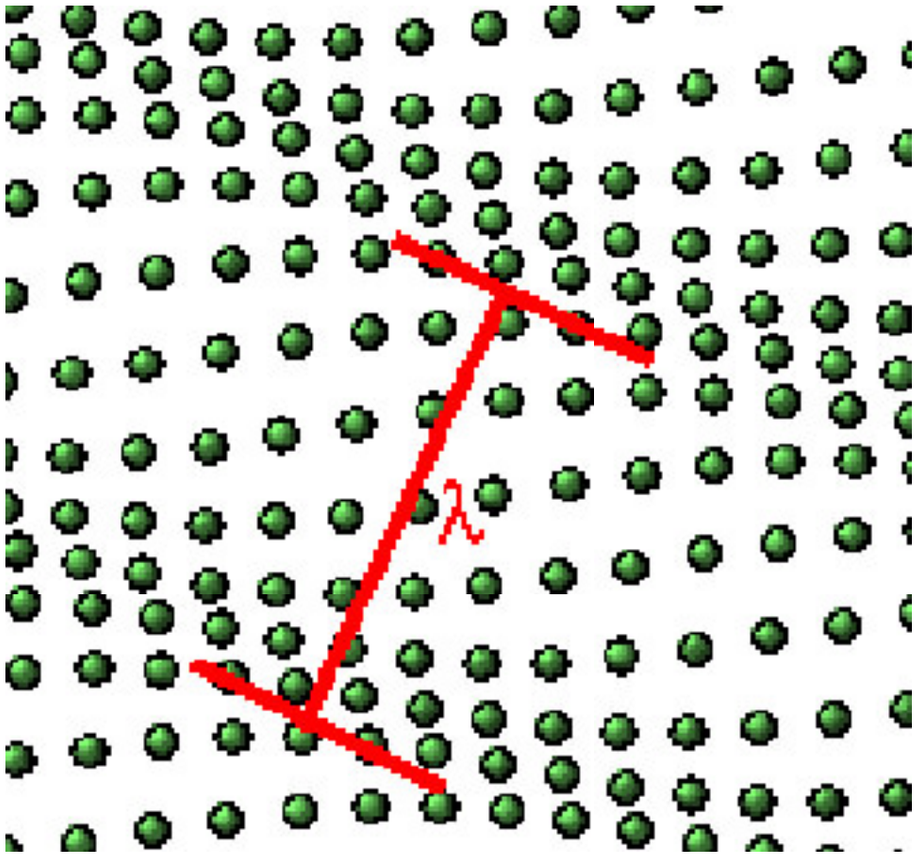
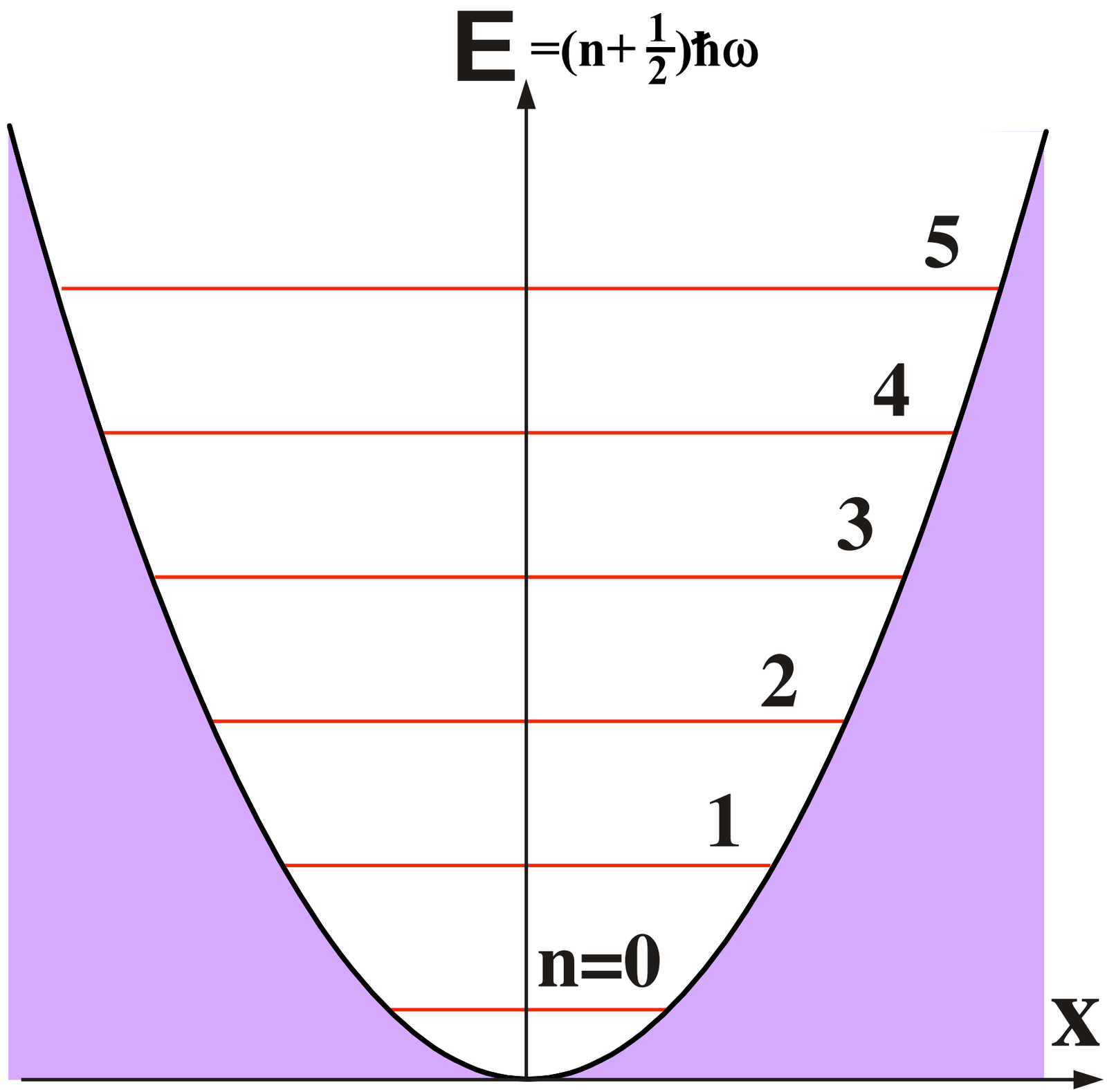
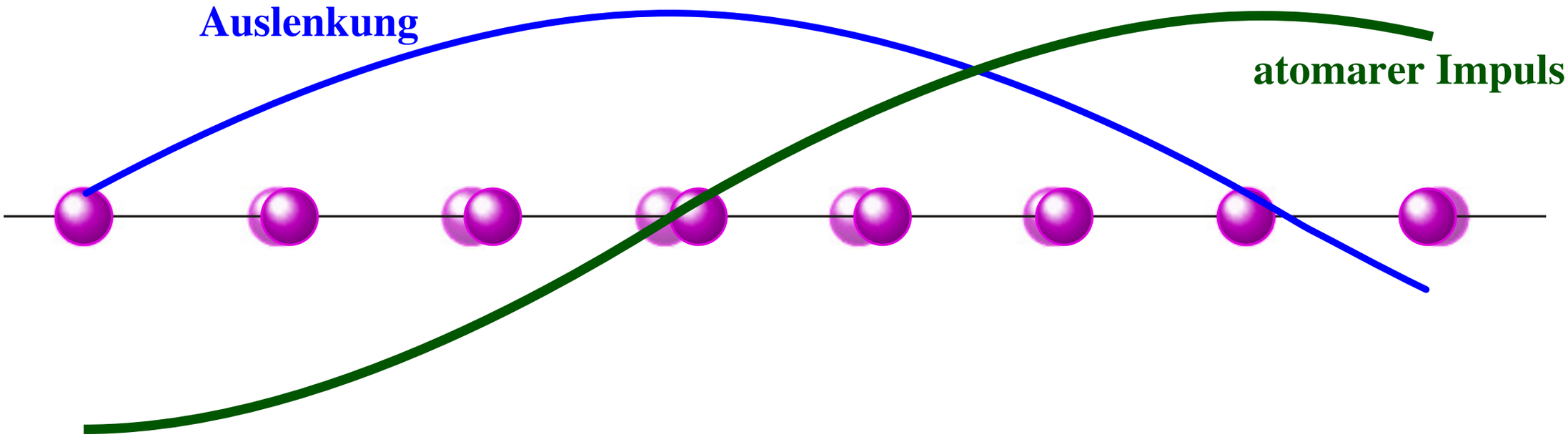
Schwingungszustände



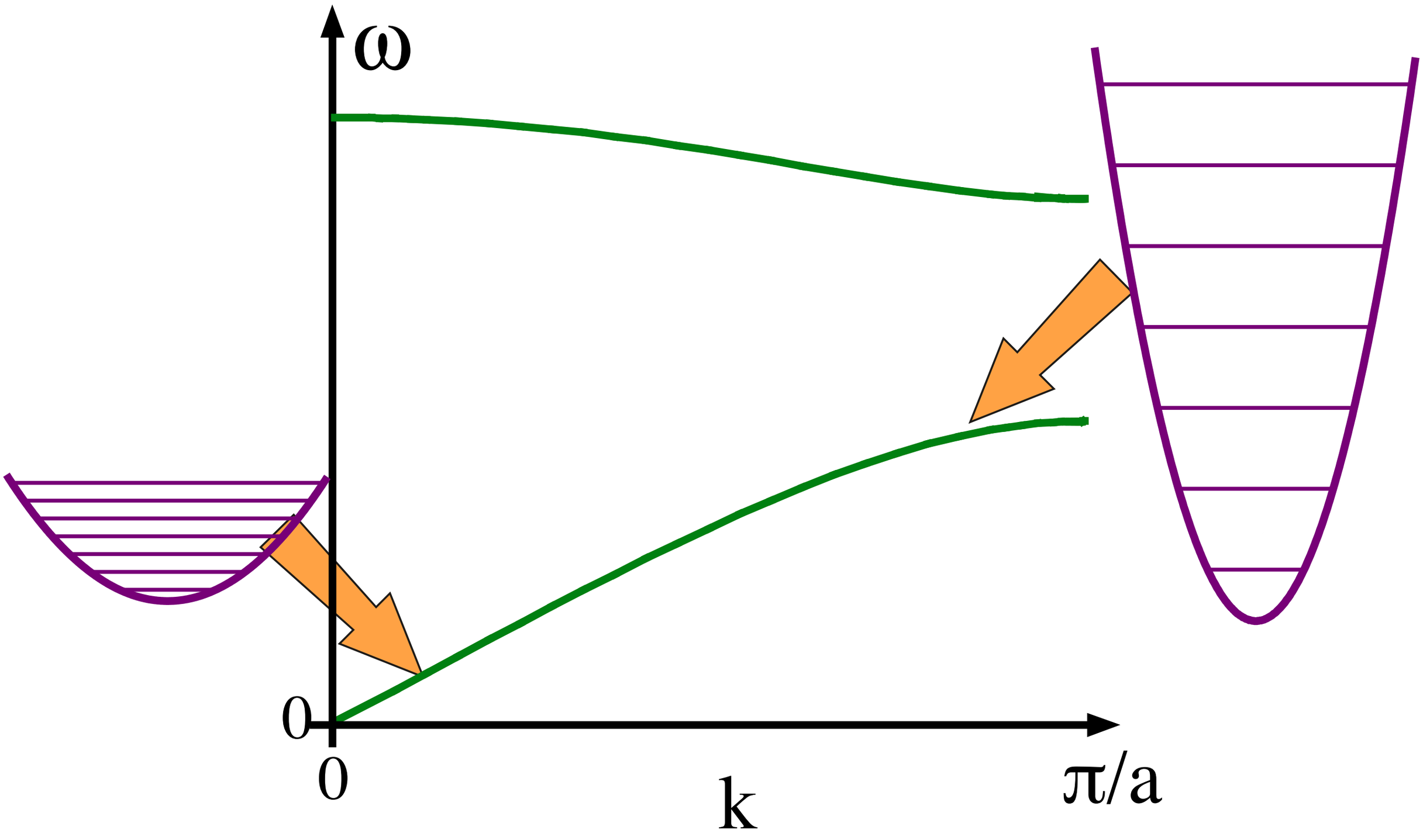
Phononen
Impuls $\vec{p} = \hbar\vec{k}$
Energie $E = \hbar\omega$
Spin $S = 1$



