

zu 3.2.3

Ausgangspunkt von wechselwirkenden Festkörperionen:

$$m_s \ddot{u}_s^\alpha(u) = - \sum_{\beta, \gamma, m} K_{s\beta}^{\alpha\gamma}(u, m) u_\beta^\gamma(m) \quad \left( \text{Newtongl. in harmonischer Näherung f. Rückstellkraft} \right)$$

Ausleitung vom s-ten Ion in der u-ten Elementarzelle eines Festkörpers,  $K \hat{=}$  Kraftkonstantenmatrix

→ System gekoppelter Oszillatoren  $\{u_\beta^\gamma(m)\}$

Ziel: Transformation zu finden um ungekoppelte Oszillatoren zu beschreiben

$$u_s^k(u) = \frac{1}{\sqrt{m_s N}} \sum_{\lambda, \alpha} A_s^\alpha(\lambda, k) q_{\lambda, \alpha}(t) e^{i\vec{k} \cdot \vec{r}_u}$$

↑
↑

Anzahl d. El.-Zellen      unbestimmte Faktoren

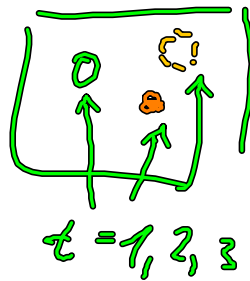
$k$  - Wellenvektor  
 $\lambda$  - Modenindex (Spinor)  
 $A$  : Vektorcharakter  
 $q$  : Zeitfunktion

Zeitabhängigkeit abh. v.  $\vec{r}_u$

Fourieransatz  $e^{i\vec{k}\cdot\vec{r}_n}$  ist immer gute Basis in periodisch fortgesetzte Systeme (Einkristalle)

nächster Schritt einsetze in die Bewegungsgleich. für  $u_s$ :

$$\sum_{\kappa, \lambda} \ddot{q}_{\kappa\lambda}(t) A_s^\alpha(\kappa, \lambda) = - \sum_{\substack{\epsilon, \beta \\ m, \kappa, \lambda}} \frac{k_{s\epsilon}^\alpha \beta (m-n)}{\sqrt{m_\epsilon m_\beta}} A_\epsilon^\beta(\kappa, \lambda) e^{i\vec{k}(\vec{r}_m - \vec{r}_n)} q_{\kappa\lambda}(t)$$



$q_{\kappa\lambda}$  wählen, so dass ein Näherungsgleichg. erfüllt:

$$\ddot{q}_{\kappa\lambda} + \omega_{\kappa\lambda}^2 q_{\kappa\lambda} = 0$$

↑  
bestimmen und diese Konstante geht in die Bestimmung von  $A_s^\alpha(\kappa, \lambda)$  ein.

die Kraftkonstante hängt nur von  $u-n$  Zell



Aufgrund der Periodizität kann  $k$  nur vom Abstand,

also  $k(u-u')$  oder

$k(\vec{r}_n - \vec{r}_{n'})$  abhängen

mittels der Ortswertgl. für  $\varphi_{k\lambda}$ :

$$(*) \quad \omega_\lambda^2(k) A_s^\alpha(k) = \sum_{t,\beta} \frac{k_{st}^{\alpha\beta}(k)}{\sqrt{m_s m_t}} A_t^\beta(k)$$

$$k_{st}^{\alpha\beta}(k) = \sum_{\substack{\vec{r}_n - \vec{r}_{n'} \\ (u-u')}} k_{st}^{\alpha\beta}(\vec{r}_n - \vec{r}_{n'}) e^{i(\vec{r}_n - \vec{r}_{n'}) \cdot \vec{k}}$$

erhält: 1) man  $\varphi_{k\lambda}(t)$  bestimmen wenn  $\omega_\lambda(k)$  bekannt

(d. unbestimmte Funktion eliminiert)

2)  $\omega_\lambda(k)$  kann man als Eigenwert

der Gleichung  $*$  finden, ebenso die

# Eigenwerten $A^*$ .

Dimension der Matrix =  $3p$

$p$  weil über alle  $T$  von einer Zelle summiert wird ( $t$ )

$3$  weil über alle 3 Raumdimensionen ( $\beta$ ) summiert wird

Zahl der Ionen in einer Zelle

„einfache Diagonalisierung mögl.“

## Ergebnisse der Festkörpertheorie

- weil  $A$  und  $\omega$  von  $\vec{k}$  abhängen

und  $p$  f. jedes  $\vec{k}$  eine Matrix diagonalisiert werden

→ das gibt dann  $3p \cdot N$  Lösungen für  $\omega_j(\vec{k})$

↑  
Anzahl period. Ebenen

↑  
 $3p$  Moden, die von der Wellenzahl  $\vec{k}$  abhängen.

