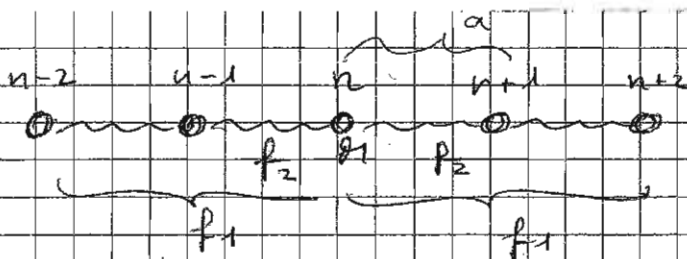


12)



$$f_2 \ll f_1$$

Bewegungsgl. f. us: "Equazione del moto"

$$M \ddot{u}_n + \phi \begin{pmatrix} n & n-1 \\ 1 & 1 \end{pmatrix} u_{n-1} + \phi \begin{pmatrix} n & n \\ 1 & 1 \end{pmatrix} u_n + \phi \begin{pmatrix} n & n+1 \\ 1 & 1 \end{pmatrix} u_{n+1} + \phi \begin{pmatrix} n & n-2 \\ 1 & 1 \end{pmatrix} u_{n-2} + \phi \begin{pmatrix} n & n+2 \\ 1 & 1 \end{pmatrix} u_{n+2} = 0$$

$$\phi \begin{pmatrix} n & n-1 \\ 1 & 1 \end{pmatrix} = \phi \begin{pmatrix} n & n+1 \\ 1 & 1 \end{pmatrix} = -f_2 \quad \leftarrow \text{Skript 9.2}$$

$$\phi \begin{pmatrix} n & n-2 \\ 1 & 1 \end{pmatrix} = \phi \begin{pmatrix} n & n+2 \\ 1 & 1 \end{pmatrix} = -f_1$$

$$\phi \begin{pmatrix} n & n \\ 1 & 1 \end{pmatrix} = 2f_2 + 2f_1$$

$$\rightarrow M \ddot{u}_n = f_2 u_{n-1} - 2f_2 u_n + 2f_1 u_n - f_2 u_{n+1} - f_1 u_{n-2} - f_1 u_{n+2}$$

$$\Rightarrow u_{s+n} = u_0 \cdot e^{i(nqa - \omega t)} \quad \rightarrow \ddot{u}_n = -u_0 \cdot \omega^2 e^{i(nqa - \omega t)}$$

$$M \ddot{u}_n + f_2 \cdot (u_{n-1} + 2u_n - u_{n+1}) + f_1 \cdot (2u_n - u_{n-2} - u_{n+2}) = 0$$

$$M \ddot{u}_n + f_2 u_0 \cdot e^{i\omega t} \cdot (-e^{i(n-1)qa} + 2 \cdot e^{inqa} - e^{i(n+1)qa}) + f_1 u_0 \cdot e^{-i\omega t} \cdot (2 \cdot e^{inqa} - e^{i(n-2)qa} - e^{i(n+2)qa}) = 0$$

$$M \ddot{u}_n + f_2 u_0 \cdot e^{-i\omega t} \cdot \frac{e^{inqa}}{2} 2(\cos(qa) - 1) + f_1 u_0 \cdot e^{-i\omega t} \cdot \frac{e^{inqa}}{2} 2(\cos(2qa) - 1) = 0$$

$$- M \omega^2 \cdot u_0 \cdot e^{inqa - i\omega t} \quad \quad \quad$$

$$\Rightarrow \frac{M \omega^2}{2} + f_2 (\cos(qa) - 1) + f_1 (\cos(2qa) - 1) = 0$$

$$\omega^2 = \frac{2}{M} [f_2 (1 - \cos(qa)) + f_1 (1 - \cos(2qa))] \quad \text{H. 9.1}$$

$$\omega^2 = \frac{4}{M} [f_2 (\sin \frac{qa}{2})^2 + f_1 (\sin qa)^2]$$

$$\omega(q) = 2 \cdot \sqrt{\frac{f_2 (\sin \frac{qa}{2})^2 + f_1 (\sin qa)^2}{M}}$$

$$2(1 - \cos \alpha) = 4(\sin \frac{\alpha}{2})^2$$

$$\alpha_1 = qa$$

$$\alpha_2 = 2qa$$

$$\Rightarrow \vec{k} \gg \vec{k}_1 \quad \vec{k}_1 \gg \vec{k}_2$$

$$\omega(q) \approx 2 \cdot \sqrt{\frac{k_2 \left(\sin \frac{qa}{2} \right)^2}{\eta}} = 2 \cdot \left| \sin \left(\frac{qa}{2} \right) \right| \cdot \sqrt{\frac{k_2}{\eta}}$$

↳ Dispersionsrelation f. akustische Phononen

"dispersione di fononi acustici"

12) anna-o

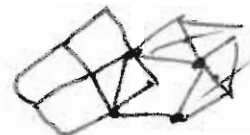
Ashcroft
Mermie

m-nächster Nachbar

$$U = \sum_n \sum_{m>0} \frac{1}{2} K_m (u(na) - u([n+m]a))^2$$

$$\epsilon_{1D} := \omega = 2 \cdot \sqrt{\sum_{m>0} K_m \frac{\sin^2(\frac{1}{2} m ka)}{m}}$$

$$13) \quad m \frac{d\vec{u}}{dt^2} = \vec{F} = (\vec{e}(\vec{e} u_e))$$



nächst. Nachbar eigentl. $\frac{1}{\sqrt{2}}$ entfernt
übernächste 1 entf.

$$\vec{R} = \frac{\vec{R}}{R}$$

$$\hat{R}_\mu \hat{R}_\nu = (\hat{R} \hat{R})_{\mu\nu}$$

$$\vec{k} = \begin{pmatrix} k \\ 0 \\ 0 \end{pmatrix} \quad D = \sum_{\vec{R}} \sin^2\left(\frac{1}{2} \vec{k} \cdot \vec{R}\right) (A \mathbb{1} + B \vec{R} \vec{R})$$

$\omega = \sqrt{\frac{2}{M}}$ λ .. EW von D -Matrix
Ursprung $\vec{R} = 0$

12 nächste Nachbarn $\frac{a}{2}(\pm \vec{x} \pm \vec{y})$ ①

$$D - \lambda \mathbb{1} = 0 \quad \text{EW-Gleichung}$$

$\frac{a}{2}(\pm \vec{y} \pm \vec{z})$ ②

$\frac{a}{2}(\pm \vec{z} \pm \vec{x})$ ③

$$\sum \sin^2\left(\frac{1}{2} \vec{k} \cdot \vec{R}\right) (A \mathbb{1} + B \vec{R} \vec{R}) - \lambda \mathbb{1} = 0$$

$$\sin^2\left(\frac{1}{2} \frac{1}{2} a (\pm \vec{x} \pm \vec{y})\right) \begin{pmatrix} k \\ 0 \\ 0 \end{pmatrix} (A \mathbb{1} + B (\pm \vec{x} \pm \vec{y})(\pm \vec{x} \pm \vec{y}) \frac{1}{2}) +$$

$$\dots \sin^2\left(\frac{1}{2} \frac{1}{2} a (\pm \vec{y} \pm \vec{z})\right) \begin{pmatrix} 0 \\ k \\ 0 \end{pmatrix} (A \mathbb{1} + B (\pm \vec{y} \pm \vec{z})(\pm \vec{y} \pm \vec{z}) \frac{1}{2}) +$$

$$\dots \sin^2\left(\frac{1}{2} \frac{1}{2} a (\pm \vec{z} \pm \vec{x})\right) \begin{pmatrix} 0 \\ 0 \\ k \end{pmatrix} (A \mathbb{1} + B (\pm \vec{z} \pm \vec{x})(\pm \vec{z} \pm \vec{x}) \frac{1}{2}) - \lambda \mathbb{1} = 0$$