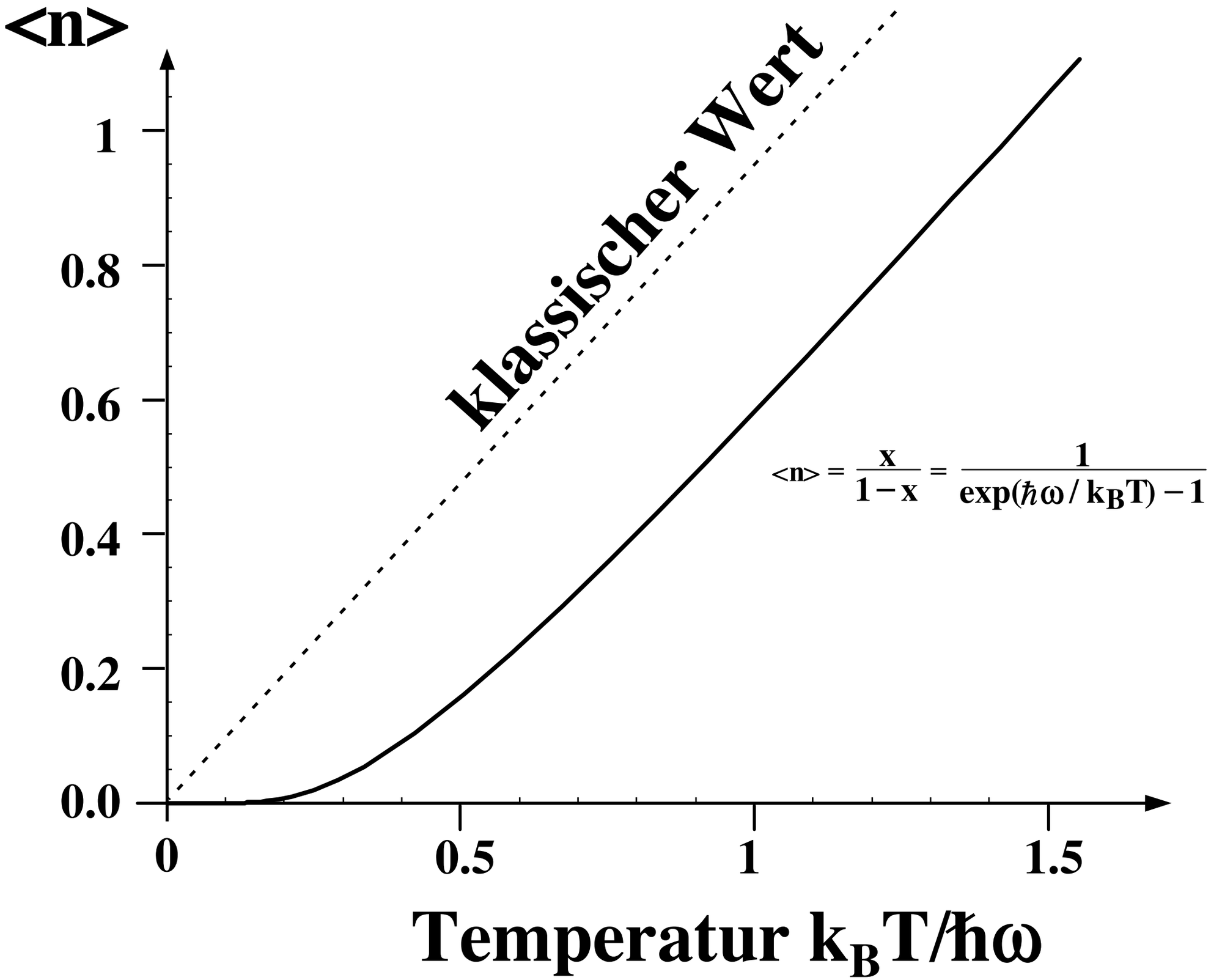
Auslenkung und Impuls



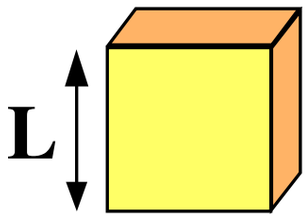
Phononenenergie



Anregung bei tiefer Temperatur



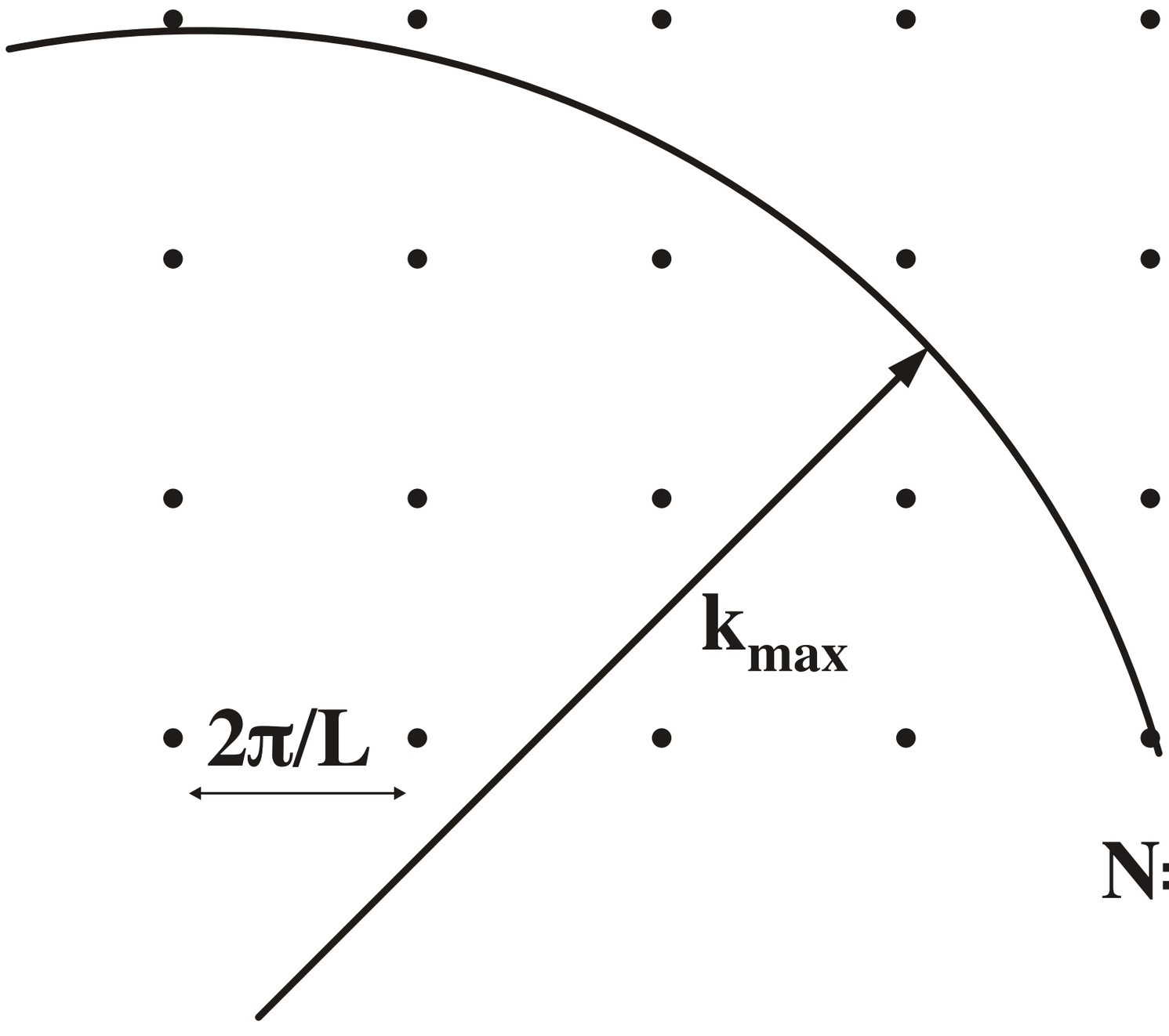
Zustände im k-Raum



Kristall

L >> a

periodische Randbedingungen

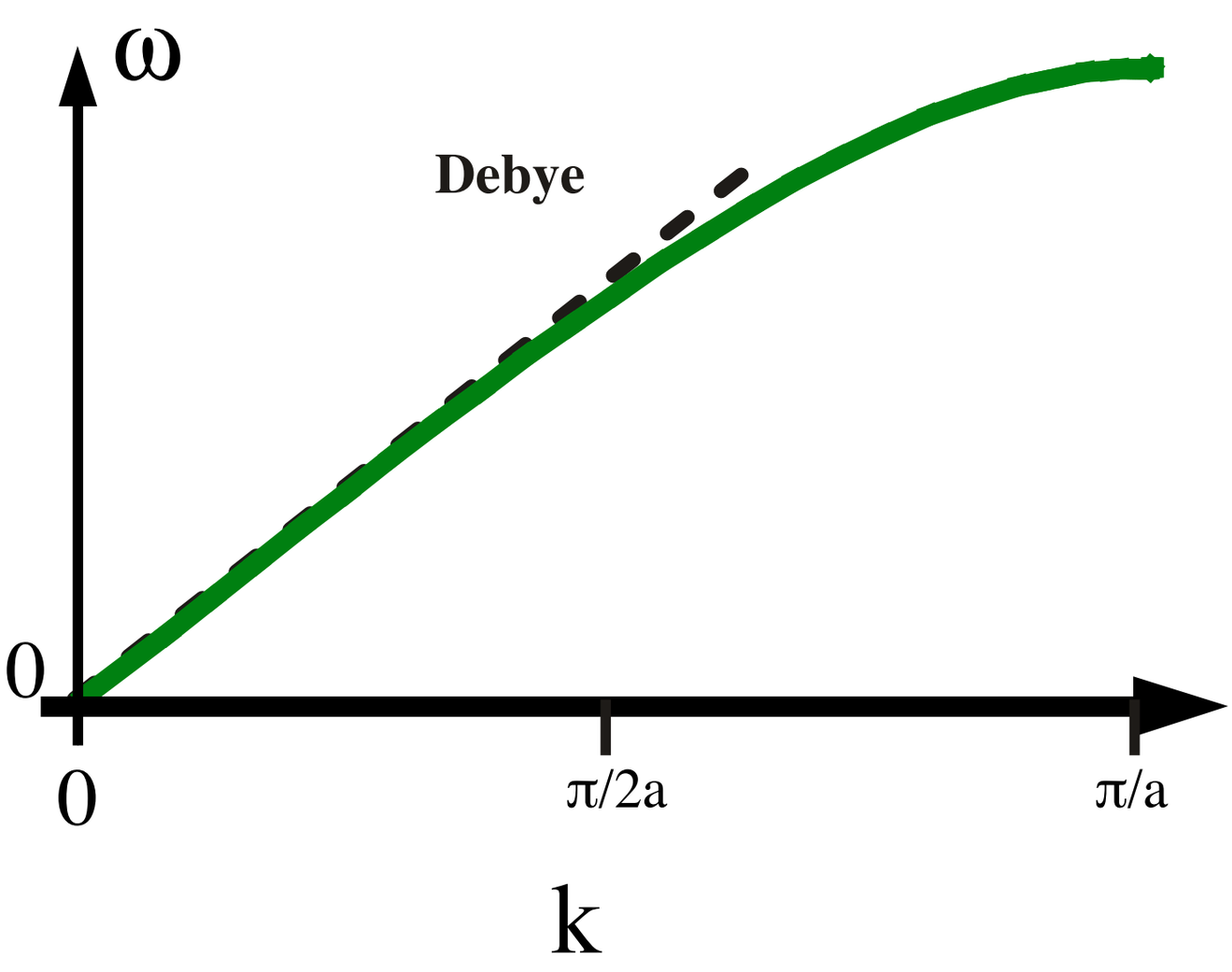


 # Zustände mit $k < k_{max}$

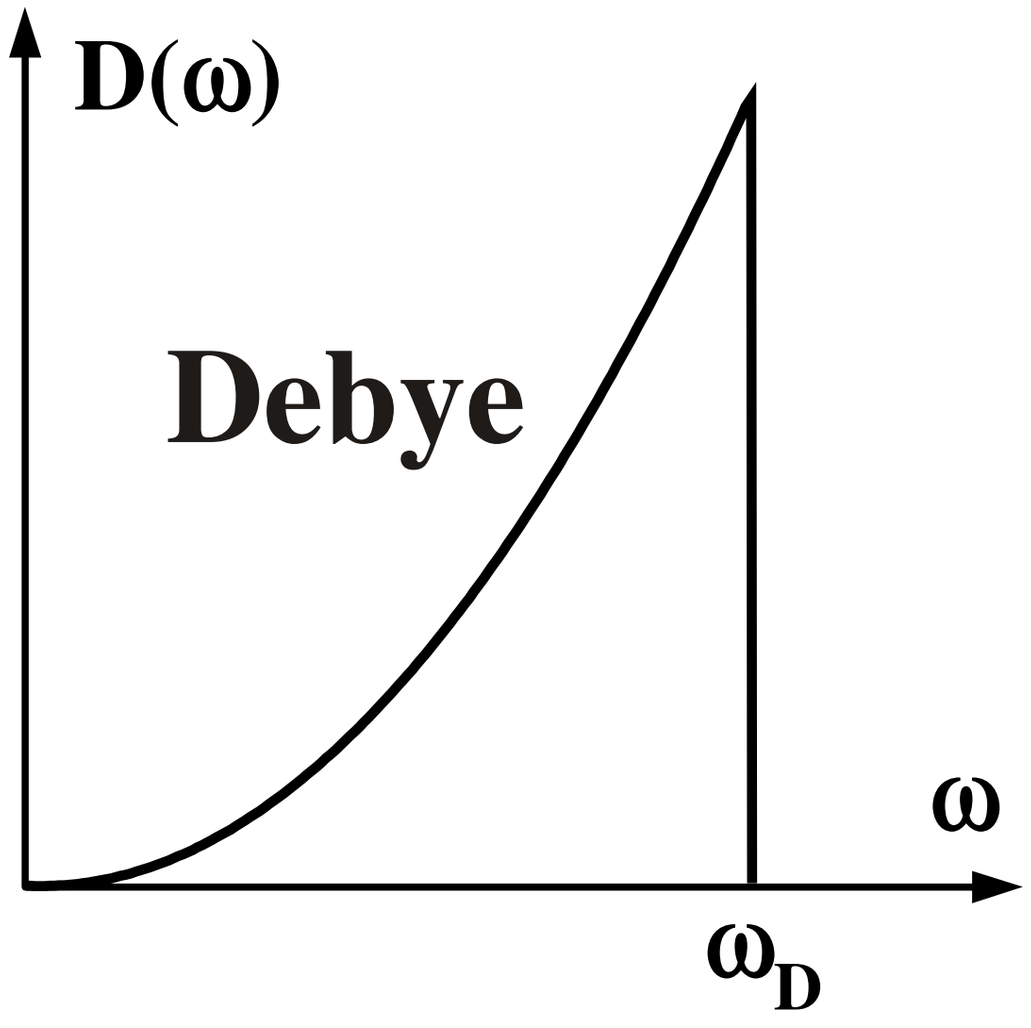
$$N = \frac{4\pi}{3} k_{max}^3 \left(\frac{L}{2\pi}\right)^3$$

Debye Näherung

Dispersion



Zustandsdichte

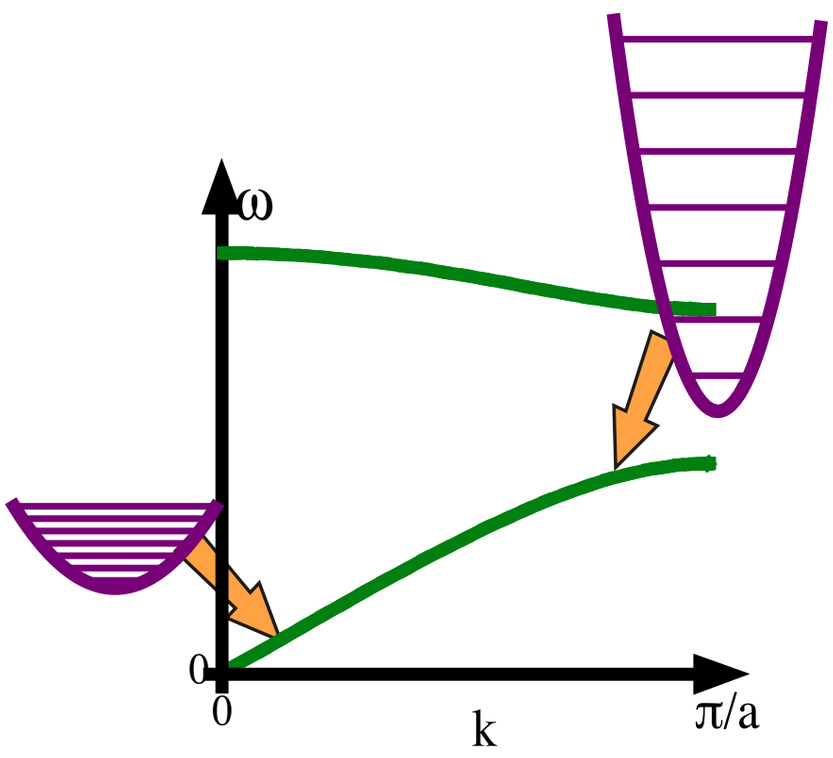


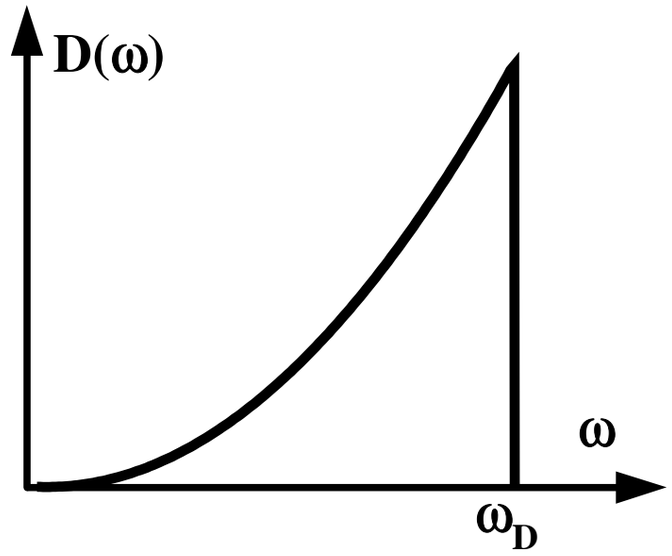
Debye Temperatur

Debye-Temperatur und Wärmeleitfähigkeit

Li	Be											B	C	N	O	F	Ne
344	1440												2230				75
0.85	2.00											0.27	1.29				
Na	Mg											Al	Si	P	S	Cl	Ar
158	400	Tieftemperaturgrenze von θ, in Kelvin										428	645				92
1.41	1.56	Wärmeleitzahl bei 300 K, in W cm^{-1} K^{-1}										2.37	1.48				
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
91	230	360.	420	380	630	410	470	445	450	343	327	320	374	282	90		72
1.02		0.16	0.22	0.31	0.94	0.08	0.80	1.00	0.91	4.01	1.16	0.41	0.60	0.50	0.02		
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn w	Sb	Te	I	Xe
56	147	280	291	275	450		600	480	274	225	209	108	200	211	153		64
0.58		0.17	0.23	0.54	1.38	0.51	1.17	1.50	0.72	4.29	0.97	0.82	0.67	0.24	0.02		
Cs	Ba	La β	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
38	110	142	252	240	400	430	500	420	240	165	71.9	78.5	105	119			
0.36		0.14	0.23	0.58	1.74	0.48	0.88	1.47	0.72	3.17		0.46	0.35	0.08			
Fr	Ra	Ac															
			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	
									200		210				120	210	
			0.11	0.12	0.16		0.13		0.11	0.11	0.11	0.16	0.14	0.17	0.35	0.16	
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	
			163		207												
			0.54		0.28	0.06	0.07										

