4 / 1 Verteilungsfunktionen

Maxwell-Boltzmann Verteilung

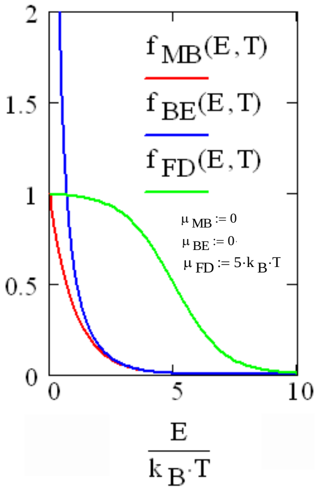
$$\mu_{MB} := 0 \cdot k_B \cdot T \qquad f_{MB}(E,T) := \frac{1}{\exp\left[\frac{(E-\mu_{MB})}{k_B \cdot T}\right]}$$

Bose-Einstein Verteilung

$$\mu_{BE} := 0 \cdot k_B \cdot T \qquad f_{BE}(E,T) := \frac{1}{\exp\left[\frac{(E-\mu_{BE})}{k_B \cdot T}\right]-1}$$

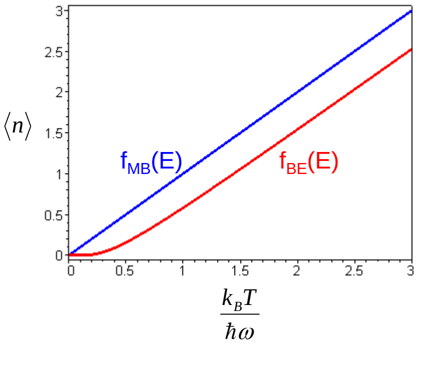
Fermi-Dirac Verteilung

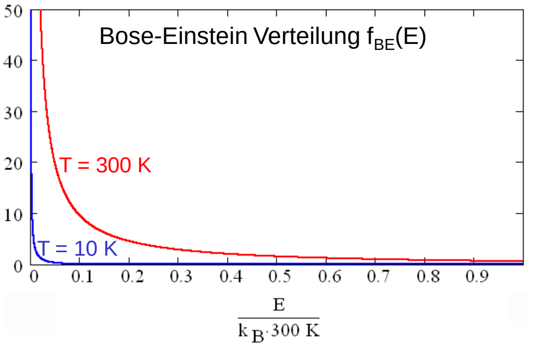
$$\mu_{FD} := 5 \cdot k_B \cdot T \qquad f_{FD}(E,T) := \frac{1}{\exp\left[\frac{(E-\mu_{FD})}{k_B \cdot T}\right]+1}$$



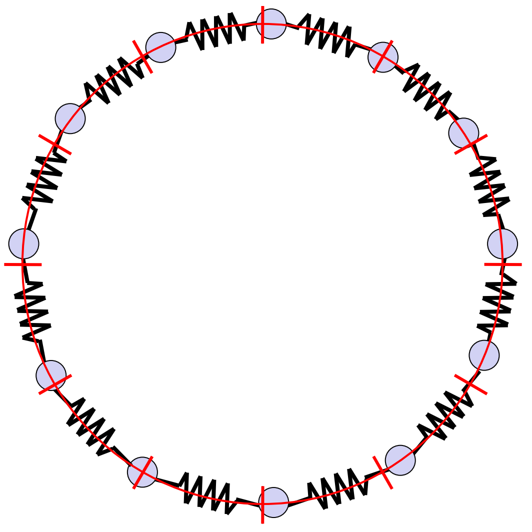
4 / 2 Bose-Einstein Verteilung

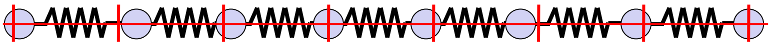
$$\langle n \rangle = f_{BE}(\omega,T) = \frac{1}{\exp(\hbar\omega / k_B T) - 1}$$



