1) $H = \alpha |x| + y z^4$ $\quad \langle x_i \frac{\partial H}{\partial x_j} \rangle = k_B T \delta_{ij}$

$\Rightarrow \langle x \frac{\partial H}{\partial x} \rangle = \langle x \alpha \ \mathrm{sign}(x) \rangle = \langle \alpha |x| \rangle \stackrel{!}{=} k_B T$

$\cancel{\langle y \frac{\partial H}{\partial y} \rangle = y z^4 = \langle H \rangle \stackrel{!}{=} k_B T}$

$\langle z \frac{\partial H}{\partial z} \rangle = \langle 4 z^4 y \rangle = k_B T$

$\Rightarrow \langle H \rangle = \langle \alpha |x| \rangle + \langle z^4 y \rangle = \underline{\underline{\frac{5}{4} k_B T}}$

✓

Ex.1 b)

In[∘]:=
```
Clear["T"]
e := h * c * B
Solve[Sum[e * J (J + 1) (2 J + 1) Exp[-J (J + 1) e / (k * T)], {J, 0, 25}] /
    Sum[(2 J + 1) Exp[-J (J + 1) e / (k * T)], {J, 0, 25}] / (k T) == 0.9, T] // N // UnitConvert
```

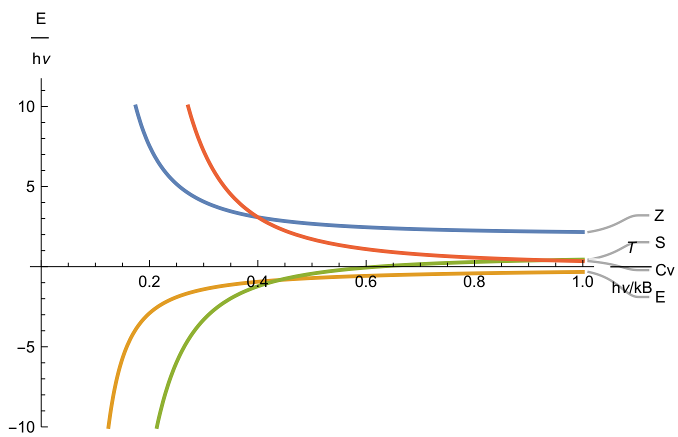
Out[∘]=
```
$Aborted
```

Dauert ewig aber findet Lösung (habs nur unabsichlich gelöscht und jetzt will ichs nicht nochmal laufen lassen). Ergebnis liegt bei 328 K wenn ich mich recht erinnere.

Ex.2

In[245]:=
```
Z := Exp[-ϵ / 2 / T] + Exp[ϵ / 2 / T]
e := ϵ / 2 Exp[-ϵ / 2 / T] - ϵ / 2 Exp[ϵ / 2 / T]
S := Log[Z] + 1 / T * e
Cv = D[e, T];
ϵ := 0.8
Plot[{Z, e, S, Cv}, {T, 0.001, 1}, AxesLabel → {T / "hν/kB", "E" / hν},
 PlotLabels → {"Z", "E", "S", "Cv"}, PlotRange → {Automatic, {-10, 10}}]
```

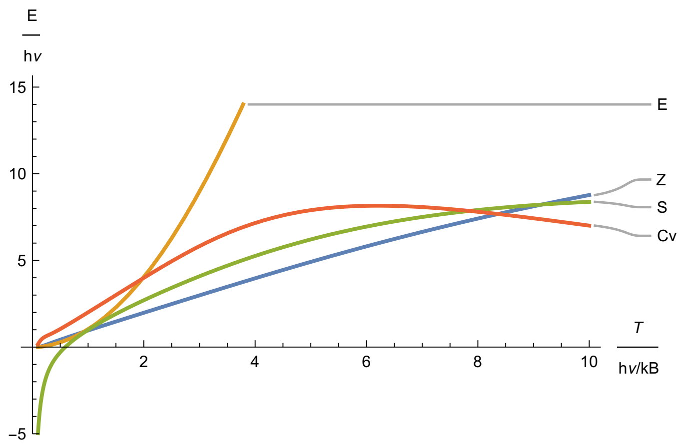
Out[250]=



In[251]:=

```
Z := Sum[Exp[-(n + 0.5) / T], {n, 0, 20}]
e := Sum[(n + 0.5) Exp[-(n + 0.5) / T], {n, 0, 20}]
S := Log[Z] + 1 / T * e
Cv = D[e, T];
Plot[{Z, e, S, Cv}, {T, 0.1, 10}, AxesLabel → {T / "hν/kB", "E" / hν},
 PlotLabels → {"Z", "E", "S", "Cv"}, PlotRange → {Automatic, {-5, 14}}]
```

Out[255]=



Ex.3

In[256]:=

```
h := h
c := c
R := R * mol
B := 10.59 /cm
ν := 2991 /cm * c
m := hydrogen chloride CHEMICAL [molecular mass]
T := 298 K ; kB := k ;
p := 1 atm ;
β := 1 / (T * kB)
```

In[264]:=

```
ztrans = (2 Pi * m / (β * h ^ 2)) ^ (3 / 2) * T * R / p // UnitConvert
zrot = 1 / (B * h * c * β)
zvib = 1 / (1 - Exp[-h ν β]) // N
ztot = ztrans * zrot * zvib
```

Out[264]=

5.204×10^{30}

Out[265]=

19.5581

Out[266]=

1.