Energie der Phononen





im Debye Modell

$$U = \frac{3\,V\,k_B^4\,T^4}{2\;\;^2\,v_S^3\,\hbar^3}\int_0^{x_D} dx\,\frac{x^3}{e^x - 1} \qquad x = \frac{\hbar\omega}{k_B T} \qquad x_D = \frac{\theta}{T} = \frac{\hbar v_S}{k_B T}\sqrt[3]{\frac{6\;\;^2 N_z}{V}}$$

$$\cdot\left(\frac{x_D}{x_D}\right)^3$$

$$U = 9\,k_B\,T\,N_z\left(\frac{T}{\theta}\right)^3\int_0^{x_D} dx\,\frac{x^3}{e^x - 1}$$

Wärmekapazität

$$U = \frac{3\,V\,\hbar}{2\,\pi^2\,v_S^3} \int_0^{\omega_D} d\omega \frac{\omega^3}{e^{\frac{\hbar\omega}{k_B T}} - 1}$$

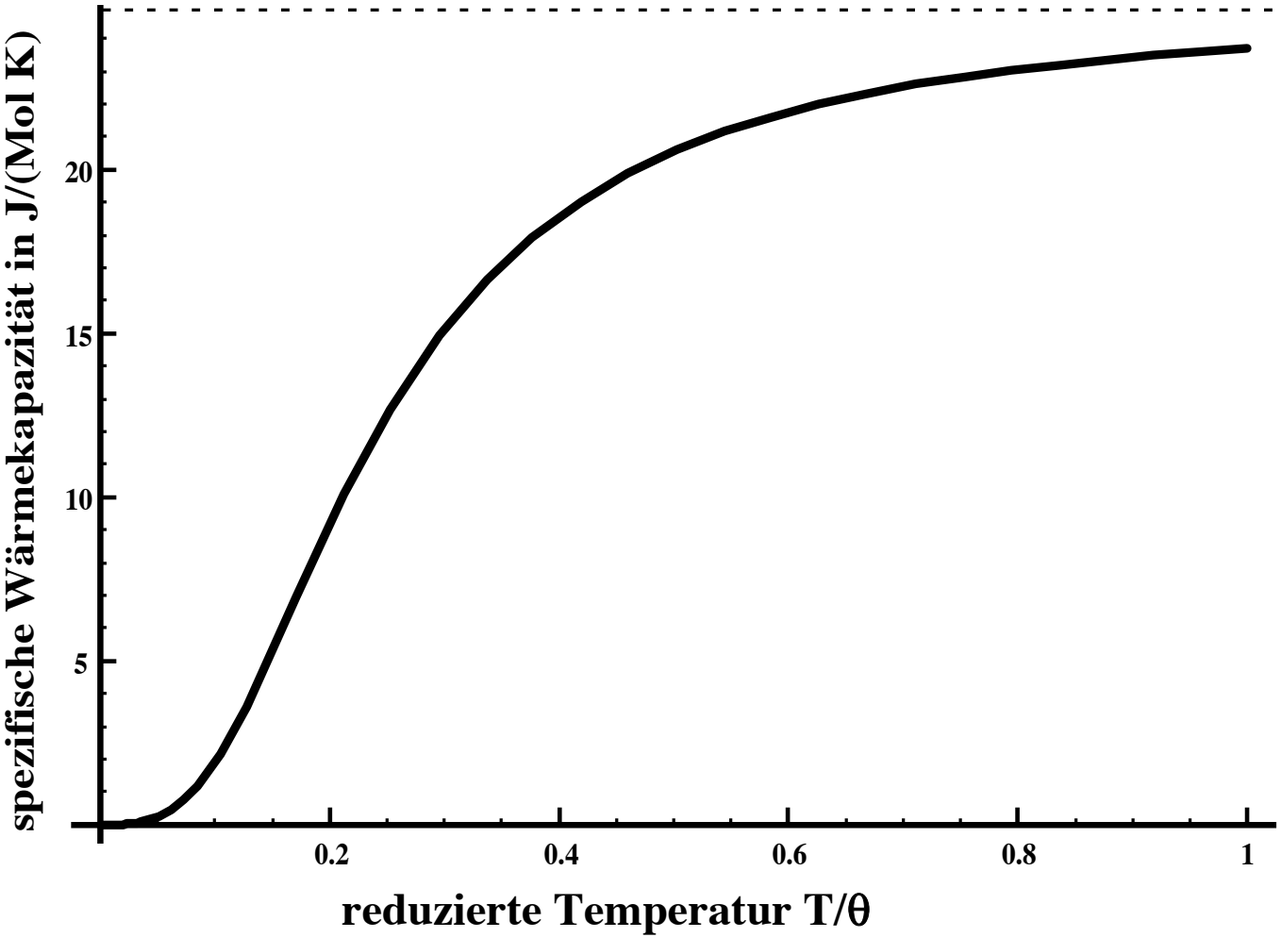
$$c_V = \frac{dU}{dT} = \frac{3\,V\,\hbar^2}{2\,\pi^2\,v_S^3\,k_B\,T^2} \int_0^{\omega_D} d\omega \frac{\omega^4\, e^{\frac{\hbar\omega}{k_B T}}}{\left(e^{\frac{\hbar\omega}{k_B T}} - 1\right)^2}$$

$$= 9\,k_B\,N_z \left(\frac{T}{\theta}\right)^3 \int_0^{x_D} dx \frac{x^4}{(e^x - 1)^2}$$