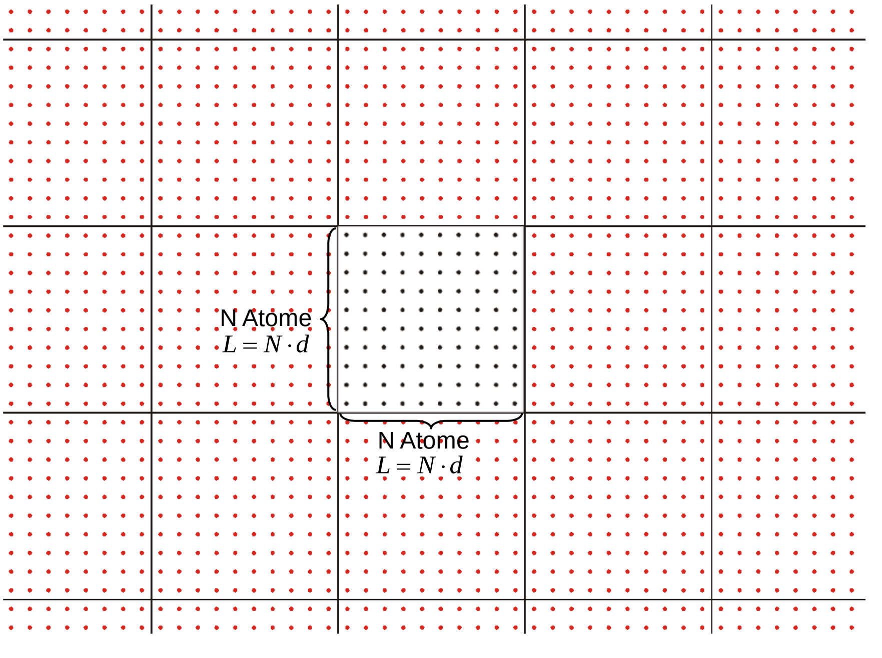


Periodische Randbedingungen

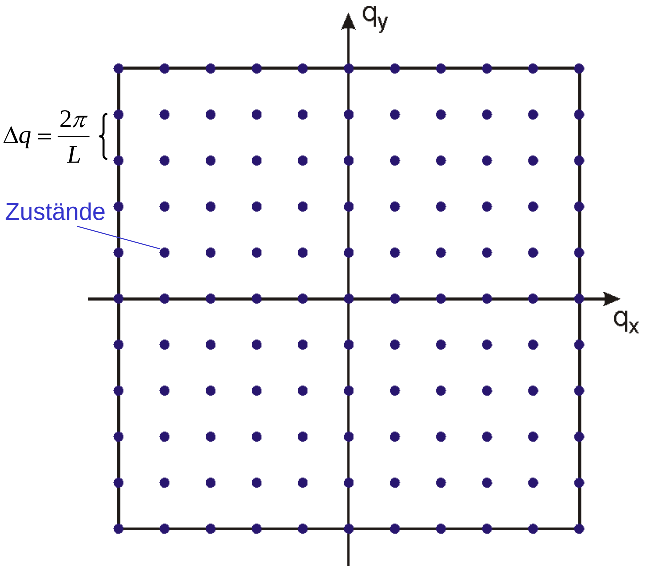




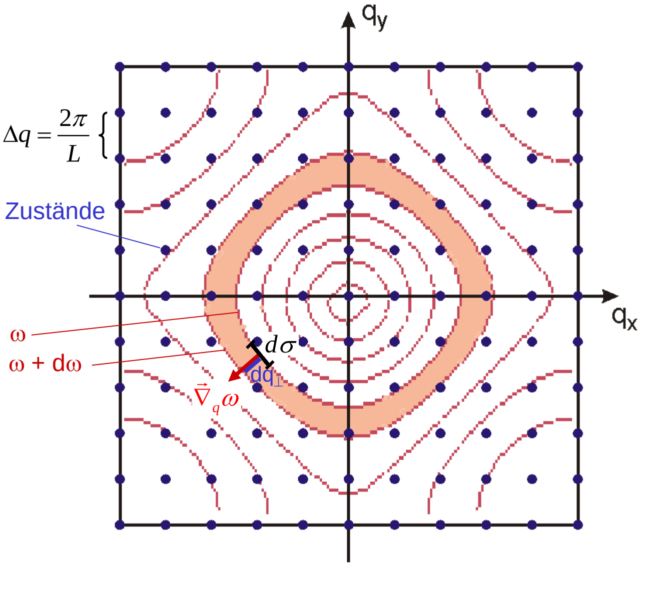
Periodische Randbedingungen



4 / 5 Periodische Randbedingungen



4 / 6 Zustandsdichte: Abzählen der Zustände

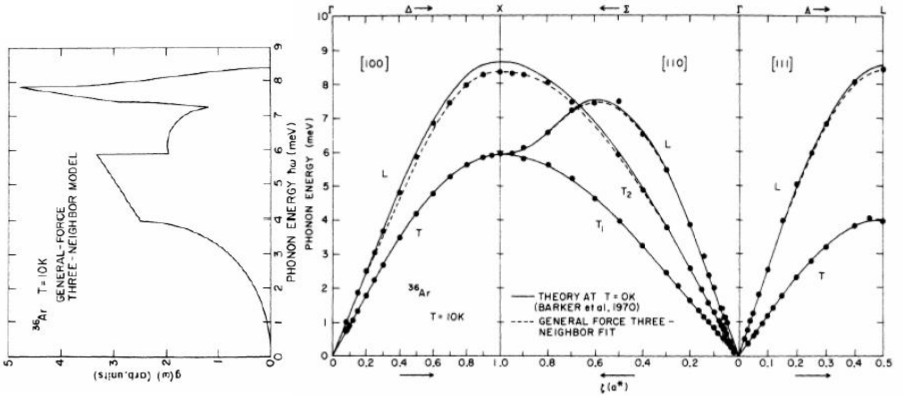


$dq_\perp$

4 / 7 Zustandsdichte

Beispiel: ^{36}Ar

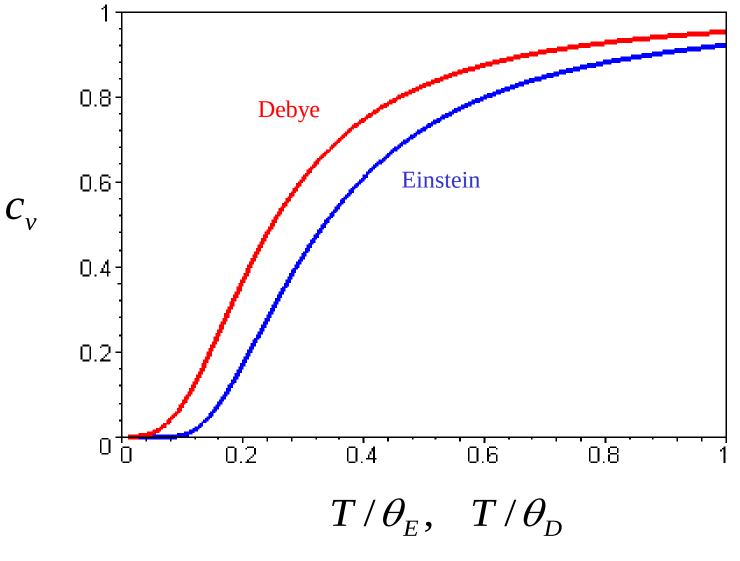
Zustandsdichte Dispersionsrelation



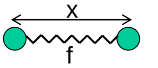
Fujii, et al., PRB 10 (1974) 3647

4 / 8 Einstein- und Debye-Modell

Verlauf der Wärmekapazität



Thermische Ausdehnung eines Oszillators



Mittlerer Abstand x bei Temperatur T gegeben durch Minimum in freier Energie $F = U + T \cdot S = U - T \cdot k_B \ln Z\,;\; Z \equiv$ Zustandssumme

Gleichgewichtsbedingung: $\left(\frac{\partial F}{\partial x}\right)_T = 0$

Harmonischer Oszillator:

$$Z = \sum_i \exp\left(-\frac{E_i}{k_B T}\right) = \frac{\exp(-\frac{1}{2}\hbar\omega / k_B T)}{1 - \exp(-\hbar\omega / k_B T)} \quad \rightarrow T \cdot S = \tfrac{1}{2}\hbar\omega + k_B T \cdot \ln\left[1 - \exp(-\hbar\omega / k_B T)\right]$$

Anharmonischer Oszillator:

