





Ex.2

a)

$$ln[\cdot]:= ek := \hbar c k$$

 $nmean := 1 / (Exp[\beta ek] - 1)$

$$N = \sum_{m=-1,1} \sum_{k} \overline{n_{k}} = 2 \frac{V}{\left(2 \pi\right)^{3}} \int d\Omega \int_{0}^{\infty} \overline{n_{k}} k^{2} dk = \frac{8 \pi V}{\left(2 \pi\right)^{3}} \int_{0}^{\infty} \frac{k^{2}}{\exp\left(\beta \hbar c k\right) - 1} dk$$

 $[x = \beta \hbar ck, dx = \beta \hbar c dk]$

$$N = \frac{8 \pi V}{(2 \pi)^3} \frac{1}{(\beta \hbar c)^3} \int_0^\infty \frac{x^2}{\exp(x) - 1} dx = \frac{8 \pi V}{(\beta \hbar c)^3} \int_0^\infty \frac{x^2}{\exp(x) - 1} dx$$

 $ln[\cdot]:= n = 8 \text{ Pi V} / (h c \beta)^3 \text{ Integrate}[x^2/(Exp[x]-1), \{x, 0, Infinity\}]$

Out[=]=
$$\frac{16 \,\pi\,\text{V Zeta[3]}}{\text{c}^3\,\text{h}^3\,\beta^3}$$

b)

$$\beta := 1/(k * T)$$

n/V/. T
$$\rightarrow$$
 = 300 K \cdots / // // N // UnitConvert

n/V/. T
$$\rightarrow$$
 = 1500 K \cdots / // // N // UnitConvert

$$n/V/. T \rightarrow \blacksquare$$
 2.73 K \cdots $\sqrt{\parallel}$ \parallel N \parallel UnitConvert

$$Out[*]= 5.47745 \times 10^{14} \text{ per meter}^3$$

$$Out[\]= 6.84681 \times 10^{16} \, per \, meter^3$$

$$Out[*]= 4.12765 \times 10^8 \text{ per meter}^3$$

c)

$$Z_k = \frac{1}{1 - \exp\left(-\beta e_k\right)}$$



$$F_k = -rac{\ln(Z_k)}{eta} = rac{1}{eta} \, \ln \left(1 - \exp \left(-eta \hbar \; c \; k
ight)
ight)$$

$$F = \sum_{m=-1,1} \sum_{k} F_{k} = 2 \sum_{k} -\frac{\ln(Z_{k})}{\beta} = \frac{8 \pi V}{\left(2 \pi\right)^{3}} \int_{0}^{\infty} k^{2} \ln\left(1 - \exp\left(-\beta \hbar c k\right)\right) d k$$

$$[x = \beta \hbar ck, dx = \beta \hbar c dk]$$

$$F = \frac{8 \pi V}{\beta (\beta h c)^3} \int_0^\infty x^2 \ln (1 - \exp(-x)) dx$$

$$F = 8 \operatorname{PiV} / (\beta \operatorname{hc})^{3} / \beta \operatorname{Integrate}[x^{2} \operatorname{Log}[1 - \operatorname{Exp}[-x]], \{x, 0, \operatorname{Infinity}]]$$

$$P = -D[F, V]$$

Out[
$$\circ$$
]= $-\frac{8 \pi^5 \text{ V}}{45 \text{ c}^3 \text{ h}^3 \beta^4}$

