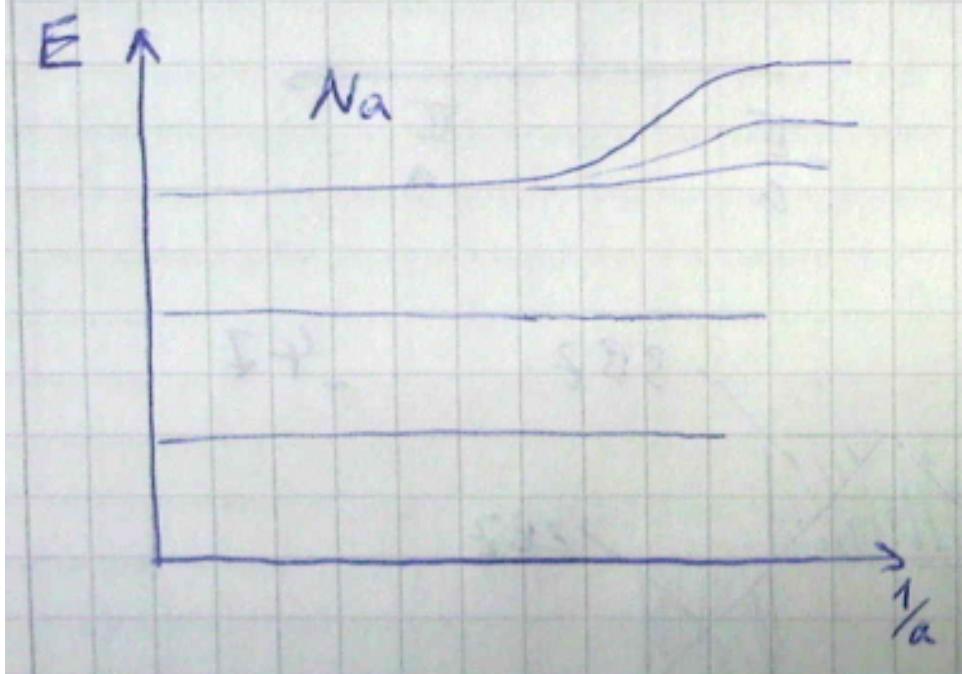


## 9.1 Tight-binding Model

'stark gebundene Elektronen'



$$\rho \propto |\psi_a - \psi_b|^2$$



Combination of Atomic Orbitals

LCAO = Linear Combination of Atomic Orbitals

$$H\phi = E\phi$$

$$H = H_A + H_S \quad (m \neq n)$$

$$H = -\frac{\hbar^2}{2m} \nabla + \tilde{V}(\vec{r} - \vec{R}_m) \quad R_m \equiv \text{Gittervektor}$$

$$H_S = \sum_{n \neq m} \tilde{V}_A(\vec{r} - \vec{R}_n)$$

Energie eigenwerte  $E_k$

$$E_k = \frac{\int \psi^* H \psi dV}{\int \psi^* \psi dV}$$

$$\psi_{\vec{k}} = \sum_m a_m \phi(\vec{r} \cdot \vec{R}_m) \quad a_m = \frac{1}{\sqrt{N}} e^{i \vec{k} \cdot \vec{R}_m} \quad N \equiv \text{Anzahl der Atome}$$

Bloch-Funktionen → orthonormal Basis lokalisierter Zustände Wnnier-Funkitonen

$$w_m(\vec{r} \cdot \vec{R}_m) = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{-i \vec{k} \cdot \vec{R}_m} \psi_{\vec{k}}(\vec{r} - \vec{R}_m)$$

$$\psi = \frac{1}{\sqrt{N}} \sum_{\vec{R}_m} e^{i \vec{k} \cdot \vec{R}_m} w_m(\vec{r} - \vec{R}_m)$$

$$E_{\vec{k}} = \underbrace{\frac{1}{\int \phi^* \phi dV}}_{=1 \text{ Wellenfkt kaum Überlappung}} \frac{1}{N} \sum_{m,n} e^{i k(R_m - R_n)} \int \phi^*(r - R_n) [H_A + H_S(\vec{r} - \vec{R}_m) \phi(\vec{r} - \vec{R}_m)] dV$$

$$\alpha = - \int \phi^*(r - R_m) H_s(\vec{r} - \vec{R}_m) \phi(\vec{r} - \vec{R}_m) dV \equiv \text{Energieänderung durch das Nachbarpotential}$$