$\pm k$

$\rightarrow$ fällt bei k weg weil $\sin^2$ symm. ist

$$\sin^2\left(\frac{1}{4} ak\right) (8A \mathbb{1} + B \frac{1}{2} (\text{Summe über alle Matrizen})) - \lambda \mathbb{1} = 0$$

$$\textcircled{1} \begin{pmatrix} \pm 1 \\ \pm 1 \\ 0 \end{pmatrix} (\pm 1 \pm 1 0) = \begin{pmatrix} \pm 1 & \pm 1 & 0 \\ \pm 1 & \pm 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \pm 1 \\ 0 \\ \pm 1 \end{pmatrix} (\pm 1 0 \pm 1) = \begin{pmatrix} \pm 1 & 0 & \pm 1 \\ 0 & 0 & 0 \\ \pm 1 & 0 & \pm 1 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} -1 & 1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & -1 \\ -1 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & -1 \\ -1 & 0 & 1 \end{pmatrix}$$

$$+ \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 8 & 0 & 0 \\ 0 & 8 & 0 \\ 0 & 0 & 8 \end{pmatrix} \rightarrow \text{Longitudinale Lsg.}$$

$$\rightarrow \text{Transversale Lsg.}$$

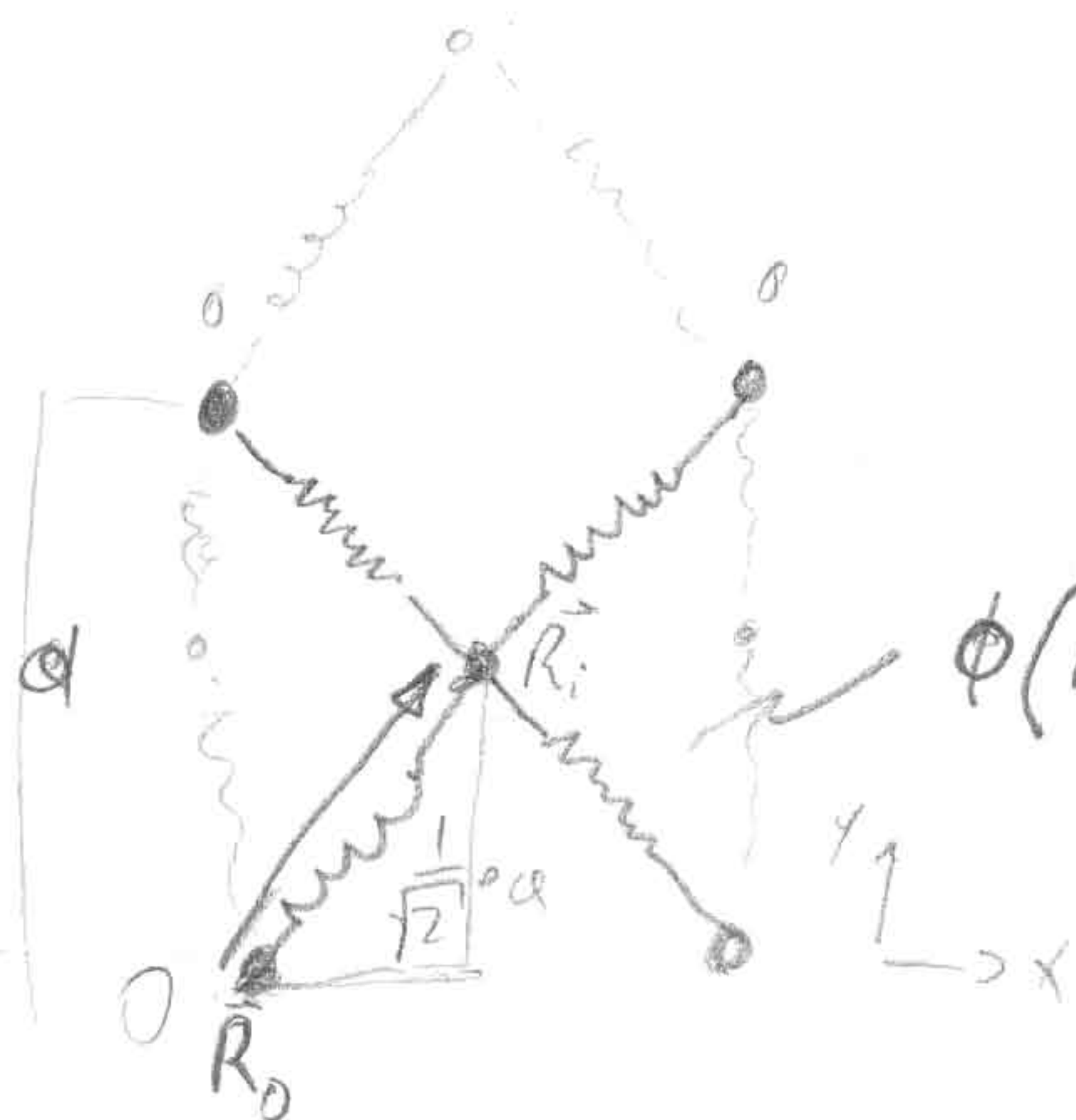
$$\lambda = \sin^2\left(\frac{1}{4} ak\right) (8A \mathbb{1} + B \frac{1}{2} 8)$$

$$\omega_L = \sqrt{\frac{8A + 4B}{M}} \sin\left(\frac{1}{4} ka\right)$$

$$\omega_T = \sqrt{\frac{8A + 2B}{M}} \sin\left(\frac{1}{4} ka\right)$$

$$\omega_L = \sqrt{\frac{8A + 4B}{M}} \sin\frac{1}{4} ka$$

15,



$$\phi(\vec{R}_0 - \vec{R}_i) = \frac{c}{2} (|\vec{R}_0 - \vec{R}_i| - |\vec{R}_0^0 - \vec{R}_i^0|)^2$$

$$\vec{R}_i^0 = \frac{a}{2} (\vec{e}_x + \vec{e}_y)$$

$$= \frac{a}{2} \begin{pmatrix} 1+0 \\ 0+1 \end{pmatrix} = \frac{a}{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\phi(\vec{R}_0 - \vec{R}_i) = \frac{c}{2} \left(\left| \vec{R}_0 - \begin{pmatrix} (1+\epsilon_{xx}) \cdot x \\ y \\ z \end{pmatrix} \right| - \left| \vec{R}_0^0 - \begin{pmatrix} x \\ y \\ z \end{pmatrix} \right| \right)^2$$

$$\vec{R}_i^0 = \frac{a}{2} \begin{pmatrix} \vec{e}_y + \vec{e}_z \\ \vec{e}_z + \vec{e}_x \\ \vec{e}_x + \vec{e}_y \end{pmatrix}$$

$$\vec{R}_i = \frac{a}{2} \begin{pmatrix} \vec{e}_y + \vec{e}_z \\ \vec{e}_z + (1+\epsilon_{xx})\vec{e}_x \\ (1+\epsilon_{xx})\vec{e}_x + \vec{e}_y \end{pmatrix}$$