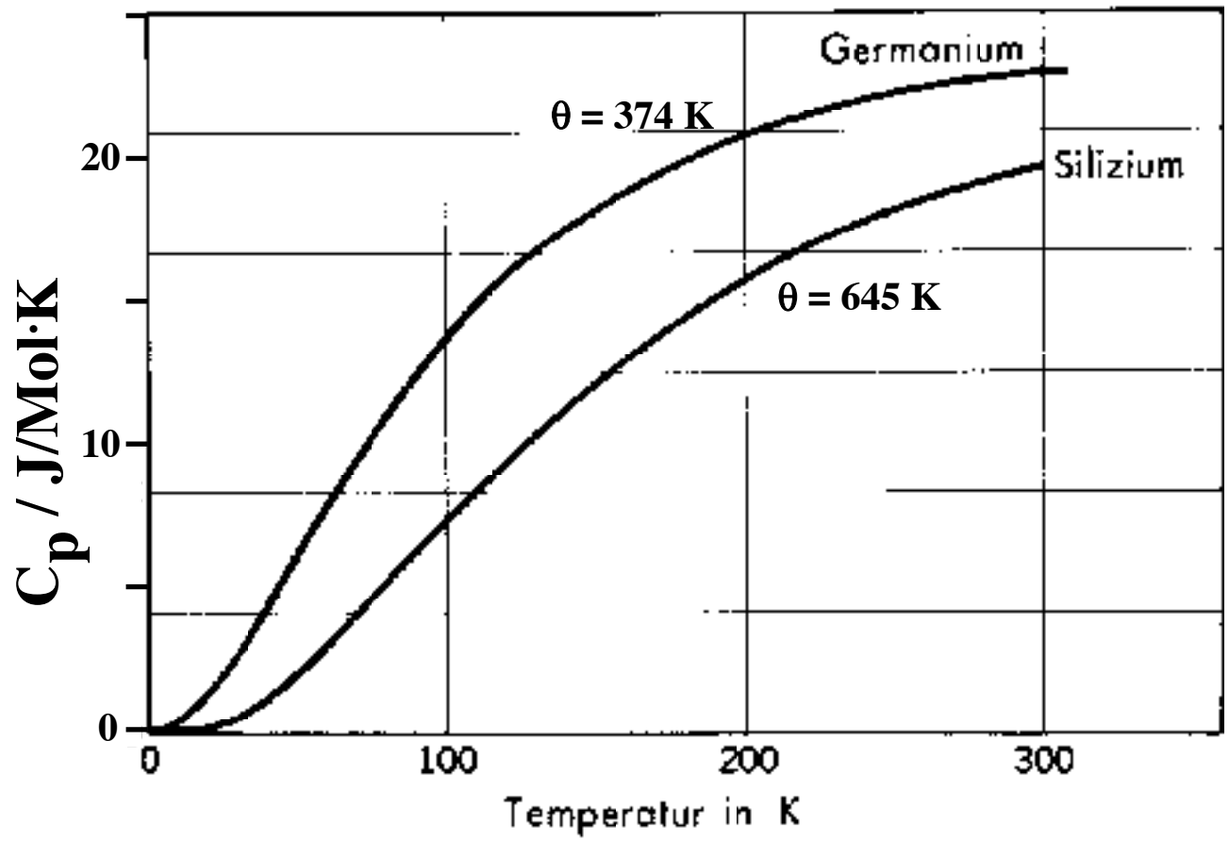
Wärmekapazität

Temperaturabhängigkeit im Debye-Modell

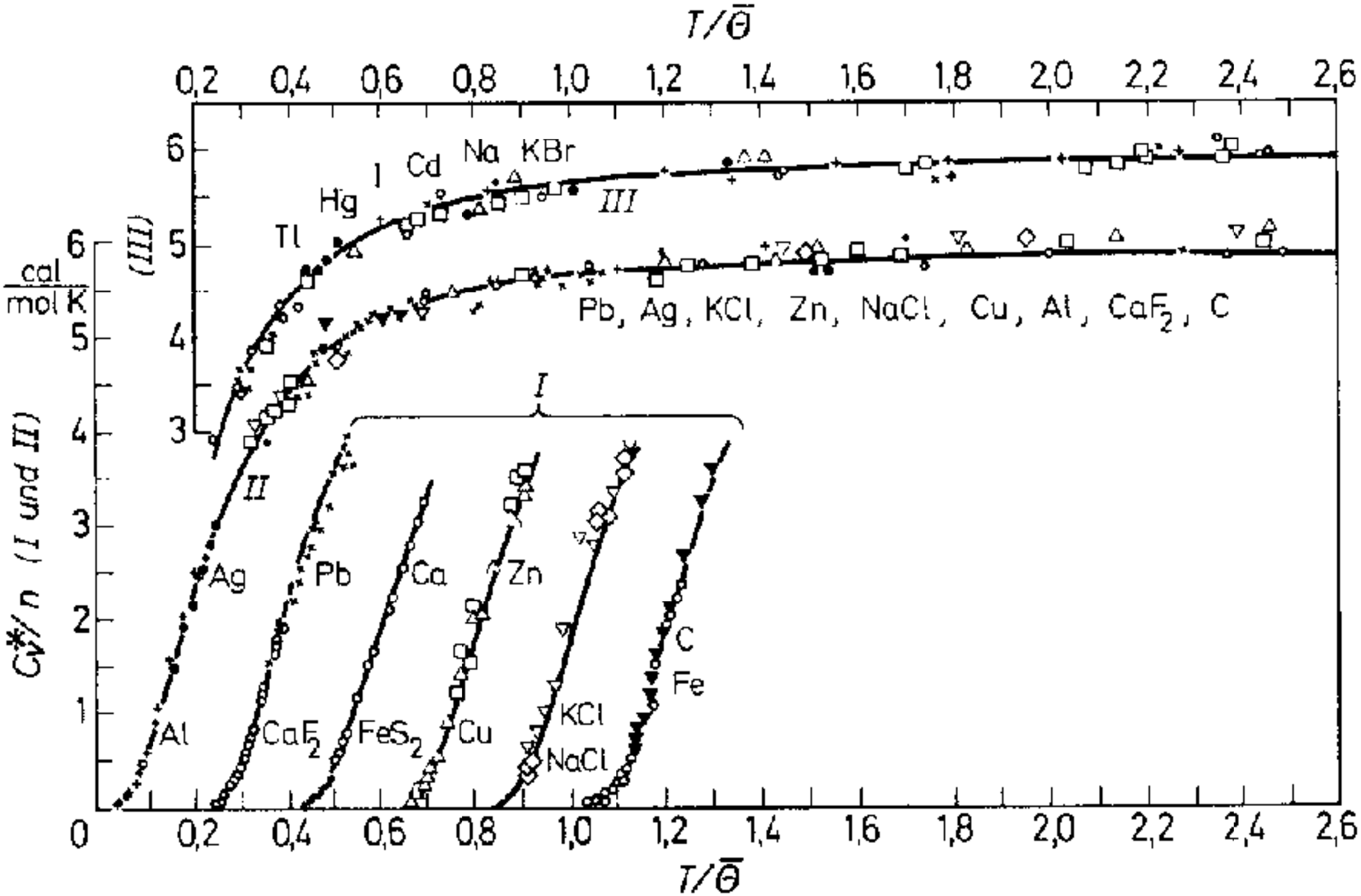
Theorie



Experiment

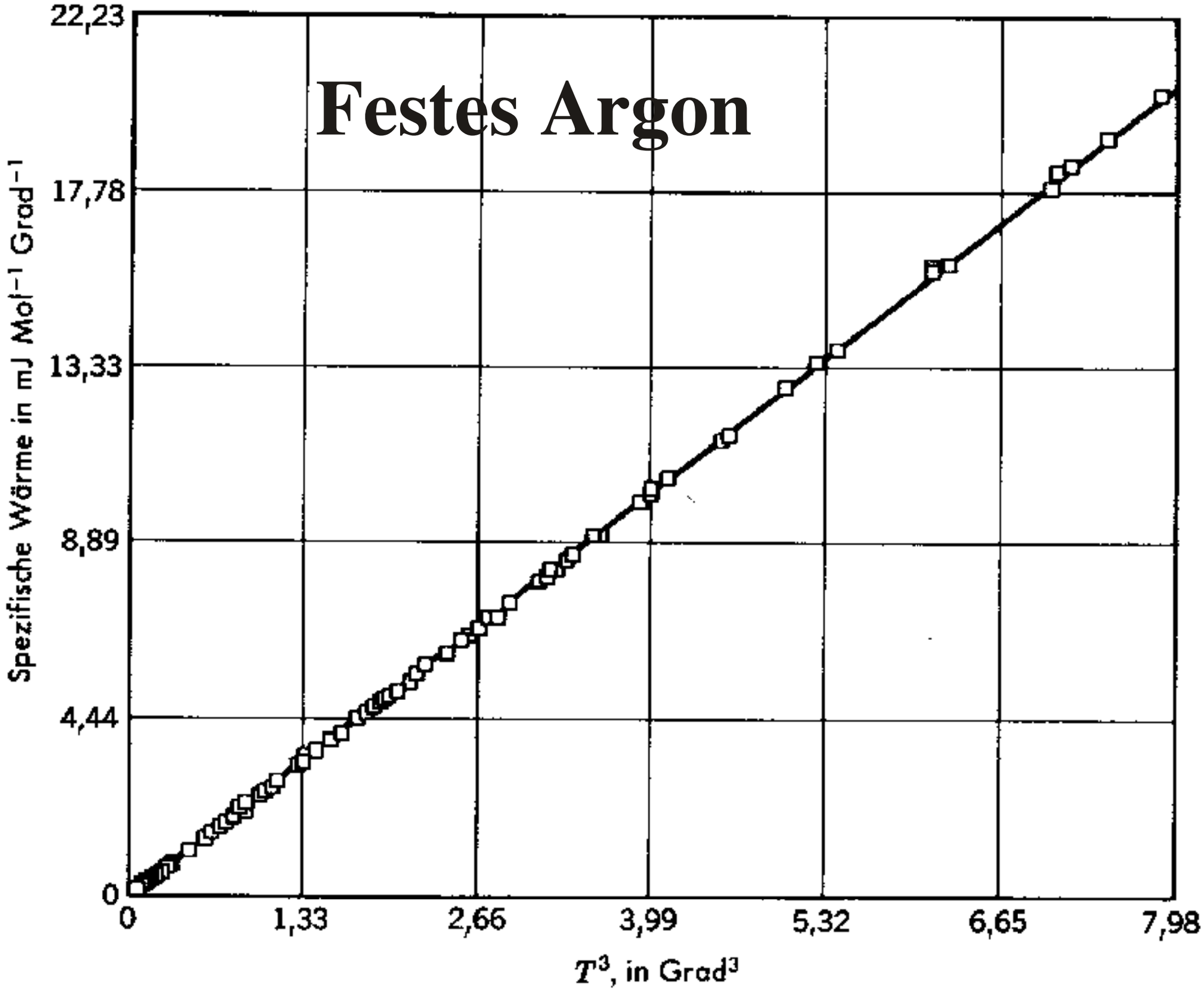


C_V vs. T

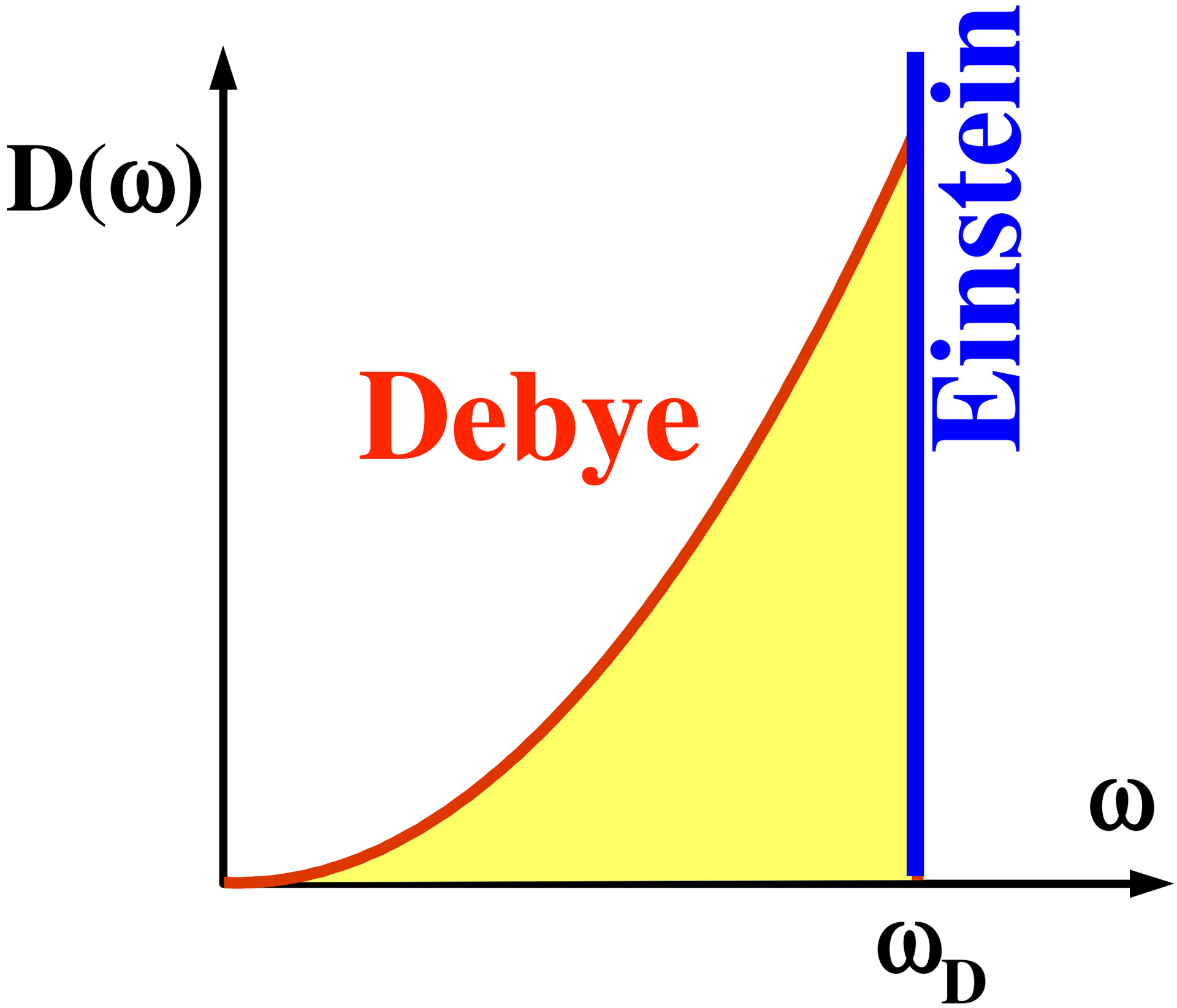


K.H. Hellwege, 'Einführung in die Festkörperphysik', Springer, Berlin (1976).