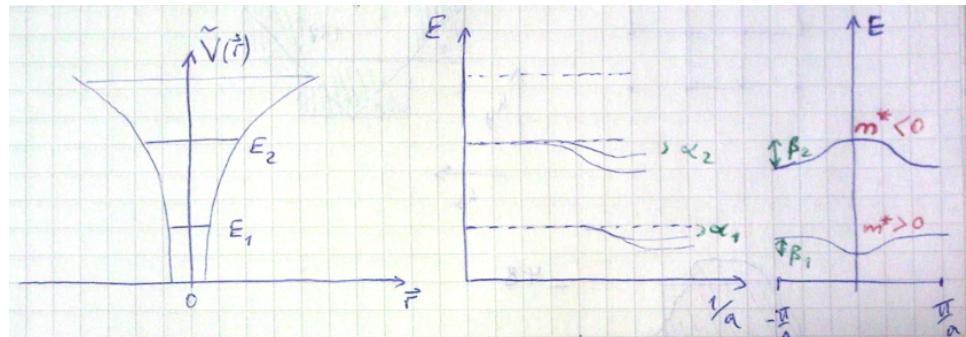
$$\beta = - \int \phi^*(r - R_n) H_S(\vec{r} - \vec{R}_m) \phi(\vec{r} - \vec{R}_n) dV \equiv \text{Energieänderung durch den Überlapp der W.F.}$$

$$E_{ki} = E_i - \alpha_i - \sum \beta_{i,n} e^{i k(R_n - R_m)} \quad (9.13)$$

$$= E_i - \alpha_i 2 \beta_i (\cos(k_x a) + \cos(k_y a)) \quad (9.14)$$

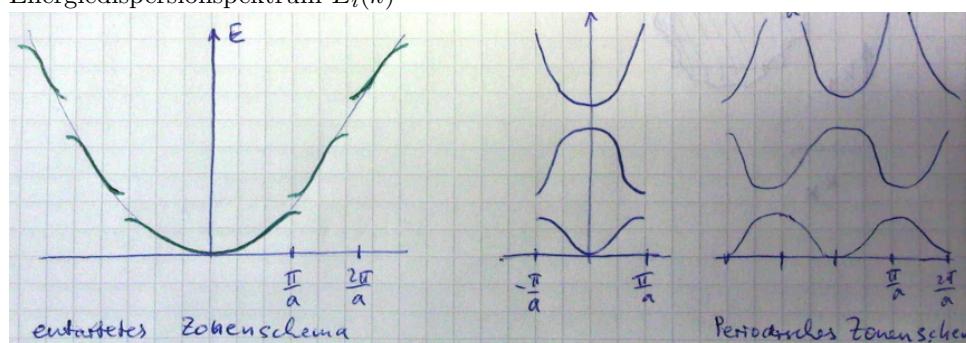
Für ein kubisch primitives Gitter  $R_m - R_n = (\pm a, 0, 0), (0 \pm a, 0), (0, a \pm a); \Rightarrow$  Entwickeln für kleine  $k$ :