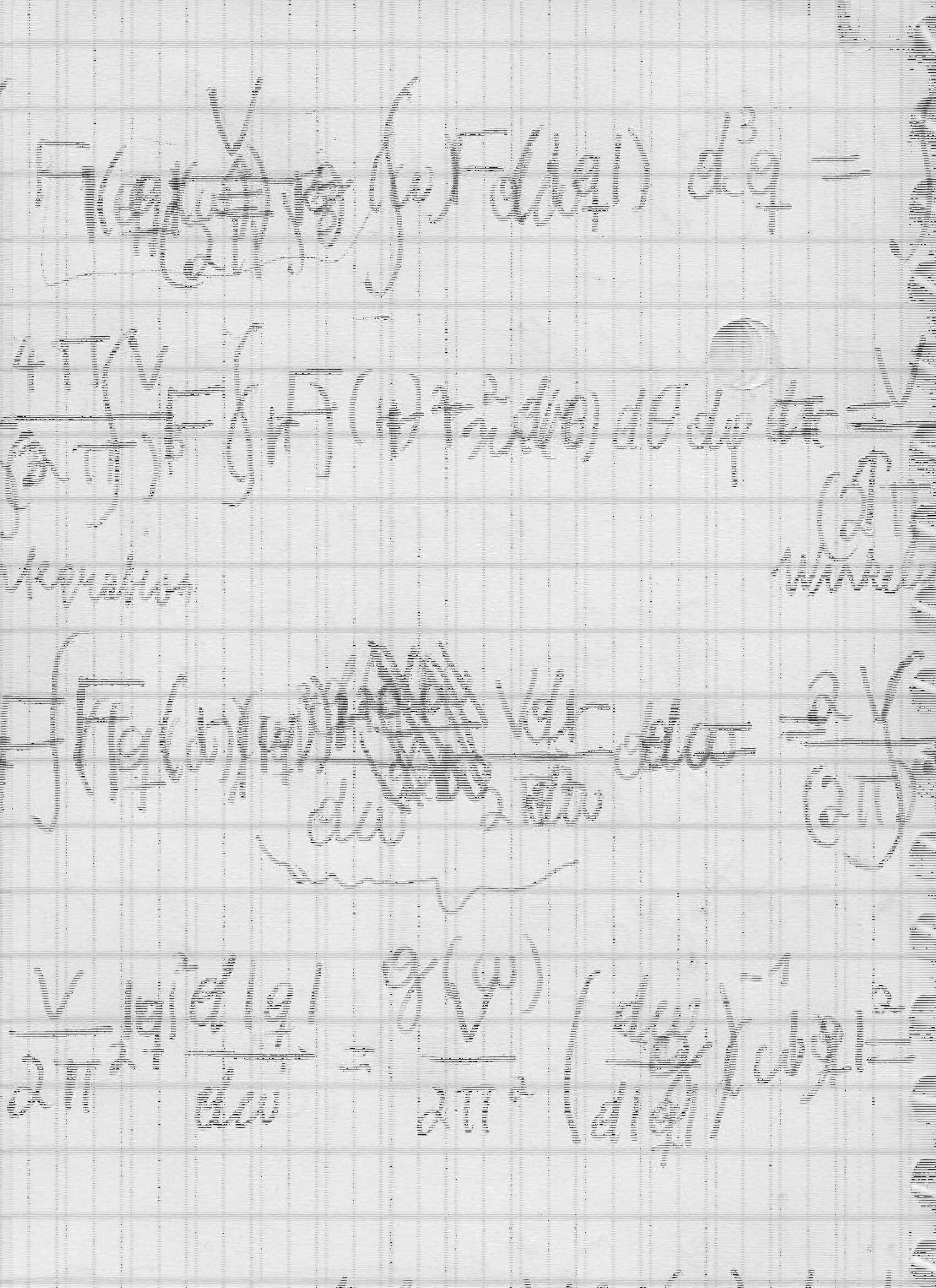
$$\vec{R}_i = \frac{a}{2} \begin{pmatrix} x(1+\epsilon_{xx}) \\ 1 \end{pmatrix}$$

$$\phi = \frac{c a^2}{2 z^2} \begin{pmatrix} x \epsilon_{xx} \\ 0 \end{pmatrix}^2$$

$$\phi' = \frac{c a^2 z}{2 z^2} \begin{pmatrix} x \epsilon_{xx} \\ 0 \end{pmatrix} \cdot \begin{pmatrix} \epsilon_{xx} \\ 0 \end{pmatrix}$$

$$\phi'' = \frac{c a^2}{2 z^2} \begin{pmatrix} \epsilon_{xx} \\ 0 \end{pmatrix} \begin{pmatrix} \epsilon_{xx} \\ 0 \end{pmatrix} = \frac{c a^2}{2 z^2} \epsilon_{xx}^2$$

$$\phi''_{\text{gesamt}} = \phi'' \cdot 4 \cdot 4 = 4 c a^2 \epsilon_{xx}^2$$

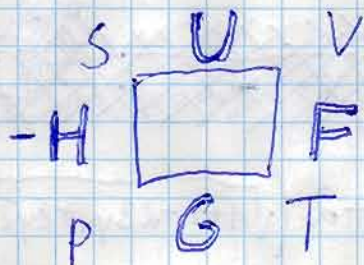


$$\epsilon_{12} = \frac{1}{2} \left(\frac{\partial v_1}{\partial x_2} + \frac{\partial v_2}{\partial x_1} \right) = \frac{1}{2} \epsilon_{yx}$$

$$\frac{\partial^2 E}{\partial \epsilon_{12}^2} = \frac{\partial^2 \left(\frac{c}{a^6} \epsilon_{yx}^2 \right)}{\partial \left(\frac{1}{2} \epsilon_{yx} \right)^2} = \frac{c}{a} \frac{4}{3} = c_{66} = c_{44}$$

19) (innere) Energie $U(S, V, N) = U$
 freie Energie $F(T, V, N) = U - TS$
 Enthalpie $H(S, p, N) = U + pV$
 freie Enthalpie $G(T, p, N) = U - TS + pV$
 großkanonisches Potential $\mathcal{J}(T, V, \mu) = U - TS - pN$
↑
chemisches Potential

Maxwell - Kasten



20) $F = U - TS$

$$F(T, V) = U(T, V) - T \int_0^T \frac{dT'}{T'} \frac{\partial}{\partial T'} E(T', V)$$

$$dF = -S dT - p dV$$

$$\Rightarrow \left(\frac{\partial F}{\partial T} \right)_V = -S$$

$$dU = T dS - p dV$$

$$\frac{dU}{dT} = \frac{T dS}{dT} - \underbrace{\frac{p dV}{dT}}_{=0} = \frac{T dS}{dT}$$

$$\Rightarrow F(T, V) = U(T, V) - T \int_0^T \frac{dT'}{T'} \frac{T'}{dT'} dS = U(T, V) - T \int_0^T dS = U(T, V) - TS \quad \square$$

Experiment: ?

