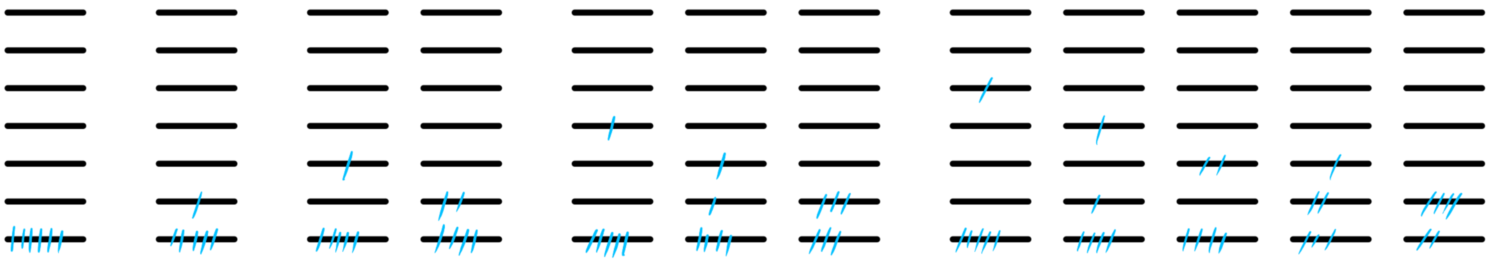
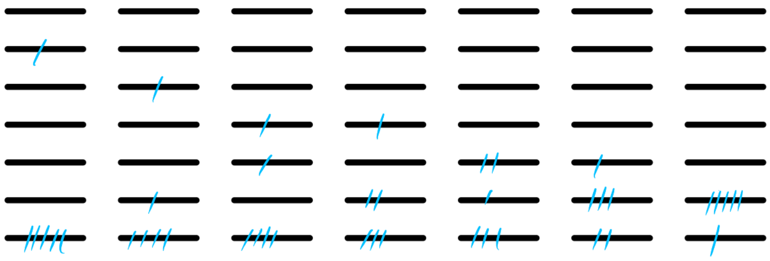
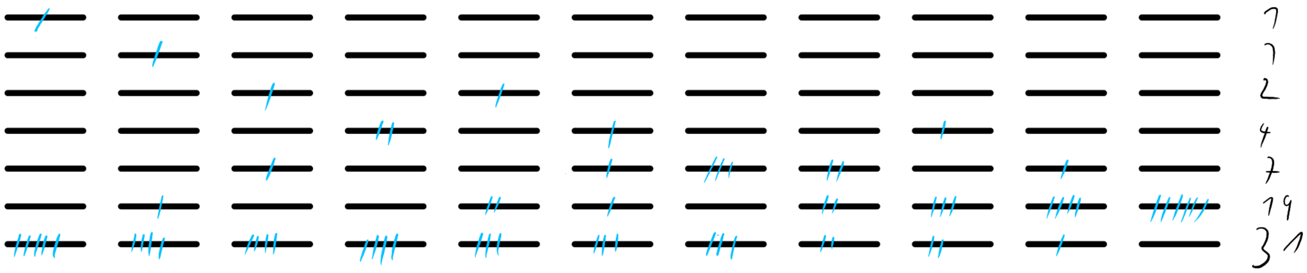
q = 0 q = 1 q = 2 q = 3 q = 4