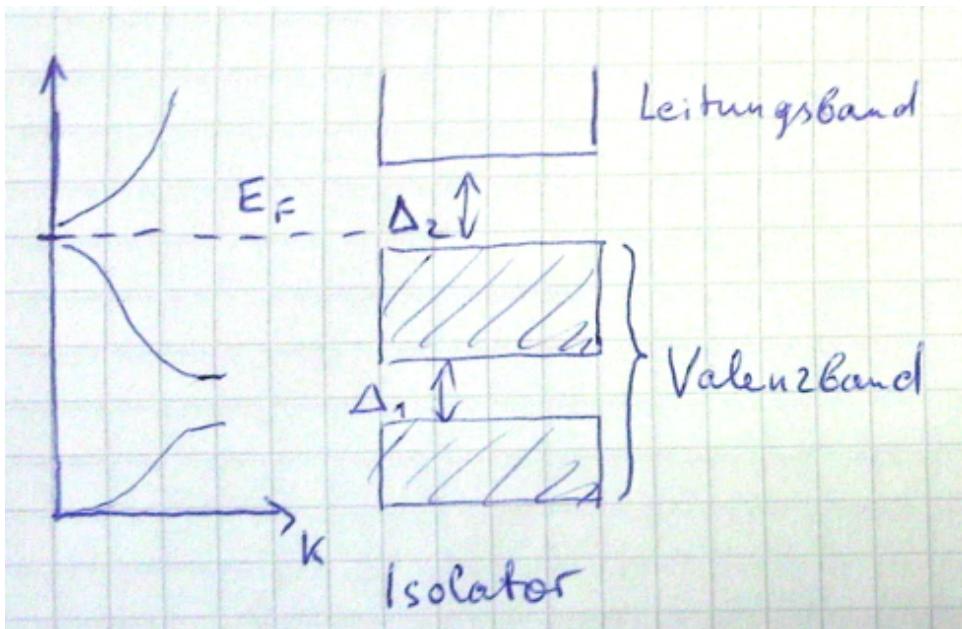
$$E_{k,i} = E_i - \alpha_i - 6\beta_i + \beta_i a^2 k^2$$



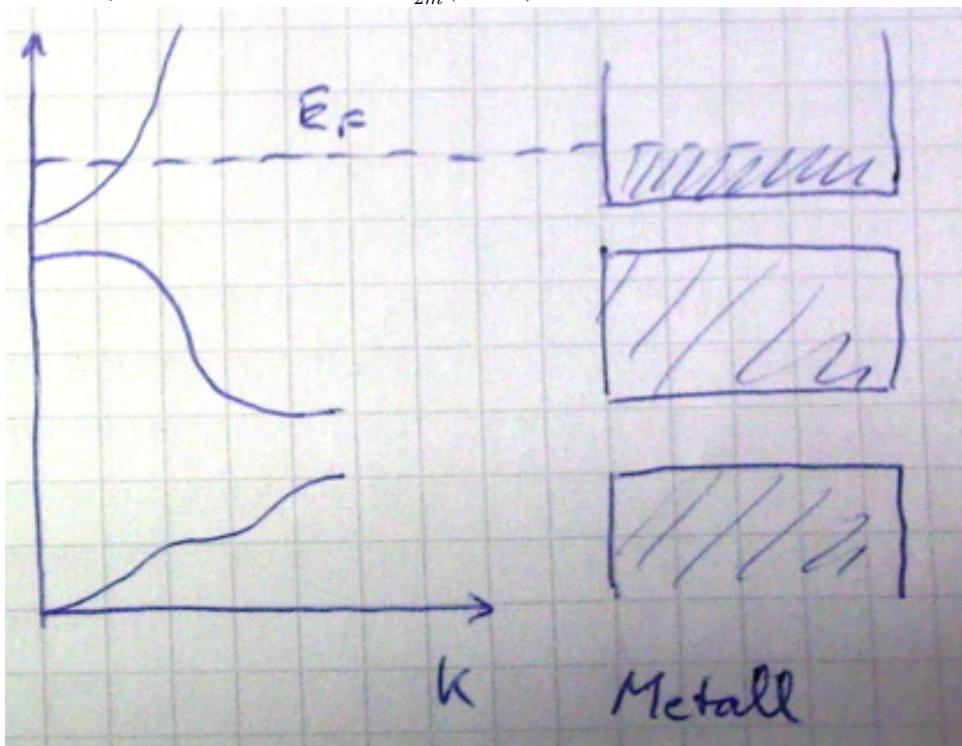
$$E_i = \frac{\hbar^2 k^2}{2m} \Rightarrow m_i^* = \frac{\hbar^2}{2\beta_i a^2}$$