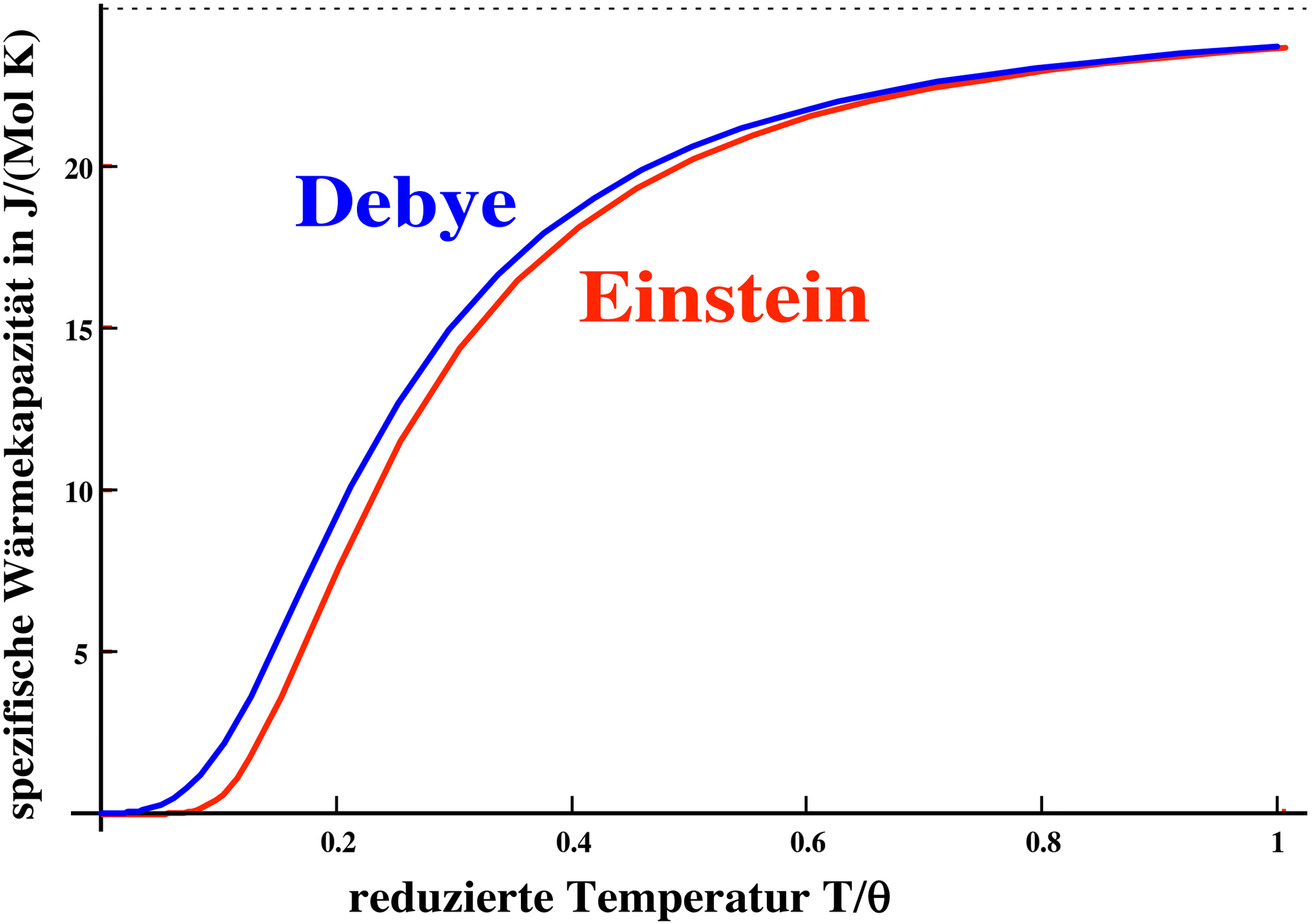
Tieftemperaturverhalten



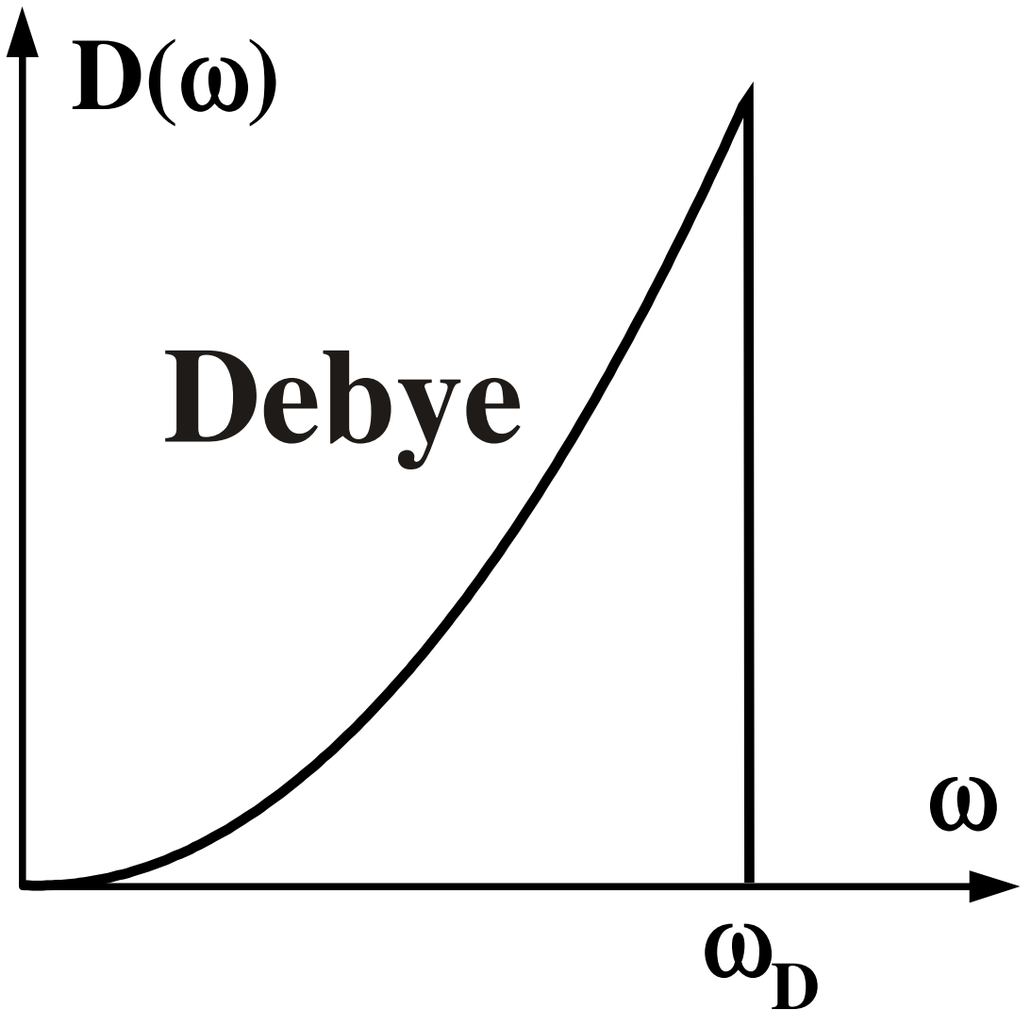
Zustandsdichten

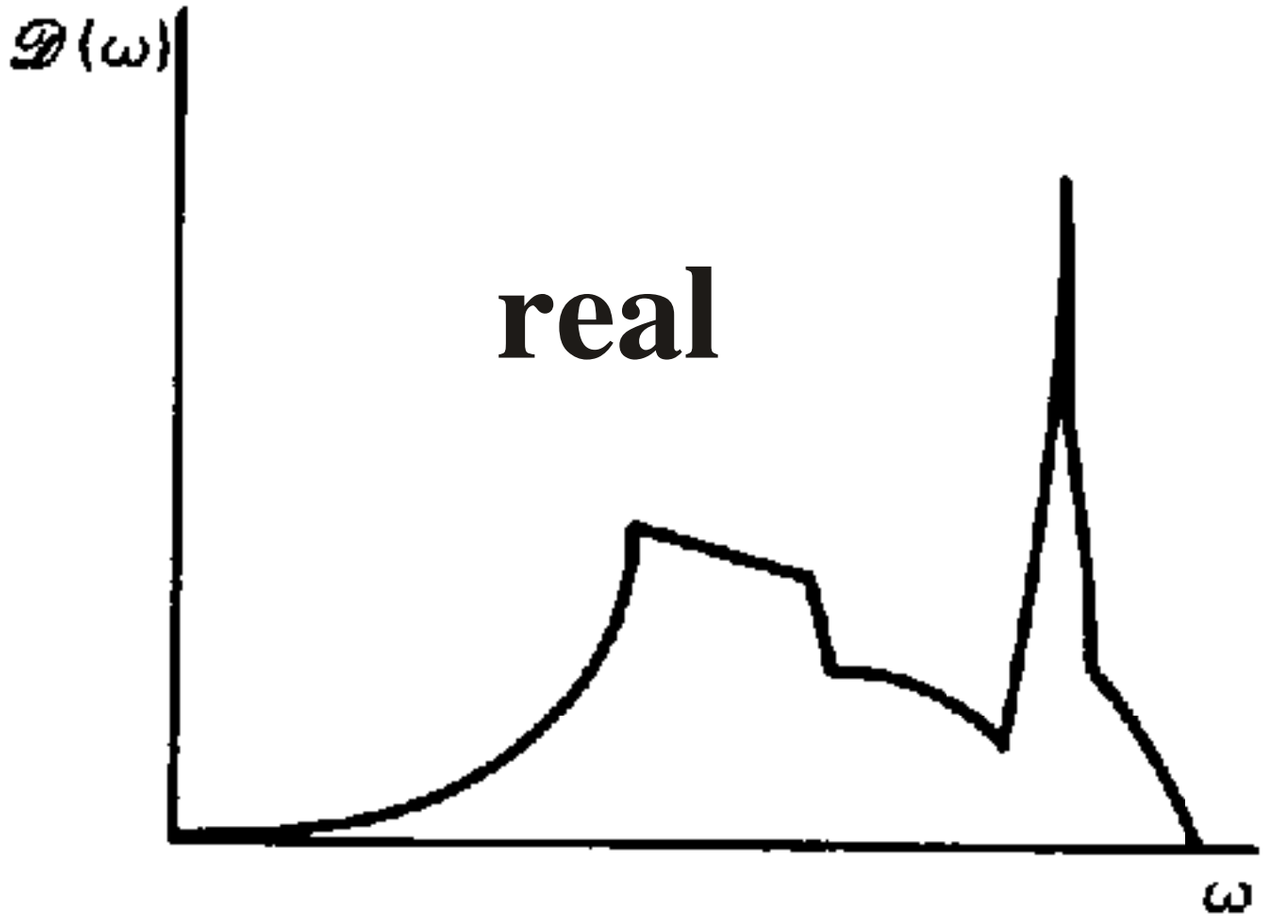


Vergleich Einstein / Debye



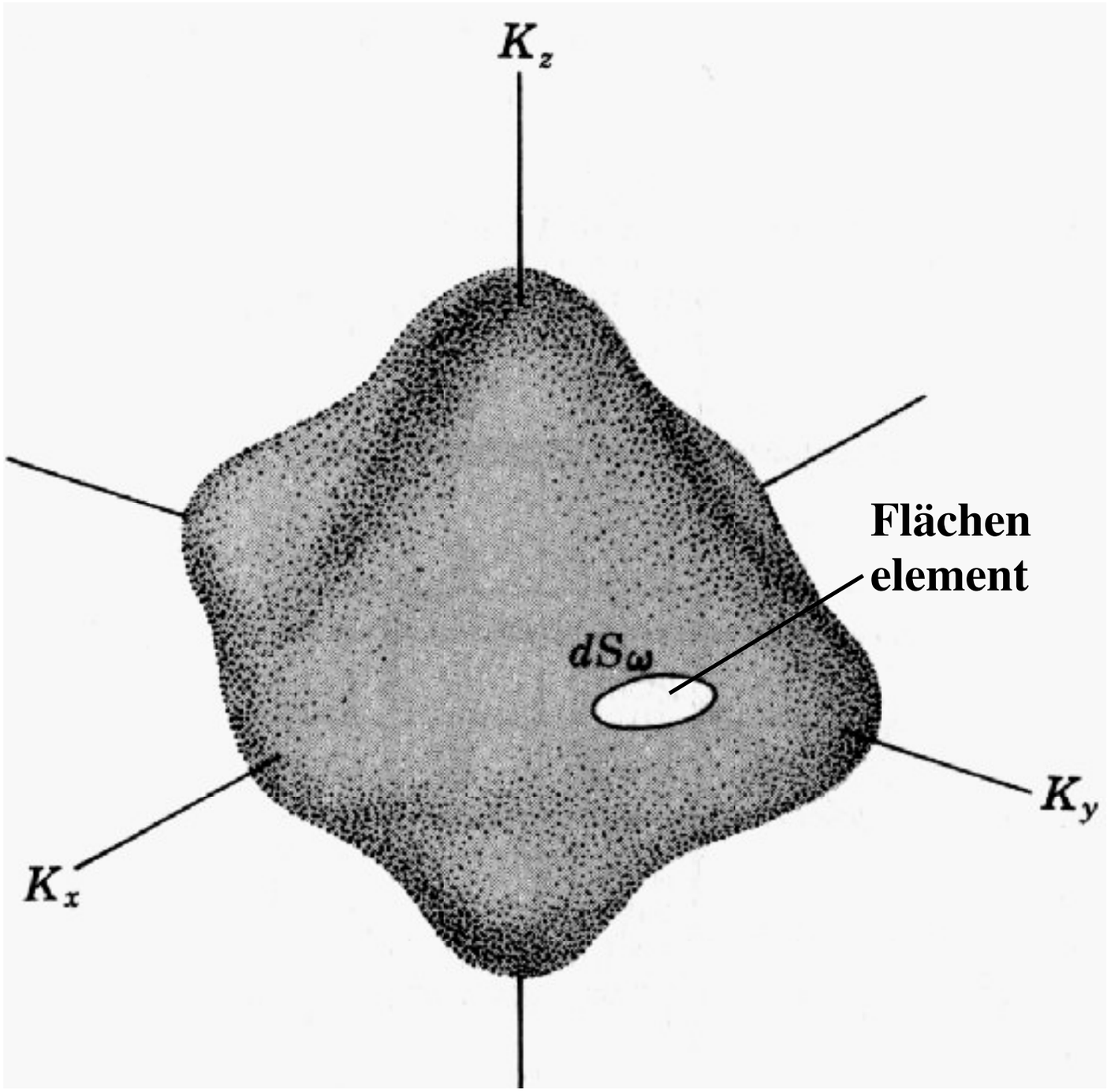
Zustandsdichten