Out[*]=
$$\frac{8 \pi^5}{45 c^3 h^3 \beta^4}$$

$$ln[-]:= \sigma := 2 Pi^5 k^4 / (15 h^3 c^2)$$

$$\beta := 1/(kT)$$

P/U

$$Out[\circ] = \frac{1}{3 \text{ V}}$$

$$\Rightarrow P = \frac{1}{3} \frac{U}{V}$$



Ex.3

$$In[1]:= Z := Exp[-U0 \beta] zvib^{(3 NN)}$$
$$zvib := Exp[-h v \beta / 2] 1 / (1 - Exp[-h v \beta])$$

$$In[3]:= U = -1 / Z D[Z, \beta] // Simplify$$

 $cV = D[U /. \{\beta \rightarrow 1 / (k T)\}, T] // Simplify$

Out[3]= U0 +
$$\frac{3\left(1 + e^{h \beta v}\right) h NN v}{2\left(-1 + e^{h \beta v}\right)}$$

Out[4]=
$$\frac{3 e^{\frac{h v}{kT}} h^2 NN v^2}{\left(-1 + e^{\frac{h v}{kT}}\right)^2 k T^2}$$

Out[5]= 0 if NN
$$\in \mathbb{R}$$
 && h k $v > 0$

Out[6]= 3 k NN



Für T->0 geht cV gegen 0, für T >> geht cV gegen 3Nk_B = 3R, was mit petit-dulong zusammenpasst

$$Z = \exp\left(-U_0\,eta
ight)^{3\,N-6} \prod_{i=1}^{N-6} z_i$$

$$\ln{(Z)} = -U_0 \beta + \ln{\left(\prod_{i=1}^{3 N-6} z_i\right)} = -U_0 \beta + \sum_{i=1}^{3 N-6} \ln{(z_i)} = -U_0 \beta + \sum_{i=1}^{3 N-6} \ln{\left(\frac{\exp\left(\frac{-h v_i}{2 k_B T}\right)}{1 - \exp\left(\frac{h v_i}{k_B T}\right)}\right)}$$

$$\operatorname{Mit} z_i = \frac{\exp\left(\frac{-h \, v_i}{2 \, k_B \, T}\right)}{1 - \exp\left(\frac{h \, v_i}{k_B \, T}\right)}$$

$$In[\cdot]:= Logz := -U0 \beta + Integrate$$

 $9 \; \text{NN/vmax^3} \; \text{v^2} \left(\text{hv} \; \beta \; / \; 2 - \text{Log} \left[\text{Exp} \left[\text{hv} \; \beta \right] - 1 \right] \right), \; \{ \text{v}, \; 0, \; \text{vmax} \}, \; \text{GenerateConditions} \; \rightarrow \; \text{False} \right]$

$$In[a]:= cV = k \beta^2 D[D[Logz, \beta], \beta] // FullSimplify$$

$$Out[-] = \frac{3}{5} \text{ k NN} \left[-\frac{4 \pi^4}{\text{h}^3 \beta^3 \text{ vmax}^3} - \frac{15 e^{\text{h} \beta \text{ vmax}} \text{h} \beta \text{ vmax}}{-1 + e^{\text{h} \beta \text{ vmax}}} + 60 \text{ Log} \left[1 - e^{\text{h} \beta \text{ vmax}} \right] + \frac{1}{\text{h}^3 \beta^3 \text{ vmax}^3} \right]$$

$$180 \left(h \beta v \max \left(h \beta v \max PolyLog[2, e^{h \beta v \max}] - 2 PolyLog[3, e^{h \beta v \max}] \right) + 2 PolyLog[4, e^{h \beta v \max}] \right) \right)$$

Analytische Lösung enthält debye-integral, welches über den Polylogarithmus ausgedrückt werden kann.

$$In[\cdot]:= Limit[cV /. \{\beta \rightarrow 1 / (k * T)\}, T \rightarrow Infinity]$$

Out[-]= 3 k NN



Bonus

 $ln[\cdot]:=$ Integrate[1/(Exp[x]-1), {x, 0, Infinity}]

... Integrate: Integral of
$$\frac{1}{-1 + e^{X}}$$
 does not converge on {0, ∞}. ①

$$Out[\cdot] = \int_0^\infty \frac{1}{-1 + e^X} dX$$

Integral divergiert => keine spontane Magnetisierung möglich