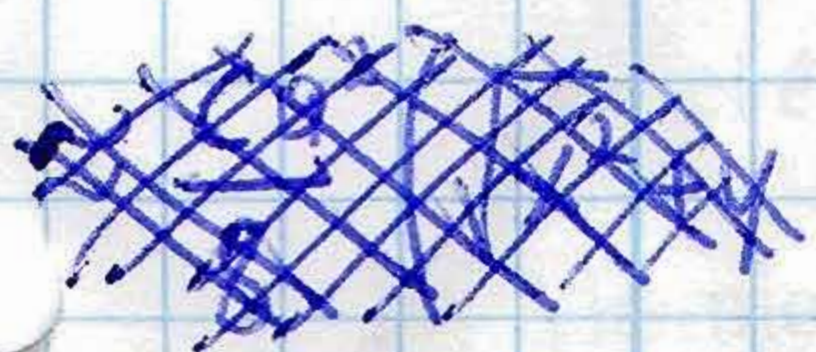
$$18) \vec{R}_i = \vec{R}_i^0 + \epsilon_{yx} \hat{e}_y (\vec{R}_i^0 \cdot \hat{e}_x)$$

$$\Phi = \frac{C}{2} (|\vec{R}_0 - \vec{R}_i| - |\vec{R}_0^0 - \vec{R}_i^0|)^2 =$$

$$= \frac{C}{2} (|\vec{R}_0 - \vec{R}_i^0 - \epsilon_{yx} \hat{e}_y (\vec{R}_i^0 \cdot \hat{e}_x)| - |\vec{R}_0^0 - \vec{R}_i^0|)^2 \quad \left\| \vec{R}_0^0 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \right.$$

$$= \frac{C a^2}{2} \left(\left| -\begin{pmatrix} x \\ y \\ z \end{pmatrix} - \epsilon_{yx} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \left(\begin{pmatrix} x \\ y \\ z \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \right) \right| - \left| \begin{pmatrix} x \\ y \\ z \end{pmatrix} \right| \right)^2 = \frac{C a^2}{8} \left(\sqrt{x^2 + (y + \epsilon_{yx} x)^2 + z^2} - \sqrt{x^2 + y^2 + z^2} \right)^2$$

$$= \frac{C a^2}{8} \left(\sqrt{x^2 + y^2 + 2\epsilon_{yx} yx + \epsilon_{yx}^2 x^2 + z^2} - \sqrt{x^2 + y^2 + z^2} \right)^2 = \frac{C a^2}{8} \Phi$$

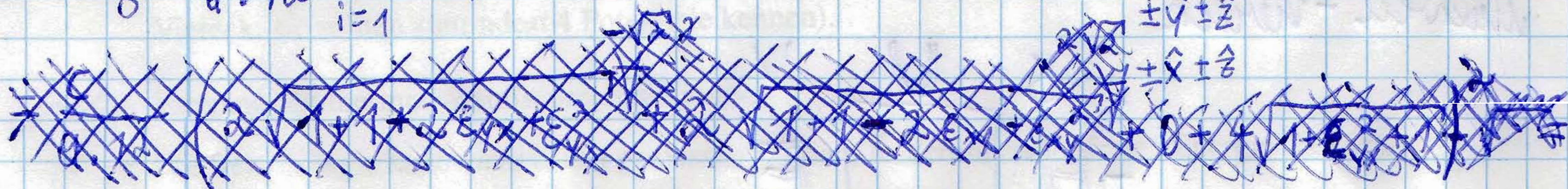


Berechne nun Gesamtenergiedichte

$$E = \frac{\sum \Phi_i}{V \cdot N}$$

$$E = \frac{C a^2}{8} \frac{8}{a^3 \cdot 12} \sum_{i=1}^{12} \Phi_i =$$

für alle nächsten Nachbarn im fcc-Gitter



$$= \frac{C}{a \cdot 12} \left(2 \left(\sqrt{1+1+2\epsilon_{yx}+\epsilon_{yx}^2} - \sqrt{2} \right)^2 + 2 \left(\sqrt{1+1-2\epsilon_{yx}+\epsilon_{yx}^2} - \sqrt{2} \right)^2 + 0 + \right. \\ \left. + 4 \left(\sqrt{2+2+\epsilon_{yx}^2} - \sqrt{2} \right)^2 \right) = \frac{C \cdot 4}{a \cdot 12} \left(\left(\sqrt{1+\epsilon_{yx}+\frac{\epsilon_{yx}^2}{2}} - 1 \right)^2 + \left(\sqrt{1-\epsilon_{yx}+\frac{\epsilon_{yx}^2}{2}} - 1 \right)^2 + \right. \\ \left. + 2 \left(\sqrt{1+\frac{\epsilon_{yx}^2}{2}} - 1 \right)^2 \right) \approx \frac{C}{a \cdot 3} \left(\left(1 + \frac{1}{2}\epsilon_{yx} - 1 \right)^2 + \left(1 - \frac{1}{2}\epsilon_{yx} - 1 \right)^2 + 2 \cdot 0 \right) =$$

Entwickle für $\epsilon_{yx} \ll 1$

$$\Rightarrow \epsilon_{yx}^2 \approx 0 \quad \text{+ Wurzel:} \quad \sqrt{1+\epsilon_{yx}} = 1 + \frac{1}{2}\epsilon_{yx}$$

$$= \frac{C}{a \cdot 3} 2 \frac{\epsilon_{yx}^2}{4} = \frac{C}{a \cdot 6} \epsilon_{yx}^2$$

$$\frac{\partial^2 E}{\partial \epsilon_{ij} \partial \epsilon_{kl}} = C_{ijkl}$$

$$\epsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

$$u_i = x_i' - x_i$$

$$u_1 = x - x = 0$$

$$u_2 = y + \epsilon_{yx} x - y = \epsilon_{yx} x$$

$$u_3 = z - z = 0$$

da $4 \rightarrow 23$ ist, würde man eigentl. ϵ_{23} berechnen, ist aber gemäß Angabe = 0 (Anfangsfehler?), einzige nichtverschwindende Komponente ist ϵ_{12} , $12 \leftrightarrow 6$, somit berechne ich $\epsilon_{12} \rightarrow C_{66}$, da jedoch kubische Symmetrie $C_{44} = C_{55} = C_{66}$, erhalte ich auch so C_{44} .

21) ① zeige, dass $(L(Lf))(x) = f(x)$ ganz allgemein gilt
 Legendre-Transform

$$(Lf)(x) = z g(z) - f(g(z)) \quad \text{gemäß Definition}$$

$$\begin{aligned} (L(Lf))(x) &= x h(x) - (Lf)(h(x)) = x h(x) - (h(x) \cdot g(h(x)) - f(g(h(x)))) = \\ &= x h(x) - h(x) \cdot x + f(x) = f(x) \quad \text{q.e.d.} \end{aligned}$$

② Anwenden auf Energie und Entalpie

$$H(P) = E(V) + PV = E(V) - \frac{dE(V)}{dV} V \quad \text{ist eine Legendre-Transform}$$

$$E'(V') = H(P) - PV' = H(P) - P \frac{dH(P)}{dP} \quad \text{ist ebenfalls eine Legendre-Transform}$$

setze ein: $E'(V') = E(V) + PV - PV' = E(V)$ gemäß ①
 $\Rightarrow V = V' \quad \text{q.e.d.}$