- zur Einigung:

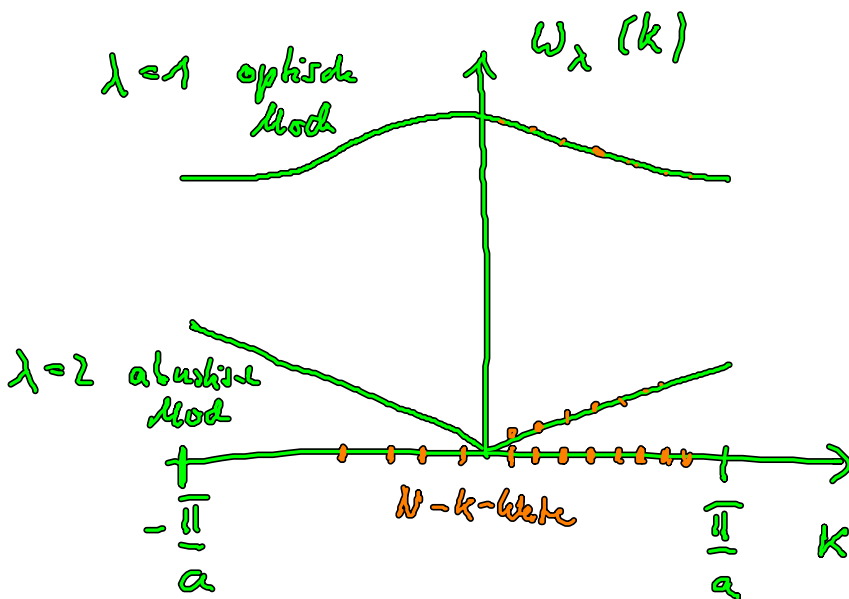
$$\ddot{q}_{\vec{k}\alpha}(t) + \omega_{\vec{k}\alpha}^2 q_{\vec{k}\alpha}(t) = 0$$

Sind brechenbar

- Wir haben damit ein System ungeschalteter, freier Oszillatoren  
vorliegen (3p N Stück)

- Dispersionsrelation:  $\omega_\lambda = \omega_\lambda(\vec{k})$  der  
angesezte Wellen  $e^{i\vec{k}\vec{r}_i} e^{-i\omega_\lambda(\vec{k})t}$

(Einung.: gedoppeltes Ploch  $\rightarrow$  Normalkoordinaten)

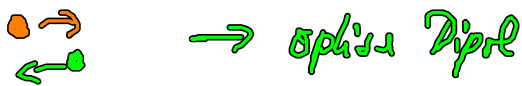


1dimensional



Lösung ~~3~~p N

- optische Mod können an optische Fasern koppeln



- akustische Mode hat die niedrigste Dispersi

$$\omega \approx v_{\text{Schall}} \cdot k$$

$\circ \rightarrow$   
 $\rightarrow$   $\rightarrow$  Kernoptisches Dipol

Der Hamiltonian für ein Festkörper kann mittels ungelockter harmonischer Oszillatoren beschrieben werden.

$$H = \sum_{k, \lambda} \hbar \omega_{\lambda}(k) \left( a_{k, \lambda}^{\dagger} a_{k, \lambda} + \frac{1}{2} \right)$$

„Phonon dispersionsrelation“

(Quantenfeld d. Ionengitters)

### 3.2.4. Masselose Quantenfelder als bosonische Oszillatoren

Boson: Photon, Phonone im Vgl. mit Exp. oder Pauli Spin-Statistik Theorem.

Zustandsumme  $\rightarrow$  Zustandsgleichungen ist jetzt Ziel

#### 3.2.4.1 Hamiltonian und Zustand

ein Oszillator:  $H = \hbar \omega \left( a^{\dagger} a + \frac{1}{2} \right)$

$$\text{Wickel - u -} : H = \sum_k \hbar \omega_k \left( a_k^\dagger a_k + \frac{1}{2} \right)$$

$k$ : Raumindex (Mod  $k$ , Wellenvektor  $\vec{k}$ )

Imp:  $k$  un  $\beta$  für jedes System spezifiziert werden.

ein Oszillator  $\epsilon_n = \hbar \omega \left( n + \frac{1}{2} \right), n = 0, 1, 2, 3 \dots$

viele Oszillatoren:  $\epsilon_n = \sum_k \hbar \omega_k \left( n_k + \frac{1}{2} \right), n_k = 0, 1, 2, 3 \dots$