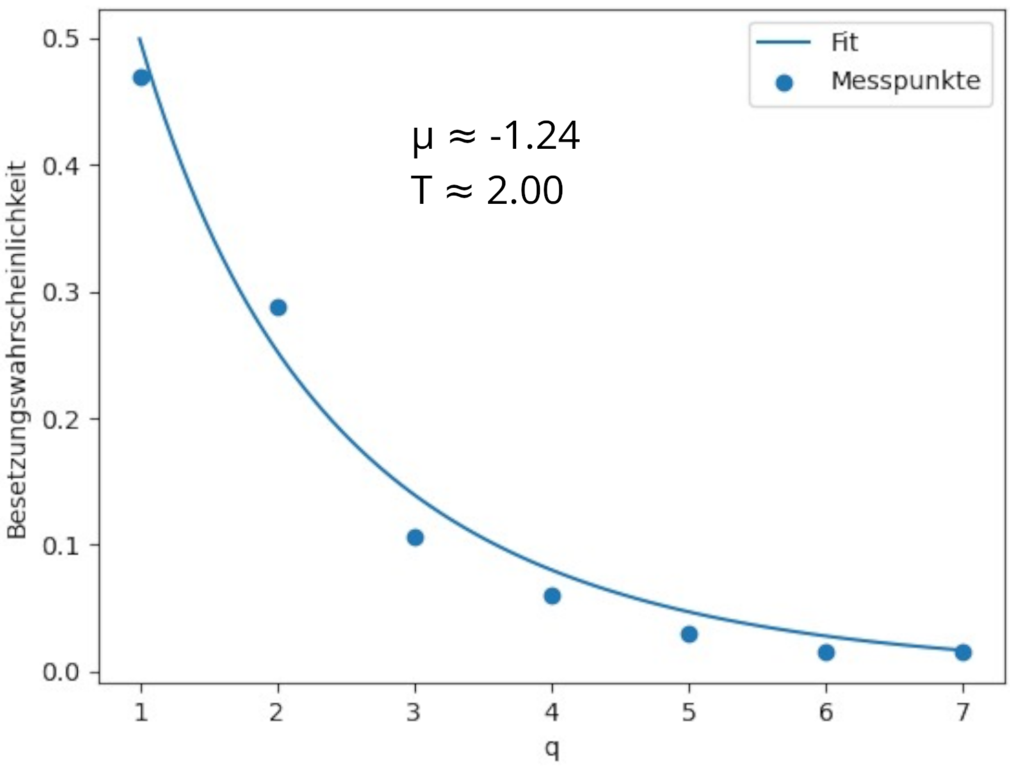


q = 5



q = 6





Ex.2

a)

```
In[∘]:= ek := ℏ c k
        nmean := 1 / (Exp[β ek] - 1)
```

$$N = \sum_{m=-1,1} \sum_{k} \overline{n_k} = 2 \frac{V}{(2\pi)^3} \int d\Omega \int_0^\infty \overline{n_k}\, k^2\, dk = \frac{8\pi V}{(2\pi)^3} \int_0^\infty \frac{k^2}{\exp(\beta\hbar c k) - 1}\, dk$$

[x = βℏck, dx = βℏc dk]

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

```
In[∘]:= n = 8 Pi V / (h c β)^3 Integrate[x^2 / (Exp[x] - 1), {x, 0, Infinity}]
```

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

b)

```
k := k ✓; h := h ⋯ ✓; c := c ✓;
β := 1 / (k * T)
n / V /. T → 300 K ⋯ ✓ // N // UnitConvert

n / V /. T → 1500 K ⋯ ✓ // N // UnitConvert

n / V /. T → 2.73 K ⋯ ✓ // N // UnitConvert
```

Out[∘]= 5.47745×10^{14} per meter^3

Out[∘]= 6.84681×10^{16} per meter^3

Out[∘]= 4.12765×10^{8} per meter^3

c)

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

$$F_k = -\frac{\ln(Z_k)}{\beta} = \frac{1}{\beta}\ln\left(1 - \exp\left(-\beta\hbar\, c\, k\right)\right)$$

$$F = \sum_{m=-1,1}\sum_k F_k = 2\sum_k -\frac{\ln(Z_k)}{\beta} = \frac{8\,\pi\, V}{(2\,\pi)^3}\int_0^\infty k^2\ln\left(1 - \exp\left(-\beta\hbar\, c\, k\right)\right)\mathrm{d}\,k$$

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

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

In[∘]:=
```
ClearAll["Global`*"]
F = 8 Pi V / (β h c)^3 / β Integrate[x^2 Log[1 - Exp[-x]], {x, 0, Infinity}]
P = -D[F, V]
```

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

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

In[∘]:=
```
σ := 2 Pi^5 k^4 / (15 h^3 c^2)
β := 1 / (k T)
U := 4 σ V / c T^4
P / U
```

Out[∘]= $\frac{1}{3\,V}$

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

Ex.3

In[1]:=
```
Z := Exp[-U0 β] zvib^(3 NN)
zvib := Exp[-h ν β / 2] 1 / (1 - Exp[-h ν β])
```

In[3]:=
```
U = -1 / Z D[Z, β] // Simplify
cV = D[U /. {β → 1 / (k T)}, T] // Simplify
```

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

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

In[5]:=
```
Limit[cV, T → 0]
Limit[cV, T → Infinity]
```

Out[5]= 0 if NN ∈ ℝ && h k ν > 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

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

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

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

In[∘]:=
```
Logz := -U0 β + Integrate[
    9 NN / νmax^3 ν^2 (h ν β / 2 - Log[Exp[h ν β] - 1]), {ν, 0, νmax}, GenerateConditions → False]
```

In[∘]:=
```
cV = k β^2 D[D[Logz, β], β] // FullSimplify
```

Out[∘]= $\frac{3}{5}\,k\,NN\left(-\frac{4\,\pi^4}{h^3\,\beta^3\,\nu max^3} - \frac{15\,e^{h\,\beta\,\nu max}\,h\,\beta\,\nu max}{-1 + e^{h\,\beta\,\nu max}} + 60\,\mathrm{Log}\left[1 - e^{h\,\beta\,\nu max}\right] + \frac{1}{h^3\,\beta^3\,\nu max^3} 180\left(h\,\beta\,\nu max\left(h\,\beta\,\nu max\,\mathrm{PolyLog}\left[2, e^{h\,\beta\,\nu max}\right] - 2\,\mathrm{PolyLog}\left[3, e^{h\,\beta\,\nu max}\right]\right) + 2\,\mathrm{PolyLog}\left[4, e^{h\,\beta\,\nu max}\right]\right)\right)$

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

In[∘]:=
```
Limit[cV /. {β → 1 / (k * T)}, T → Infinity]
```

Out[∘]= 3 k NN

Bonus

In[∘]:=
```
Integrate[1 / (Exp[x] - 1), {x, 0, Infinity}]
```

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

Out[∘]= $\int_0^\infty \frac{1}{-1 + e^x}\, dx$

Integral divergiert => keine spontane Magnetisierung möglich