Vorteile der Legendre-Transform: transportiert Information auch über das Verhalten der Ableitung
 nützliche Eigenschaften

$$\frac{d(Lf)(z)}{dz} = g(z) = x(z)$$

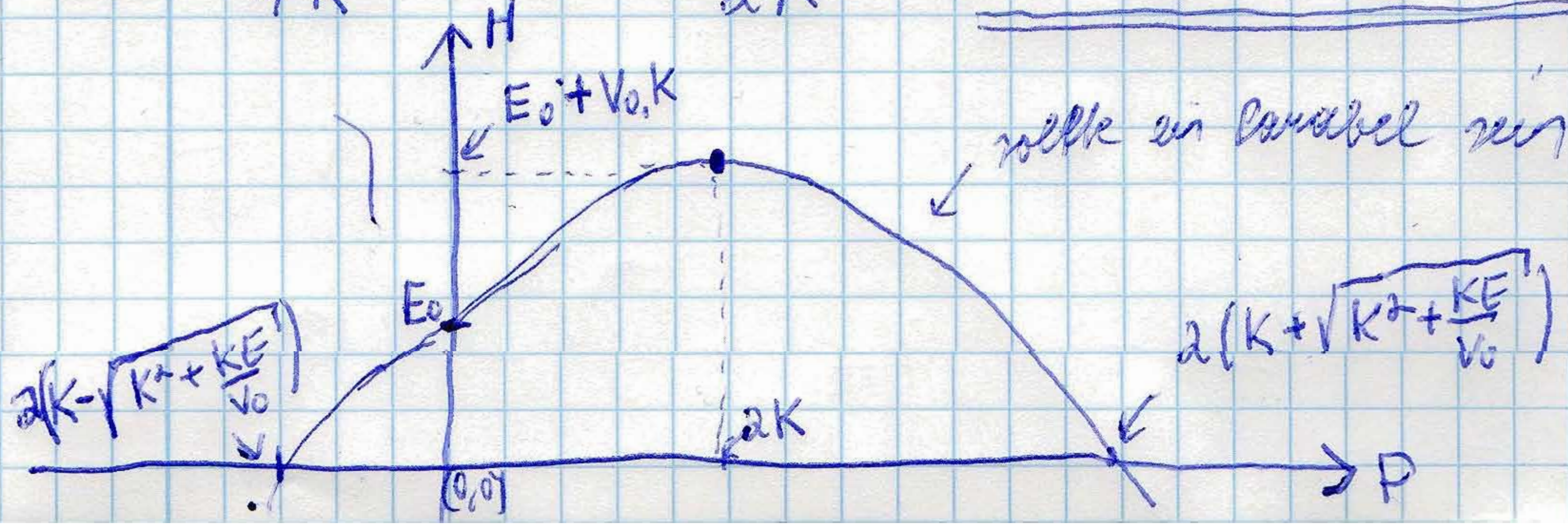
$$\frac{d^2(Lf)(z)}{dz^2} = \frac{dx}{dz}$$

$$\frac{d^2(Lf)(x)}{dx^2} = \frac{dz}{dx}$$

22) $E(V) = E_0 + \frac{K}{V_0} (V - V_0)^2$

$$\frac{dE}{dV} = \frac{K}{V_0} 2(V - V_0) = -P \quad \Rightarrow \quad V = V_0 - \frac{V_0 P}{2K}$$

$$\begin{aligned} H &= E - \frac{dE}{dV} V = E_0 + \frac{K}{V_0} \left(V_0 - \frac{V_0 P}{2K} - V_0 \right)^2 + P \left(V_0 - \frac{V_0 P}{2K} \right) = \\ &= E_0 + \frac{V_0 P^2}{4K} + P V_0 - \frac{V_0 P^2}{2K} = E_0 + P V_0 - \frac{1}{4} V_0 \frac{P^2}{K} = H \end{aligned}$$



$$23) a) P_j = e^{-\beta \epsilon_j} (1 - e^{-\beta \epsilon})$$

$$\epsilon = h c k$$

$$K = 214 \text{ cm}^{-1}$$

$$\beta = \frac{1}{k_B T}$$

$$\gamma = \frac{h c}{k_B T} \Big|_{T=25^\circ\text{C}} = \frac{1}{207 \text{ cm}^{-1}}$$

$$P_1 = e^{-\gamma K} (1 - e^{-\gamma K})$$

$$P_2 = e^{-2\gamma K} (1 - e^{-\gamma K})$$

$$P_1 + P_2 = e^{-\gamma K} - e^{-2\gamma K} + e^{-2\gamma K} - e^{-3\gamma K} = e^{-\gamma K} - e^{-3\gamma K} \approx 0,310663$$

$\sim 31\%$ sind in den ersten und zweiten angeregten Zustand

$$b) (i) P_0 = P_1 \cdot 2$$

$$1 \cdot \left(1 - e^{-\frac{h c k}{k_B T}}\right) = e^{-\frac{h c k}{k_B T}} \left(1 - e^{-\frac{h c k}{k_B T}}\right) \cdot 2$$

$$\frac{1}{2} = e^{-\frac{h c k}{k_B T}} \Rightarrow T = \frac{-h c k}{k_B \ln\left(\frac{1}{2}\right)} = \underline{\underline{444,685 \text{ K}}}$$

$$(ii) P_0 = P_1$$

$$\left(1 - e^{-\frac{h c k}{k_B T}}\right) = e^{-\frac{h c k}{k_B T}} \left(1 - e^{-\frac{h c k}{k_B T}}\right)$$

$$1 = e^{-\frac{h c k}{k_B T}} \Rightarrow 0 = -\frac{h c k}{k_B T} \quad \text{gilt nur für } \underline{\underline{T \rightarrow \infty}}$$

$$24) U = \frac{3}{2} N k_B T \quad \text{Energie eines idealen Gases}$$

$$C_v = \frac{\partial U}{\partial T} \Big|_v = \frac{3}{2} N k_B \underset{\substack{\uparrow \\ \text{für ein Mol}}}{=} \underline{\underline{12,466 \frac{\text{J}}{\text{mol} \cdot \text{K}}}}$$

$$25) Z = \sum_i e^{-\beta \epsilon_i} = e^{-\beta \epsilon_0} + \underset{\substack{\uparrow \\ \text{Entartung}}}{2} \cdot e^{-\beta \epsilon_1} = \underline{\underline{1 + 2 e^{-\beta \epsilon}}} \quad \text{mit } \beta = \frac{1}{k_B T}$$

$\epsilon_0 = 0; \epsilon_1 = \epsilon$

$$U = -\frac{\partial}{\partial \beta} \ln(Z^N) = -N \frac{\partial}{\partial \beta} \ln(1 + 2 e^{-\beta \epsilon}) = -N \frac{1}{1 + 2 e^{-\beta \epsilon}} (-2 \epsilon e^{-\beta \epsilon}) = 2 N \epsilon \frac{1}{e^{\beta \epsilon} + 2}$$

$$C_v = \frac{\partial U}{\partial T} \Big|_v = \frac{\partial}{\partial T} \left(2 N \epsilon \frac{1}{e^{\frac{\epsilon}{k_B T}} + 2} \right) = 2 N \epsilon \frac{-1}{\left(e^{\frac{\epsilon}{k_B T}} + 2\right)^2} e^{\frac{\epsilon}{k_B T}} \left(-\frac{\epsilon}{k_B T^2}\right) =$$

$$= \underline{\underline{\frac{2 N \epsilon^2}{k_B} T^{-2} \frac{e^{\frac{\epsilon}{k_B T}}}{\left(e^{\frac{\epsilon}{k_B T}} + 2\right)^2}}}$$

$$27) p_n = c e^{-\frac{E_n}{k_B T}}$$

$$\sum_n p_n = 1$$

$$E_n = \hbar \omega (n + \frac{1}{2})$$

$$\Rightarrow \sum_n e^{-\frac{E_n}{k_B T}} = \frac{1}{c} = \sum_n e^{-\frac{\hbar \omega}{k_B T} (n + \frac{1}{2})} = e^{-\frac{1}{2} \frac{\hbar \omega}{k_B T}} \cdot \sum_n e^{-\frac{\hbar \omega}{k_B T} n} = e^{-\frac{1}{2} \frac{\hbar \omega}{k_B T}} \frac{1}{1 - e^{-\frac{\hbar \omega}{k_B T}}}$$

$$\Rightarrow c = \left(1 - e^{-\frac{\hbar \omega}{k_B T}}\right) e^{\frac{1}{2} \frac{\hbar \omega}{k_B T}}$$