↑  
Besetzungszahl der Mod  $k$ ,  
z.B. Vielmodresonator

Zustand  $|u\rangle = |n_1, n_2, \dots, n_k, \dots, n_N\rangle$   
für Vielmodfall

### 3.2.42. Zustandssummen von ungelockten Oszillatoren

(i) Zustandssumme f. 1 Oszillator:

$$Z_k = \sum_{\text{alle Zustände } \{n\}} e^{-\beta \epsilon_n}, \quad \epsilon_n = \left( n + \frac{1}{2} \right) \hbar \omega$$

masselose Objekte

$\mu = 0$   
(kan. = großkanonische Summe)

$$z_k = \sum_{u=0}^{\infty} e^{-\beta u \epsilon} e^{-\beta \frac{\epsilon}{2}}$$

$u=0$  geometrisch Reihe

Boson, deshalb 0,  $\infty$  Summe

$$= \frac{1}{1 - e^{-\beta \epsilon}} e^{-\beta \frac{\epsilon}{2}}$$

$$\ln z_k = -\frac{\beta \epsilon}{2} - \ln(1 - e^{-\beta \epsilon})$$

$\sim F$

freie Energie

Bsp. für Anwendung ist bekannter Zustand gleich.

$$E = -\partial_{\beta} \ln z_k$$

$$= \frac{\epsilon}{2} + \frac{e^{-\beta \epsilon} \cdot \epsilon}{1 - e^{-\beta \epsilon}}$$



$$E = \hbar\omega \frac{1}{e^{\beta\hbar\omega} - 1} + \frac{\hbar\omega}{2}$$

Energie des Oszillators im Wärmebad  
der Temperatur  $T$ .

Bemerkung:

a) kalt  $T \rightarrow 0, \beta \rightarrow \infty \Rightarrow E \rightarrow \frac{\hbar\omega}{2}$

Im Mittel ist das System mit der Grundzustands-  
Energie ausgestattet

b) warm  $T \rightarrow \infty, \beta \rightarrow 0 \Rightarrow$

$$\frac{1}{e^{\beta\hbar\omega} - 1} \approx \frac{1}{1 + \beta\hbar\omega - 1} = \frac{kT}{\hbar\omega}$$

$$E = kT$$

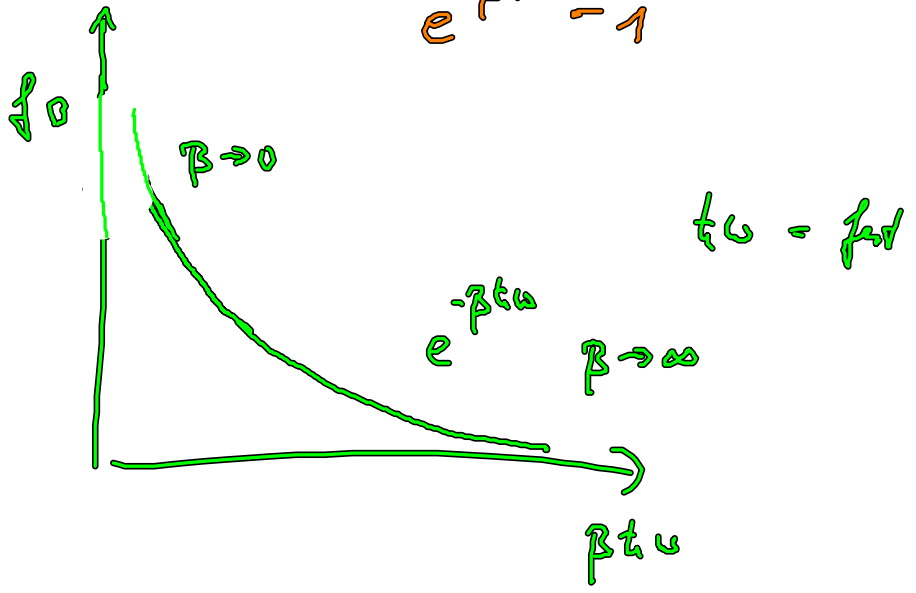
Im Mittel ist das System mit der klassisch

Energie ausgestattet  $\rightarrow$  klassisch freier Fall ( $T \rightarrow \infty$ )

c) mittlerer Anzahl von Oszillatorkvanta



$$\rho_B = \frac{1}{e^{\beta \epsilon_u} - 1}$$



~~(Bosonen sind besetzt sind im Grundzustand kommen darf zurück zu besetzen.)~~

diskutieren wir in Detail in der Anwendung.