Energiedispersionspektrum  $E_i(k)$

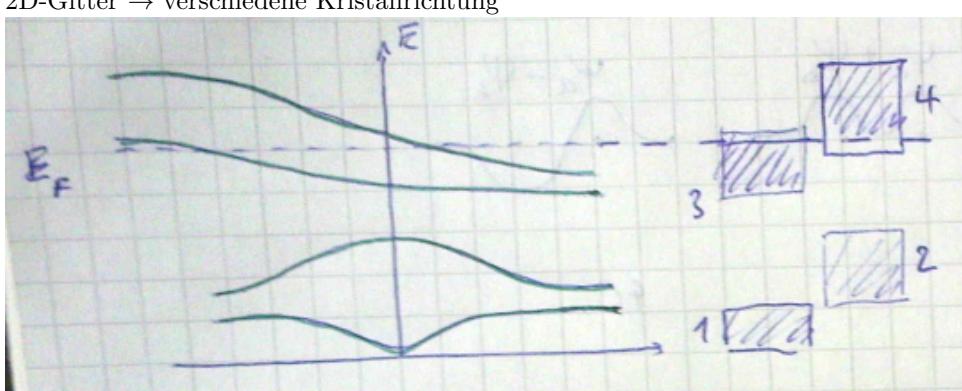




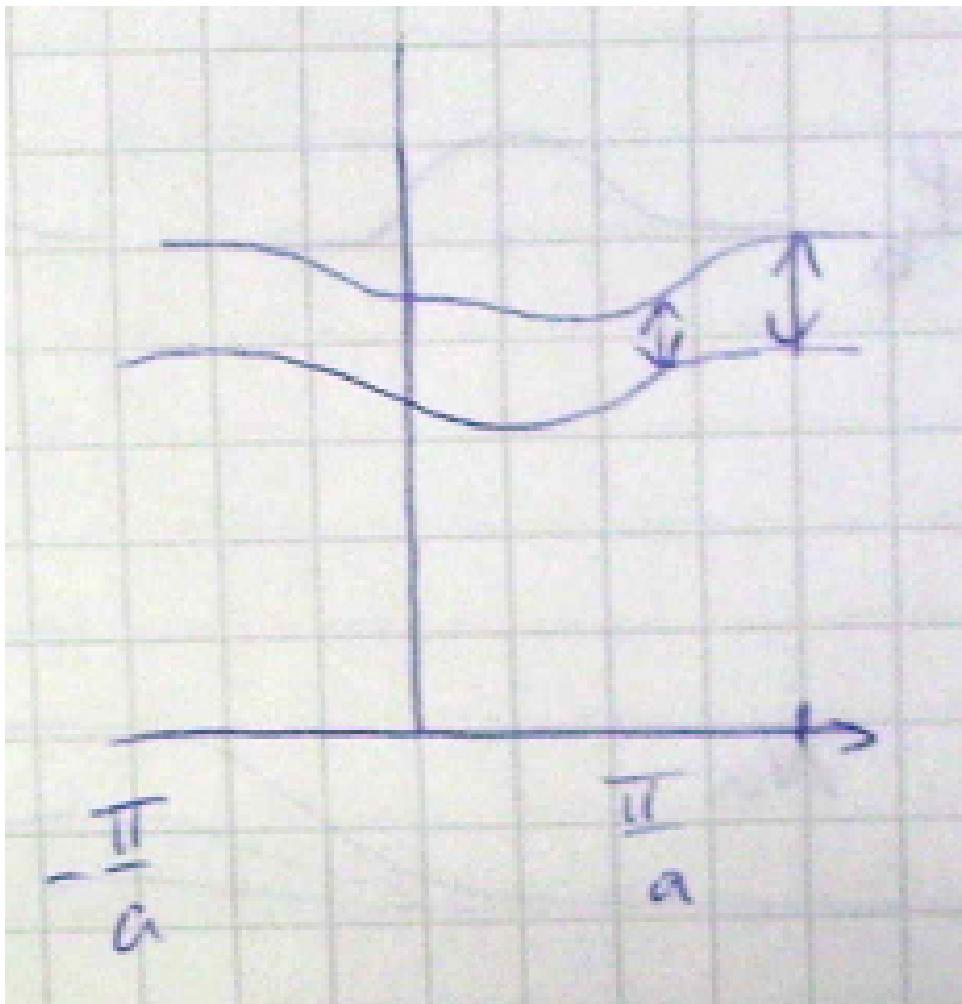
Isolator,  $\rho = 10^7 - 10^{14} \Omega m$ ;  $E_F = \frac{\hbar^2}{2m}(3\pi^2 n_e)^{2/3}$