$$p_n = e^{+\frac{1}{2} \frac{\hbar \omega}{k_B T}} \left(1 - e^{-\frac{\hbar \omega}{k_B T}}\right) e^{-\frac{\hbar \omega}{k_B T} (n + \frac{1}{2})} = e^{-\frac{\hbar \omega}{k_B T} n} \cdot \left(1 - e^{-\frac{\hbar \omega}{k_B T}}\right)$$

$$\sum_n E_n \cdot p_n = \sum_n \hbar \omega (n + \frac{1}{2}) e^{-\frac{\hbar \omega}{k_B T} n} \left(1 - e^{-\frac{\hbar \omega}{k_B T}}\right) =$$

$$= \hbar \omega \left(\frac{1}{2} \sum_n e^{-\frac{\hbar \omega}{k_B T} n} + \sum_n n \cdot e^{-\frac{\hbar \omega}{k_B T} n} \right) \left(1 - e^{-\frac{\hbar \omega}{k_B T}}\right) =$$

$$= \hbar \omega \left(\frac{1}{2} \left(1 - e^{-\frac{\hbar \omega}{k_B T}}\right) \left(1 - e^{-\frac{\hbar \omega}{k_B T}}\right)^{-1} + \left(1 - e^{-\frac{\hbar \omega}{k_B T}}\right) \frac{e^{\frac{\hbar \omega}{k_B T}}}{(-1 + e^{\frac{\hbar \omega}{k_B T}})^2} \right) =$$

$$= \hbar \omega \left(\frac{1}{2} + e^{\frac{\hbar \omega}{k_B T}} \frac{(1 - e^{-\frac{\hbar \omega}{k_B T}})}{(1 - e^{-\frac{\hbar \omega}{k_B T}})(-1 + e^{\frac{\hbar \omega}{k_B T}})} \right) = \hbar \omega \left(\frac{1}{2} + \frac{1}{(e^{\frac{\hbar \omega}{k_B T}} - 1)} \right) = \hbar \omega \left(\bar{n}(\omega) + \frac{1}{2} \right)$$

Bose-Einstein-Statistik

28 a)

$$g(\omega) = \delta(\omega - \omega_E)$$

$$U = 3(N-1) \int g(\omega) \hbar \omega \left(\bar{n}(\omega) + \frac{1}{2} \right) d\omega = 3(N-1) \int \delta(\omega - \omega_E) \left(\frac{\hbar \omega}{e^{\frac{\hbar \omega}{k_B T}} - 1} + \frac{\hbar \omega}{2} \right) d\omega =$$

$$= 3(N-1) \left(\frac{\hbar \omega_E}{e^{\frac{\hbar \omega_E}{k_B T}} - 1} + \frac{\hbar \omega_E}{2} \right)$$

$$C_V = \frac{\partial U}{\partial T} = 3(N-1) \frac{\partial}{\partial T} \left(\frac{\hbar \omega_E}{e^{\frac{\hbar \omega_E}{k_B T}} - 1} + \frac{\hbar \omega_E}{2} \right) = 3(N-1) \hbar \omega_E \frac{\frac{\hbar \omega_E}{k_B T^2} \cdot e^{\frac{\hbar \omega_E}{k_B T}}}{(e^{\frac{\hbar \omega_E}{k_B T}} - 1)^2} =$$

$$= 3(N-1) k_B \frac{\hbar^2 \omega_E^2}{k_B^2 T^2} \frac{e^{\frac{\hbar \omega_E}{k_B T}}}{(e^{\frac{\hbar \omega_E}{k_B T}} - 1)^2}$$

28b)

$$y = \frac{\hbar \omega_E}{k_B T}$$

$$\lim_{T \rightarrow \infty} C_V = \lim_{y \rightarrow 0} C_V = \lim_{y \rightarrow 0} 3(N-1) k_B y^2 \frac{e^y}{(e^y - 1)^2} = \lim_{y \rightarrow 0} 3(N-1) k_B \frac{2ye^y + y^2 e^y}{2(e^y - 1)} =$$

$$\lim_{y \rightarrow 0} 3(N-1) k_B \frac{2ye^y + 2e^y + 2ye^y + y^2 e^y}{2e^y} = \lim_{y \rightarrow 0} 3(N-1) k_B \left(1 + 2y + \frac{1}{2}y^2\right) = \underline{\underline{(3N-1) k_B}}$$

weil für große T , die thermische Wärme proportional zu den Freiheitsgraden ist.

$$C_V \stackrel{\text{für } y \rightarrow \text{sehr gross}}{\underset{\hat{=} T \rightarrow 0}{\approx}} 3(N-1) k_B y^2 \frac{e^y}{(e^y - 1)^2} \approx 3(N-1) k_B y^2 \frac{e^y}{(e^y)^2} \approx 3(N-1) k_B y^2 e^{-y} \approx 3(N-1) k_B e^{-y}$$

für sehr große y
dominiert die e -Funktion

bei Debye Modell

$$C_V \xrightarrow{T \rightarrow \infty} 3 N k_B$$

$$C_V \xrightarrow{T \rightarrow 0} \frac{12 \pi^4 N k_B}{5 \theta_D^3} T^3$$

26)

wenn N hinreichend groß, und Funktion $\rightarrow$ ^{Gitter} periodisch

dann kann man analog zum Übergang von Fourierreihe und Fouriertrafo eine Umwandlung der Summe in ein Integral durchführen

Die Periodizität im Ortsraum ist a = Abstand der Atome, jedoch im Raum der Wellenzahl (vgl. Impulsraum) entspricht das gemäß der Fouriertransformation eine Periodizität von $\frac{2\pi}{a}$, deshalb sind die Grenzen des Integrals $\frac{\pi}{a}$ und $-\frac{\pi}{a}$

im 2D-Fall

$$\frac{1}{N^2} \sum_{n_1=1}^N \sum_{n_2=1}^N = \left(\frac{2\pi}{a}\right)^2 \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} dk_1 dk_2$$

$$29) \quad G_1(T, p) = G_2(T, p)$$

$$\text{in GGW: } T_1 = T_2 \quad \mu_1 = \mu_2$$

$$p_1 = p_2 = p_c \quad \text{am Phasenübergang}$$

$$G = U - TS + pV$$

$$F = U - TS$$

$$\Rightarrow G = F + pV$$

$$G_1 = G_2 \Rightarrow F_1 + p_c V_1 = F_2 + p_c V_2$$

$$\Rightarrow F_1 - F_2 = p_c (V_2 - V_1) \Rightarrow \underline{\underline{p_c = - \frac{F_1 - F_2}{V_1 - V_2} = - \frac{\Delta F}{\Delta V}}}$$

$$30) \quad \text{laut Skript 7.3.1}$$

$$N_{AA} = \frac{N_A^2}{N} \frac{Z}{2}$$

$$N_{BB} = \frac{N_B^2}{N} \frac{Z}{2}$$

$$N_{AB} = \frac{N_A N_B}{N} Z$$

$$N = N_A + N_B$$

mit hier $N_{AB} + N_{BA}$, anders als im Skript

$$N_A = \sum_i \frac{1}{2} (s_i + 1) = \frac{1}{2} \sum_i (s_i + 1) = \frac{1}{2} \left(\sum_i s_i + \sum_i 1 \right) = \frac{1}{2} \left(\sum_i s_i + Z \right)$$

$$N_B = \sum_i \frac{1}{2} (-s_i + 1) = \frac{1}{2} \left(-\sum_i s_i + Z \right) \quad \text{nützliche Formel: } \left(\sum_i a_i \right)^2 = 2 \sum_i \sum_{i < j} a_i a_j + \sum_i a_i^2$$