Die Bose verteilung gibt an, welche mittleren Zahl von Quanta bei einer fest Temperatur vorliegen.

Sie zeigt ein Singularität für  $\beta \rightarrow 0$ ,

für  $\beta \rightarrow \infty$  wird  $f_B \rightarrow 0$ , weil  $T \rightarrow 0$  (im Mittel in tiefen  $u$ -Zuständen)

(ii) Viel-Oszillatoren Zustandssumme

$$\omega \rightarrow \omega_k \quad (k \rightarrow \vec{k}, \lambda)$$

↑  
viel Oszillatoren (z.B. Moden d. elektromagn. Felds)

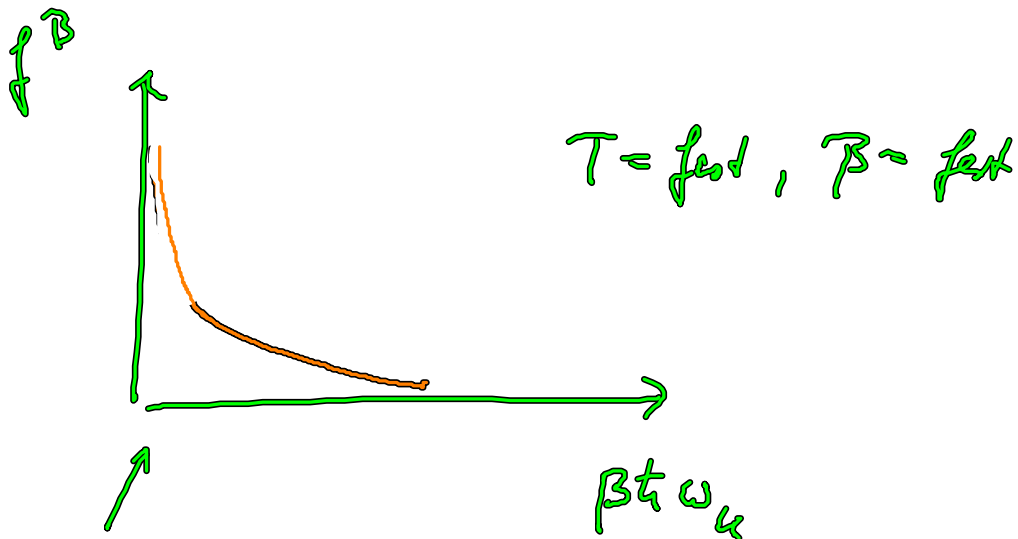
$$\begin{aligned}
 Z_k &= \sum_{\text{alle Zustände}} e^{-\beta \epsilon_n} \\
 &= \sum_{\substack{\text{alle mögl.} \\ \{n_k\} \text{ Summe}}} e^{-\beta \sum_k n_k \epsilon_k} \quad \begin{array}{l} \text{über alle Zustände mit } \epsilon_n \text{ enthält} \\ n_k: 0 - \infty \end{array} \\
 &= \sum_{n_1=0}^{\infty} e^{-\beta \epsilon \omega_1 (n_1 + \frac{1}{2})} \dots \sum_{n_k=0}^{\infty} e^{-\beta \epsilon \omega_k (n_k + \frac{1}{2})} \quad \text{1052.11.10.11.12.13.14.15.16.17.18.19.20.21.22.23.24.25.26.27.28.29.30.31.32.33.34.35.36.37.38.39.40.41.42.43.44.45.46.47.48.49.50.51.52.53.54.55.56.57.58.59.60.61.62.63.64.65.66.67.68.69.70.71.72.73.74.75.76.77.78.79.80.81.82.83.84.85.86.87.88.89.90.91.92.93.94.95.96.97.98.99.100.101.102.103.104.105.106.107.108.109.110.111.112.113.114.115.116.117.118.119.120.121.122.123.124.125.126.127.128.129.130.131.132.133.134.135.136.137.138.139.140.141.142.143.144.145.146.147.148.149.150.151.152.153.154.155.156.157.158.159.160.161.162.163.164.165.166.167.168.169.170.171.172.173.174.175.176.177.178.179.180.181.182.183.184.185.186.187.188.189.190.191.192.193.194.195.196.197.198.199.200.201.202.203.204.205.206.207.208.209.210.211.212.213.214.215.216.217.218.219.220.221.222.223.224.225.226.227.228.229.230.231.232.233.234.235.236.237.238.239.240.241.242.243.244.245.246.247.248.249.250.251.252.253.254.255.256.257.258.259.260.261.262.263.264.265.266.267.268.269.270.271.272.273.274.275.276.277.278.279.280.281.282.283.284.285.286.287.288.289.290.291.292.293.294.295.296.297.298.299.300.301.302.303.304.305.306.307.308.309.310.311.312.313.314.315.316.317.318.319.320.321.322.323.324.325.326.327.328.329.330.331.332.333.334.335.336.337.338.339.340.341.342.343.344.345.346.347.348.349.350.351.352.353.354.355.356.357.358.359.360.361.362.363.364.365.366.367.368.369.370.371.372.373.374.375.376.377.378.379.380.381.382.383.384.385.386.387.388.389.390.391.392.393.394.395.396.397.398.399.400.401.402.403.404.405.406.407.408.409.410.411.412.413.414.415.416.417.418.419.420.421.422.423.424.425.426.427.428.429.430.431.432.433.434.435.436.437.438.439.440.441.442.443.444.445.446.447.448.449.450.451.452.453.454.455.456.457.458.459.460.461.462.463.464.465.466.467.468.469.470.471.472.473.474.475.476.477.478.479.480.481.482.483.484.485.486