Metall:  $\rho = 10^{-4} - 10^{-8} \Omega m$ ;  
2D-Gitter  $\rightarrow$  verschiedene Kristallrichtung

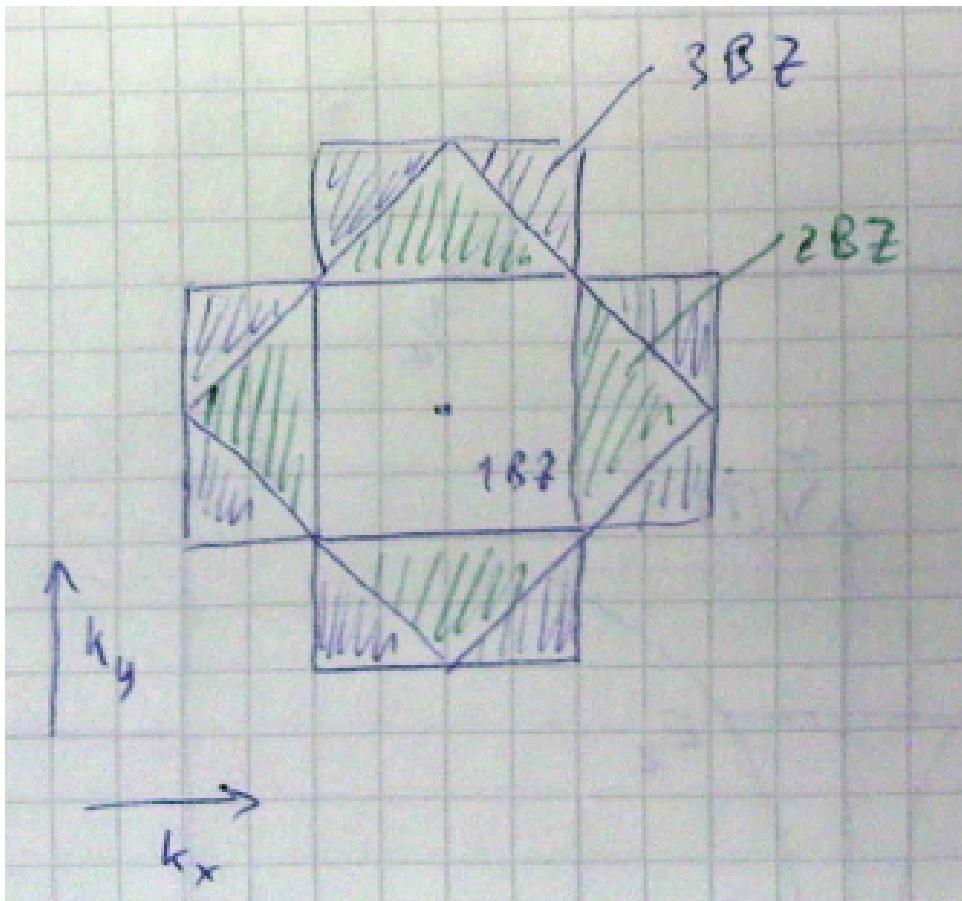


Halbmetalle As, Sb(Antimon), Bi



## 9.2 Brillouin-Zonen und Fermi- Flächen

Brillouin-Zonen und Fermi Flächen (2D BZ)



an der zonengrenze (stehende Wellen)

$$\frac{\partial \omega}{\partial k} = \frac{1}{\hbar} \vec{\nabla} E_{\perp} = 0$$