$$H = N_{AA} E_{AA} + N_{BB} E_{BB} + N_{AB} E_{AB} = \frac{Z}{2N} \left(N_A^2 E_{AA} + N_B^2 E_{BB} + 2 N_A N_B E_{AB} \right) =$$

$$= \frac{Z}{2(N_A + N_B)} \left(\frac{1}{4} \left(\sum_i s_i + Z \right)^2 E_{AA} + \frac{1}{4} \left(-\sum_i s_i + Z \right)^2 E_{BB} + \frac{2}{4} \left(\sum_i s_i + Z \right) \left(-\sum_i s_i + Z \right) E_{AB} \right) =$$

$$= \frac{Z}{\left(\sum_i s_i + Z \right) - \left(\sum_i s_i + Z \right)} \frac{1}{4} \left(\left(\sum_i s_i \right)^2 + 2Z \left(\sum_i s_i \right) + Z^2 \right) E_{AA} + \left(\left(\sum_i s_i \right)^2 - 2Z \left(\sum_i s_i \right) + Z^2 \right) E_{BB} +$$

$$+ 2 \left(-\left(\sum_i s_i \right)^2 + Z^2 \right) E_{AB} = \frac{1}{8} \left(\left(2 \sum_i \sum_{i < j} s_i s_j + \sum_i s_i^2 + Z^2 + 2Z \left(\sum_i s_i \right) \right) E_{AA} + \right.$$

$$+ \left(2 \sum_i \sum_{i < j} s_i s_j + \sum_i s_i^2 + Z^2 - 2Z \left(\sum_i s_i \right) \right) E_{BB} + 2 \left(-2 \sum_i \sum_{i < j} s_i s_j + \sum_i s_i^2 + Z^2 \right) E_{AB} =$$

$$= \frac{1}{4} (E_{AA} + E_{BB} - 2 E_{AB}) \sum_i \sum_{i < j} s_i s_j + \frac{1}{4} \left(Z^2 (E_{AA} + E_{BB}) + Z \left(\sum_i s_i \right) (E_{AA} - E_{BB}) \right) =$$

$$= \underline{\underline{J \sum_{i < j} s_i s_j + \text{const}}}$$

in Kurzschreibweise $\sum_{i < j}$

$$31) \quad E(k) = \frac{\hbar^2}{2m} k^2 \quad dE = \frac{\hbar^2 k}{m} dk$$

a) durch Quantenbedingungen $\rightarrow$ $D(\vec{k}) = 2 \frac{V}{(2\pi)^3}$
in 3D

$$D(\vec{k}) dk^3 = D(E) dE = 2 \frac{V}{(2\pi)^3} \underbrace{4\pi k^2 dk}_{\text{Kugelkoordin.}}$$

$$\Rightarrow \underline{D(E) = \frac{V}{(2\pi)^3} \left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2}}$$

$$D(k) = \frac{dE}{dk} D(E) = \frac{\hbar^2 k}{m} \frac{V}{(2\pi)^3} \left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2} = \frac{V}{(2\pi)^3} \frac{\hbar^2 k}{m} \left(\frac{2m}{\hbar^2}\right)^{3/2} \left(\frac{\hbar^2 k^2}{2m}\right)^{1/2}$$

$$\Rightarrow \underline{D(k) = \frac{V \cdot 2}{(2\pi)^2} k^2}$$

b) durch Quantenbedingung $\rightarrow$ $D(\vec{k}) = 2 \frac{A}{(2\pi)^2}$
in 2D

$$D(\vec{k}) dk^2 = D(E) dE = 2 \frac{A}{(2\pi)^2} \underbrace{2\pi k dk}_{\text{Polarkoordin.}}$$

$$\Rightarrow \underline{D(E) = \frac{A}{2\pi} \left(\frac{2m}{\hbar^2}\right)} = \text{const.}$$

$$D(k) = \frac{dE}{dk} D(E) = \frac{A}{2\pi} \left(\frac{2m}{\hbar^2}\right) \cdot \left(\frac{\hbar^2 k}{m}\right)$$

$$\Rightarrow \underline{D(k) = \frac{A}{\pi} k}$$

32) a) $1 \text{ \AA} = 10^{-10} \text{ m}$; $1 \text{ eV} = 1,602 \cdot 10^{-19} \text{ J}$; $m_e = 9,109 \cdot 10^{-31} \text{ kg}$

$\hbar = 1,055 \cdot 10^{-34} \text{ Js}$; $k_B = 1,381 \cdot 10^{-23} \text{ J/K} = 8,617 \cdot 10^{-5} \text{ eV/K}$

$$T_F = \frac{\hbar^2}{2m k_B} (3\pi^2 n)^{2/3} = \frac{\hbar^2 (3\pi^2)^{2/3}}{2m k_B} n^{2/3} = \frac{(3\pi^2)^{2/3}}{2} \frac{(1,055 \cdot 10^{-34} \text{ Js})^2 \cdot (10^{-10})^{-2}}{(9,109 \cdot 10^{-31} \text{ kg}) \cdot (1,381 \cdot 10^{-23} \text{ J/K})} (n [\text{\AA}^{-3}])^{2/3}$$

$$\approx 423054 \text{ K} \frac{1}{\text{\AA}^2} (n [\text{\AA}^{-3}])^{2/3}$$

$$E_F = k_B \cdot T_F = 36,45 \frac{\text{eV}}{\text{\AA}^2} (n [\text{\AA}^{-3}])^{2/3}$$

b)

	$n [\text{\AA}^{-3}]$	$T_F [\text{K}]$	$E_F [\text{eV}]$
Li	0,05	57417	4,948
Ru	0,013	23390	2,015
Al	3 \cdot 0,071	150886	13,002

33) $E_F = \frac{\hbar^2}{2m k_B} (3\pi^2)^{2/3} n^{2/3}$

bei $T=0\text{K}$ alle Elektronen im Grundzustand $\Rightarrow$ Fermi-Energie

im 3D-Fall: $n(E) = \frac{(2m)^{3/2}}{2\pi^2 \hbar^3} \sqrt{E}$ laut Vorlesungs-Skript

Energie pro Volumen: $\frac{U}{V} = \int_0^{E_F} n(E) \cdot E \cdot dE = \frac{(2m)^{3/2}}{2\pi^2 \hbar^3} \int_0^{E_F} E^{3/2} dE = \frac{(2m)^{3/2}}{2\pi^2 \hbar^3} \cdot \frac{2}{5} E_F^{5/2}$

$$= \frac{3}{5} n E_F \quad \text{mit } n = \frac{N}{V} \Rightarrow \underline{\underline{\langle E \rangle = \frac{U}{N} = \frac{3}{5} E_F}}$$

im 2D-Fall: $n(E) = C$

Energie pro Fläche: $\frac{U}{A} = \int_0^{E_F} n(E) \cdot E \cdot dE = C \int_0^{E_F} E \cdot dE = \frac{C}{2} E_F^2$

$$\Rightarrow \underline{\underline{\langle E \rangle = \frac{U}{N} = \frac{A}{N} \frac{C}{2} E_F^2 = \frac{C}{2} E_F^2}}$$

in Konstante kann auch noch eine E_F "versteckt" sein; vgl. 3D-Fall

34)

Damit zwei Operatoren die selben Eigenfunktionen muss der Kommutator aus beiden vernachlässigen.