.487.488.489.490.491.492.493.494.495.496.497.498.499.500.501.502.503.504.505.506.507.508.509.510.511.512.513.514.515.516.517.518.519.520.521.522.523.524.525.526.527.528.529.530.531.532.533.534.535.536.537.538.539.540.541.542.543.544.545.546.547.548.549.550.551.552.553.554.555.556.557.558.559.560.561.562.563.564.565.566.567.568.569.570.571.572.573.574.575.576.577.578.579.580.581.582.583.584.585.586.587.588.589.590.591.592.593.594.595.596.597.598.599.600.601.602.603.604.605.606.607.608.609.610.611.612.613.614.615.616.617.618.619.620.621.622.623.624.625.626.627.628.629.630.631.632.633.634.635.636.637.638.639.640.641.642.643.644.645.646.647.648.649.650.651.652.653.654.655.656.657.658.659.660.661.662.663.664.665.666.667.668.669.670.671.672.673.674.675.676.677.678.679.680.681.682.683.684.685.686.687.688.689.690.691.692.693.694.695.696.697.698.699.700.701.702.703.704.705.706.707.708.709.710.711.712.713.714.715.716.717.718.719.720.721.722.723.724.725.726.727.728.729.730.731.732.733.734.735.736.737.738.739.740.741.742.743.744.745.746.747.748.749.750.751.752.753.754.755.756.757.758.759.760.761.762.763.764.765.766.767.768.769.770.771.772.773.774.775.776.777.778.779.780.781.782.783.784.785.786.787.788.789.790.791.792.793.794.795.796.797.798.799.800.801.802.803.804.805.806.807.808.809.810.811.812.813.814.815.816.817.818.819.820.821.822.823.824.825.826.827.828.829.830.831.832.833.834.835.836.837.838.839.840.841.842.843.844.845.846.847.848.849.850.851.852.853.854.855.856.857.858.859.860.861.862.863.864.865.866.867.868.869.870.871.872.873.874.875.876.877.878.879.880.881.882.883.884.885.886.887.888.889.890.891.892.893.894.895.896.897.898.899.900.901.902.903.904.905.906.907.908.909.910.911.912.913.914.915.916.917.918.919.920.921.922.923.924.925.926.927.928.929.930.931.932.933.934.935.936.937.938.939.940.941.942.943.944.945.946.947.948.949.950.951.952.953.954.955.956.957.958.959.960.961.962.963.964.965.966.967.968.969.970.971.972.973.974.975.976.977.978.979.980.981.982.983.984.985.986.987.988.989.990.991.992.993.994.995.996.997.998.999.1000} \\
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 \end{array}
 \end{aligned}$$

analy Redng. :

$$\ln Z_k = \sum_k \frac{\epsilon \omega_k}{2} + \sum_k \frac{\epsilon \omega_k}{e^{\beta \epsilon \omega_k} - 1}$$

$$\langle n_k \rangle = \int_0^\infty f_k^{\beta} = \frac{1}{e^{\beta \hbar \omega_k} - 1}$$

- Bei unabhängigen Oszillatoren zerfällt die Zustandssumme in ein Produkt von Einzellozillator Zustandssummen.
- Die mittlere Zahl der Quanta im  $k$ -ten Oszillator ist durch die Bose verteilg. gegeben:



$\omega_k \rightarrow 0$

dh. wieder ungeladene Oszillatoren

→ man beobachtet die Tendenz,

dass sich Bosonen f. festgehaltenen  $T$

in Zustand kleinsten Energie (Grundzustand)

versammeln.