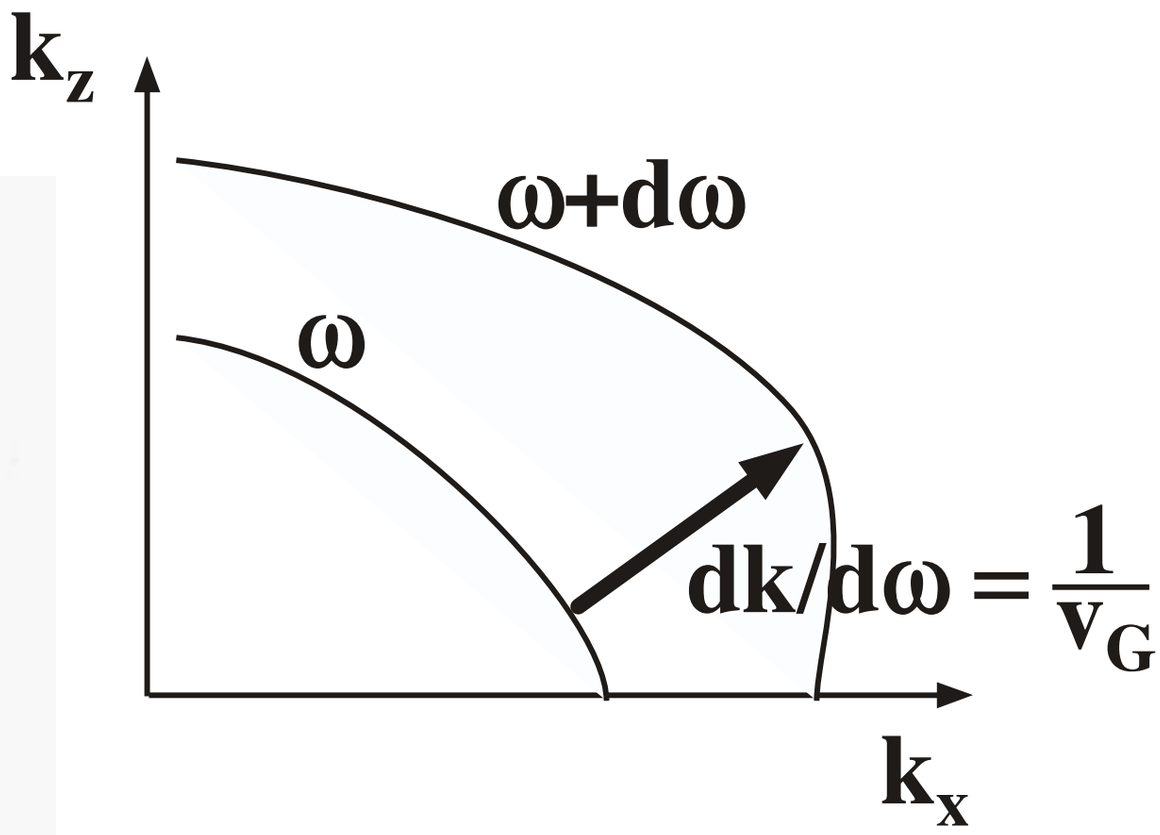




Zustandsdichte in 3D

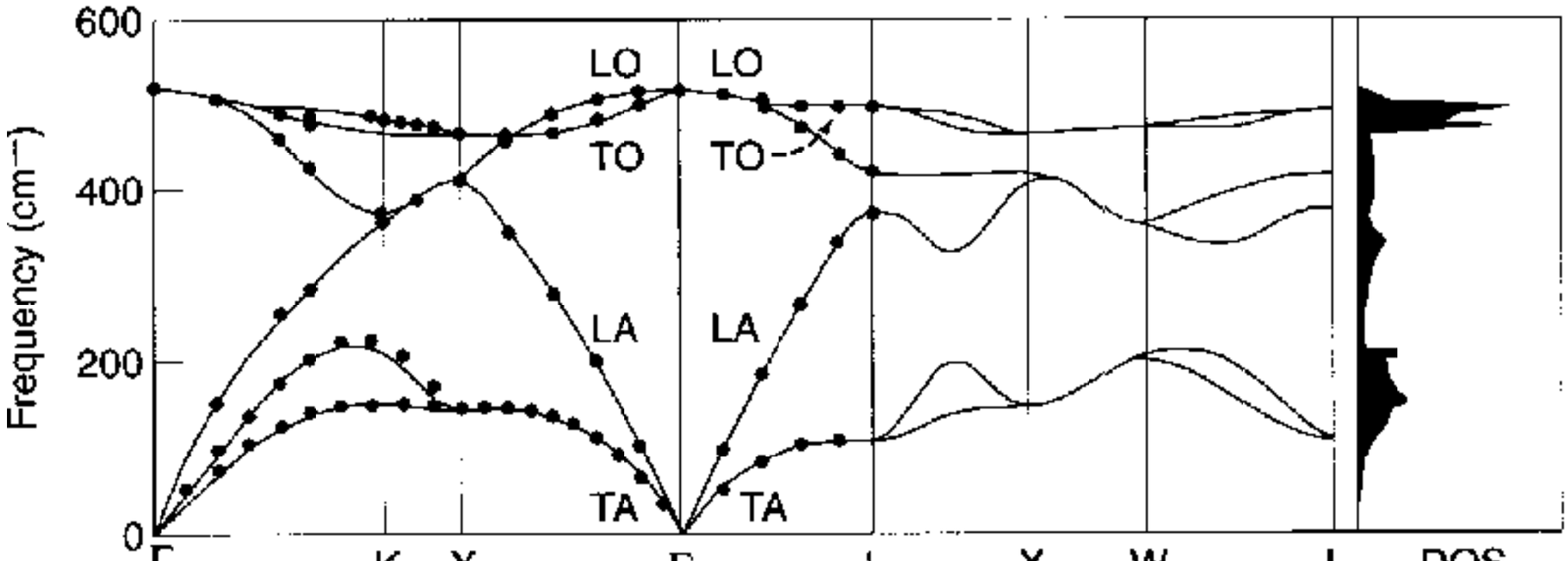
Iso-Frequenzfläche



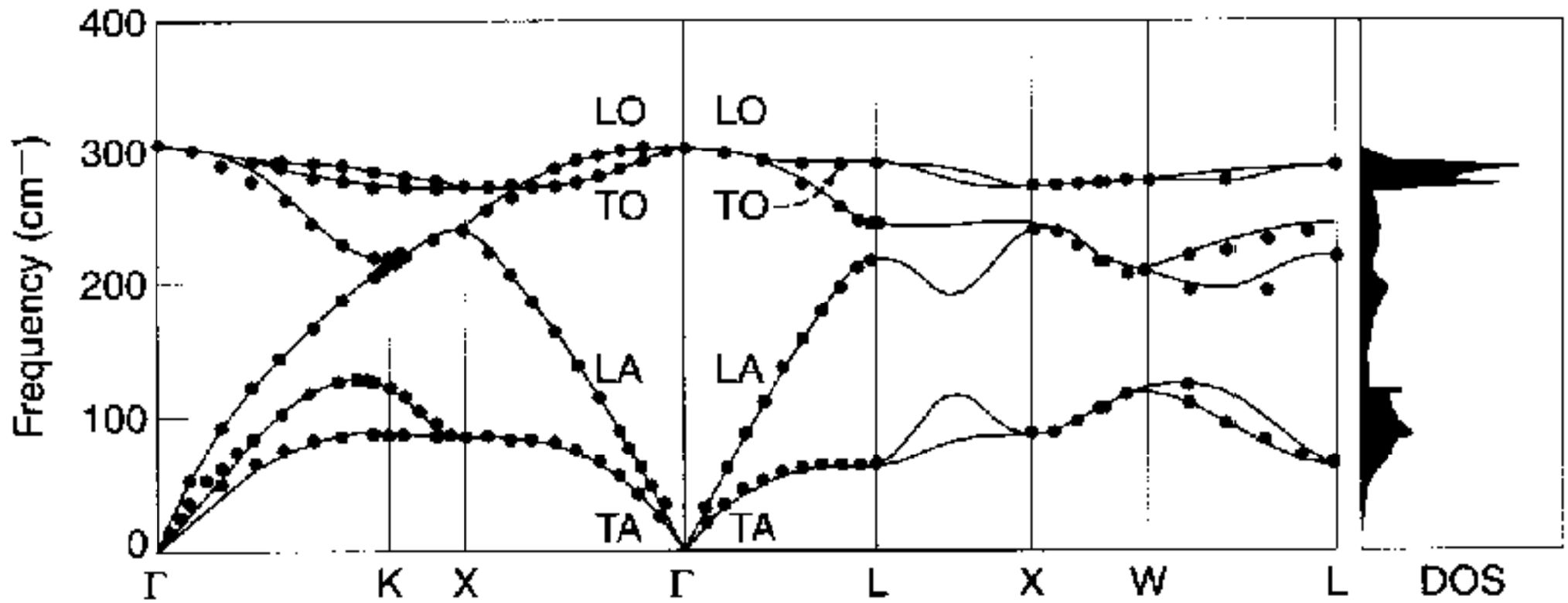


Dispersion und Zustandsdichte

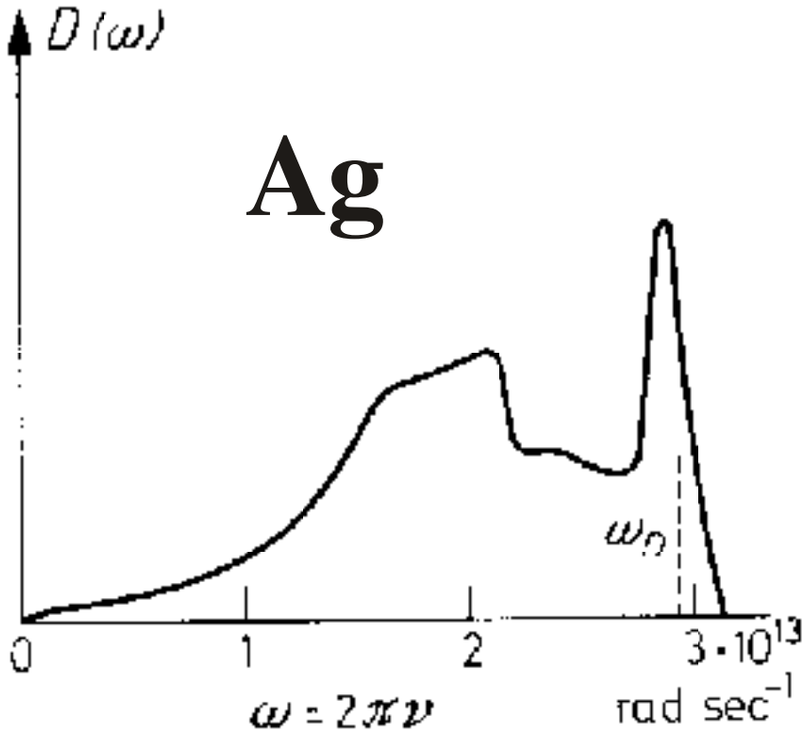
Si