$$[\vec{P}, H] = [\vec{P}, \frac{\vec{P}^2}{2m} + V(\vec{r})] = [\vec{P}, \frac{\vec{P}^2}{2m}] + [\vec{P}, V(\vec{r})] =$$

$$= \frac{1}{2m} ([\vec{P}, \vec{P}] \vec{P} + \vec{P} [\vec{P}, \vec{P}]) + [\vec{P}, V(\vec{r})] = [\vec{P}, V(\vec{r})] = \vec{P} \cdot V(\vec{r}) - V(\vec{r}) \cdot \vec{P} = \dots$$

$$[\vec{P}, \vec{P}] = 0$$

in Nebenrechnung angewendet auf Testfunktion $\Psi(\vec{r})$

$$\vec{P} = -i\hbar \vec{\nabla}$$

$$(\vec{P} \cdot V(\vec{r}) - V(\vec{r}) \cdot \vec{P}) \Psi(\vec{r}) = (-i\hbar \vec{\nabla}) (V(\vec{r}) \cdot \Psi(\vec{r})) - V(\vec{r}) \cdot (-i\hbar \vec{\nabla} \cdot \Psi(\vec{r})) =$$

$$= (-i\hbar \vec{\nabla} \cdot V(\vec{r})) \cdot \Psi(\vec{r}) + V(\vec{r}) \cdot (-i\hbar \vec{\nabla} \cdot \Psi(\vec{r})) - V(\vec{r}) \cdot (-i\hbar \vec{\nabla} \cdot \Psi(\vec{r})) =$$

$$= (-i\hbar \vec{\nabla} \cdot V(\vec{r})) \cdot \Psi(\vec{r})$$

$$\Rightarrow [\vec{P}, H] = \vec{P} \cdot V(\vec{r}) \neq 0, \text{ wäre nur Null wenn } V(\vec{r}) = \text{const, ist aber laut Angabe genau nicht der Fall.}$$

35)

$$\text{Blochtheorem: } \Psi(x+R) = e^{iKR} \Psi(x)$$

$$\Psi(x) = C_1 e^{ik_1 x} + C_{-1} e^{-ik_1 x}$$

$$K_1 = \frac{\pi}{a}$$

$$e^{-i\pi} = 1 = e^{i\pi}$$

$$\Psi(x+R) = C_1 e^{ik_1(x+R)} + C_{-1} e^{-ik_1(x+R)} = C_1 e^{ik_1 x} e^{ik_1 R} + C_{-1} e^{-ik_1 x} e^{-ik_1 R} =$$

$$= C_1 e^{ik_1 x} e^{i\pi \frac{R}{a}} + C_{-1} e^{-ik_1 x} e^{-i\pi \frac{R}{a}} = C_1 e^{ik_1 x} 1^{\frac{R}{a}} + C_{-1} e^{-ik_1 x} 1^{\frac{R}{a}} =$$

$$= 1^{\frac{R}{a}} (C_1 e^{ik_1 x} + C_{-1} e^{-ik_1 x}) = e^{i\pi \frac{R}{a}} (C_1 e^{ik_1 x} + C_{-1} e^{-ik_1 x}) = e^{iK_1 R} \cdot \Psi(x)$$

q.e.d.

$$\sin(x) = \frac{1}{2i} (e^{ix} - e^{-ix})$$

$$V(x) = 2V \sin(2\pi x/a)$$

$$= \frac{2V}{2i} (e^{i2\pi \frac{x}{a}} - e^{-i2\pi \frac{x}{a}})$$

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x) + V(x) \Psi(x) - E \Psi(x) \right) = 0$$

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} (C_1 e^{i\frac{\pi}{a}x} + C_{-1} e^{-i\frac{\pi}{a}x}) + V(x) (C_1 e^{i\frac{\pi}{a}x} + C_{-1} e^{-i\frac{\pi}{a}x}) - E (C_1 e^{i\frac{\pi}{a}x} + C_{-1} e^{-i\frac{\pi}{a}x}) \right) =$$

$$\frac{\hbar^2 \pi^2}{2m a^2} C_1 e^{i\frac{\pi}{a}x} + \frac{\hbar^2 \pi^2}{2m a^2} C_{-1} e^{-i\frac{\pi}{a}x} + \frac{V}{i} C_1 e^{i\frac{\pi}{a}x} (e^{i2\pi \frac{x}{a}} - e^{-i2\pi \frac{x}{a}}) +$$

$$+ \frac{V}{i} C_{-1} e^{-i\frac{\pi}{a}x} (e^{i2\pi \frac{x}{a}} - e^{-i2\pi \frac{x}{a}}) - E C_1 e^{i\frac{\pi}{a}x} - E C_{-1} e^{-i\frac{\pi}{a}x} =$$

$$\text{bereichne ab nun: } b = \frac{\hbar^2 \pi^2}{2m a^2}$$

$\Rightarrow$

$$= bC_1 e^{i\frac{\pi}{a}x} + bC_{-1} e^{-i\frac{\pi}{a}x} + \frac{V}{i}C_1 \left(\underbrace{e^{-i\frac{\pi}{a}x} + e^{i3\frac{\pi}{a}x}}_{\substack{=0 \\ \text{laut Angabe}}} \right) + \frac{V}{i}C_{-1} \left(\underbrace{e^{i\frac{\pi}{a}x} - e^{-i3\frac{\pi}{a}x}}_{=0} \right) +$$

$$- EC_1 e^{i\frac{\pi}{a}x} - EC_{-1} e^{-i\frac{\pi}{a}x} = 0$$

zerlege in 2 Gleichungen

$$(bC_1 + \frac{V}{i}C_{-1} - EC_1) e^{i\frac{\pi}{a}x} = 0 \quad \text{und} \quad (bC_{-1} - \frac{V}{i}C_1 - EC_{-1}) e^{-i\frac{\pi}{a}x} = 0$$

schreibe neu in Matrix und Vektor um

$$\begin{pmatrix} b-E & \frac{V}{i} \\ -\frac{V}{i} & b-E \end{pmatrix} \begin{pmatrix} C_1 \\ C_{-1} \end{pmatrix} = 0 = \left(\begin{pmatrix} b & \frac{V}{i} \\ -\frac{V}{i} & b \end{pmatrix} + 1E \right) \begin{pmatrix} C_1 \\ C_{-1} \end{pmatrix}$$

vergleiche mit Angabe: $\Rightarrow \bar{H} = \begin{pmatrix} \frac{\hbar^2 \pi^2}{2m a^2} & \frac{V}{i} \\ -\frac{V}{i} & \frac{\hbar^2 \pi^2}{2m a^2} \end{pmatrix}$

Teil d. Matrixgleichung entspricht Eigenwertgleichung für E $(\bar{H} - 1E) = 0$

$$\Downarrow \det(\bar{H} - 1E) = 0$$

$$(b-E)^2 - V^2 = 0 = b^2 - 2bE + E^2 - V^2 = 0$$

$$\Rightarrow \underline{E_{1,2}} = b \pm \sqrt{b^2 - b^2 + V^2} = b \pm V = \underline{\frac{\hbar^2 \pi^2}{2m a^2} \pm V}$$

Ansatz ist bei $k_1 = \frac{\pi}{a}$ gültig, weil nur hier die Terme $e^{\pm i3k_1 x}$ wegen ihrer 2π -Periodizität im Exponenten, Termen $e^{\pm i k_1 x}$ entsprechen und daher mit einer Neudefinition der Vorfaktoren zusammengezogen werden können.

Dispersionsrelation $\omega = \omega(k)$ $E = \hbar \omega \Rightarrow$

$$\omega_{\pm}(k) = \frac{\hbar}{2m} k^2 (\pm) V$$