„Quasi-harmonische Näherung“: $\omega = \omega(x)\,;\; E = (n + \frac{1}{2}) \cdot \hbar\omega(x)$

$\rightarrow$ zeitl. Mittelwert des Abstands x $\neq$ Minimum des Potentials x_0

Entwicklung von U um x_0: $U = U(x_0) + \frac{1}{2} f \cdot (x - x_0)^2$

Berechnung von mittlerem Abstand x über Gleichgewichtsbedingung:

$$\left(\frac{\partial U}{\partial x}\right)_T = f \cdot (x - x_0)\,;\quad \left(\frac{\partial (T \cdot S)}{\partial x}\right)_T = \tfrac{1}{2}\hbar\frac{\partial\omega}{\partial x} + \hbar\frac{\exp(-\hbar\omega / k_B T)}{1 - \exp(-\hbar\omega / k_B T)} \cdot \frac{\partial\omega}{\partial x} = \underbrace{\frac{\partial\omega}{\partial x} \cdot \frac{1}{\omega}}_{\frac{\partial(\ln\omega)}{\partial x} = \frac{\partial(\ln\omega)}{\partial(\ln x)} \cdot \frac{1}{x_0}} \cdot \langle E(\omega, T)\rangle$$

$$\rightarrow \quad x - x_0 = -\frac{1}{f x_0} \cdot \frac{\partial(\ln\omega)}{\partial x} \cdot \langle E(\omega, T)\rangle$$

$$\boxed{\alpha \equiv \frac{1}{x_0} \cdot \frac{dx}{dT} = -\frac{1}{x_0^2 f} \cdot \frac{\partial(\ln\omega)}{\partial(\ln x)} \cdot \frac{\partial}{\partial T}\langle E(\omega, T)\rangle}$$

(nach Ibach/Lüth)