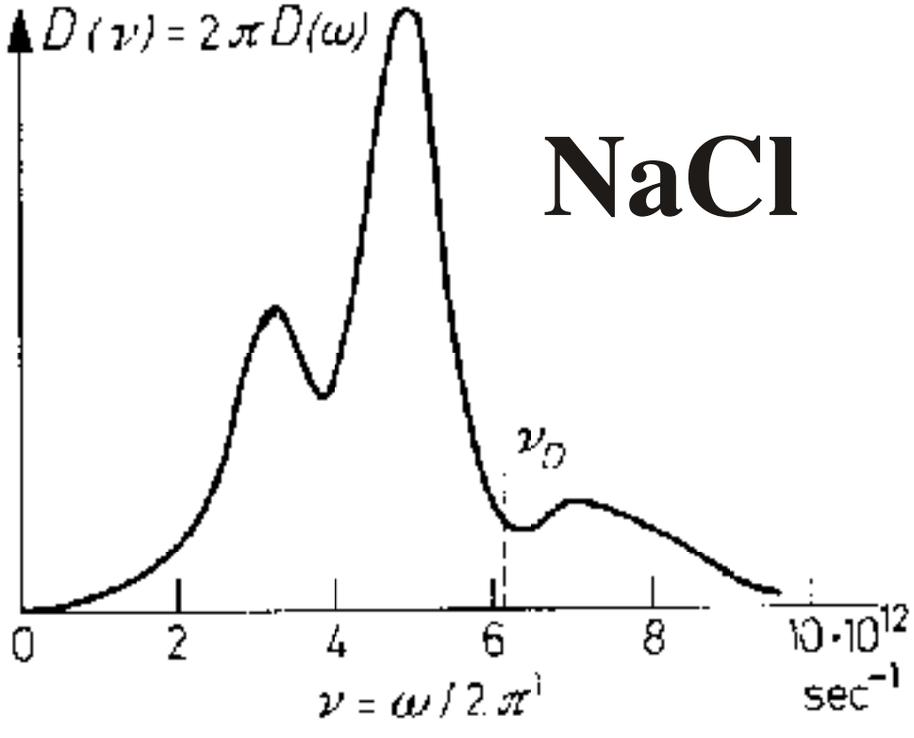


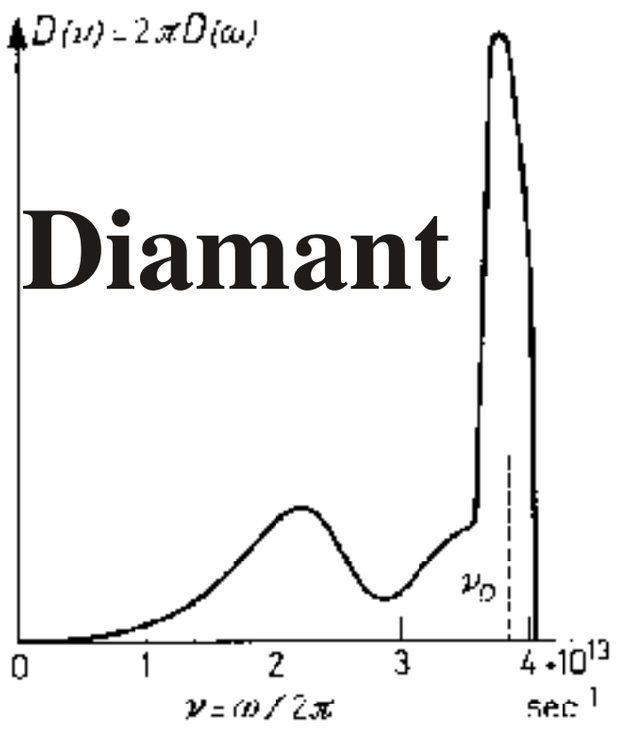
Ge



Zustandsdichte : Beispiele

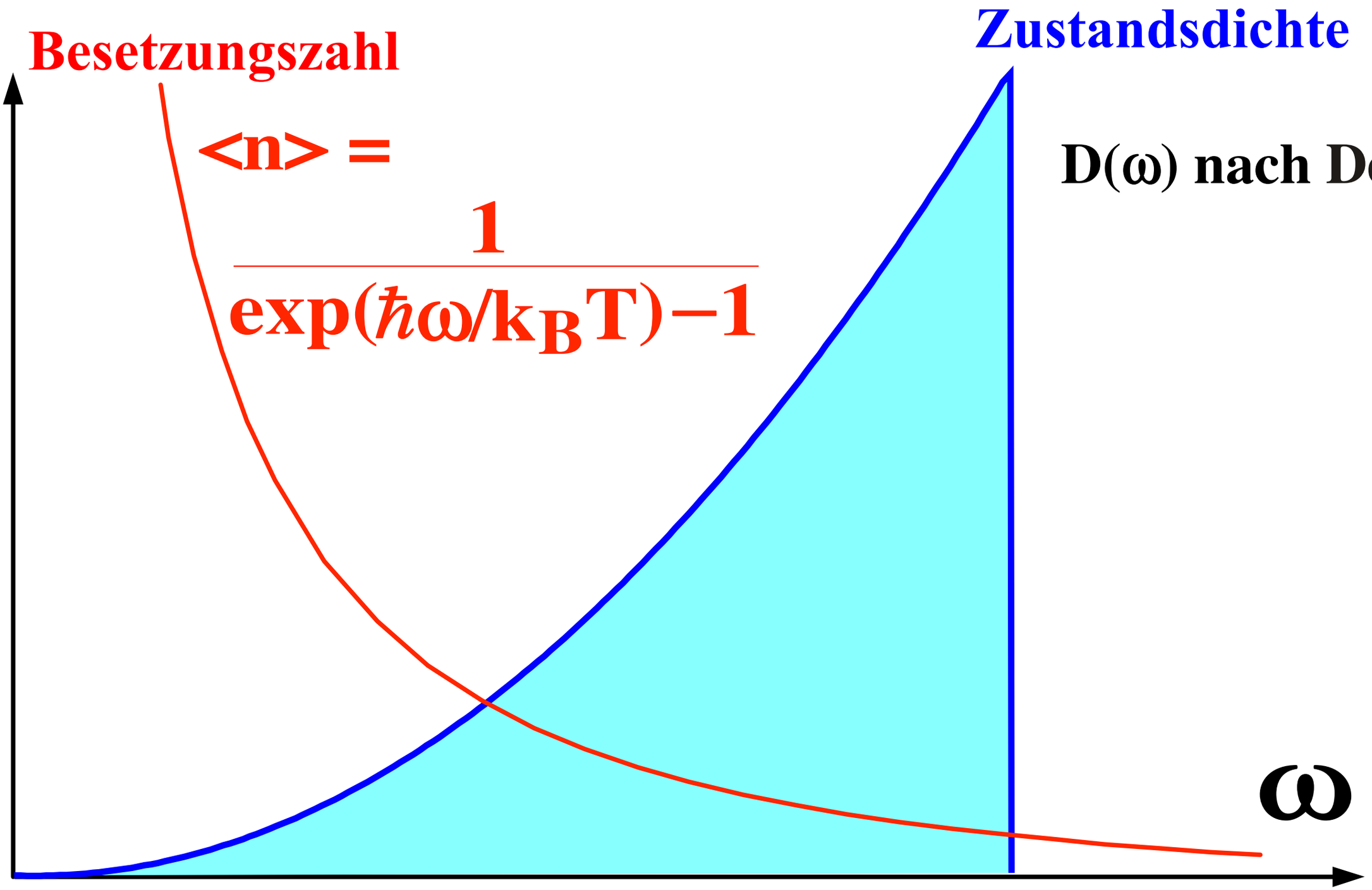






Phononendichte

 # Phononen pro Frequenzeinheit



Phononendichte

 # Phononen pro Frequenzeinheit