Out[267]=

1.01783×10^{32}

In[268]:=

```
Utrans = UnitConvert[3 / (2 β), "eV"] // N
Urot = UnitConvert[1 / β, "eV"] // N
Uvib = UnitConvert[h ν Exp[-h ν β] / (1 - Exp[-h ν β]), "eV"] // N
Utot = -Utrans + Urot + Uvib
```

Out[268]=

0.0385195 eV

Out[269]=

0.0256797 eV

Out[270]=

1.98422×10^{-7} eV

Out[271]=

-0.0128396 eV

In[272]:=

```
cVtrans = UnitConvert[3 / 2 * kB, "eV/K"] // N
cVrot = UnitConvert[kB, "eV/K"] // N
cVvib = UnitConvert[β h ^ 2 ν ^ 2 Exp[-h ν β] / (T (1 - Exp[-h ν β]) ^ 2), "eV/K"] // N
cVtot = -cVtrans + cVrot + cVvib
```

Out[272]=

0.00012926 eV/K

Out[273]=

0.0000861733 eV/K

Out[274]=

9.61539×10^{-9} eV/K

Out[275]=

-0.0000430771 eV/K

Ex.4

a) - d) sind am papier (siehe unten) hier habe ich das anstrengende zeug gemacht

In[276]:=

```
Clear["β", "B", "m"]
a := β J
b := β B m
mat := {{Exp[a + b], Exp[-a]}, {Exp[-a], Exp[a - b]}}
eig = Eigenvalues[mat]
```

Out[280]=

$$\left\{\frac{1}{2} e^{-J\beta - B m \beta}\left(e^{2 J \beta} + e^{2 J \beta + 2 B m \beta} - \sqrt{e^{4 J \beta} + 4 e^{2 B m \beta} - 2 e^{4 J \beta + 2 B m \beta} + e^{4 J \beta + 4 B m \beta}}\right),\right.$$
$$\left.\frac{1}{2} e^{-J\beta - B m \beta}\left(e^{2 J \beta} + e^{2 J \beta + 2 B m \beta} + \sqrt{e^{4 J \beta} + 4 e^{2 B m \beta} - 2 e^{4 J \beta + 2 B m \beta} + e^{4 J \beta + 4 B m \beta}}\right)\right\}$$

In[281]:=

```
Z = eig[[1]] ^ n + eig[[2]] ^ n // FullSimplify
```

Out[281]=

$$2^{-n}\left(\left(e^{-((J+B m) \beta)}\left(e^{2 J \beta} + e^{2 (J+B m) \beta} - \sqrt{e^{4 J \beta} + 4 e^{2 B m \beta} + e^{4 (J+B m) \beta} - 2 e^{4 J \beta + 2 B m \beta}}\right)\right)^{n} +\right.$$
$$\left.\left(e^{-((J+B m) \beta)}\left(e^{2 J \beta} + e^{2 (J+B m) \beta} + \sqrt{e^{4 J \beta} + 4 e^{2 B m \beta} + e^{4 (J+B m) \beta} - 2 e^{4 J \beta + 2 B m \beta}}\right)\right)^{n}\right)$$

In[282]:=

```
F = -n / β * Log[eig[[2]]]
M = -1 / n * D[F, B]
```

Out[282]=

$$-\frac{n\,\mathrm{Log}\left[\frac{1}{2}\,e^{-J\beta-Bm\beta}\left(e^{2J\beta}+e^{2J\beta+2Bm\beta}+\sqrt{e^{4J\beta}+4\,e^{2Bm\beta}-2\,e^{4J\beta+2Bm\beta}+e^{4J\beta+4Bm\beta}}\right)\right]}{\beta}$$

Out[283]=

$$\left(2\,e^{J\beta+Bm\beta}\left(-\frac{1}{2}\,e^{-J\beta-Bm\beta}\left(e^{2J\beta}+e^{2J\beta+2Bm\beta}+\sqrt{e^{4J\beta}+4\,e^{2Bm\beta}-2\,e^{4J\beta+2Bm\beta}+e^{4J\beta+4Bm\beta}}\right)m\,\beta+\frac{1}{2}\,e^{-J\beta-Bm\beta}\left(2\,e^{2J\beta+2Bm\beta}\,m\,\beta+\frac{8\,e^{2Bm\beta}\,m\,\beta-4\,e^{4J\beta+2Bm\beta}\,m\,\beta+4\,e^{4J\beta+4Bm\beta}\,m\,\beta}{2\,\sqrt{e^{4J\beta}+4\,e^{2Bm\beta}-2\,e^{4J\beta+2Bm\beta}+e^{4J\beta+4Bm\beta}}}\right)\right)\right)\Big/\left(\left(e^{2J\beta}+e^{2J\beta+2Bm\beta}+\sqrt{e^{4J\beta}+4\,e^{2Bm\beta}-2\,e^{4J\beta+2Bm\beta}+e^{4J\beta+4Bm\beta}}\right)\beta\right)$$

In[284]:=

```
M /. {J → 0} // FullSimplify
Limit[M, β → Infinity] // FullSimplify
```

Out[284]=

$$\left(-1+\frac{2\,e^{2Bm\beta}}{\sqrt{\left(1+e^{2Bm\beta}\right)^2}}\right)m$$

Out[285]=

m if Bm > 0 && Bm < 2J

In[286]:=

$$\mathtt{MJ0} = \left(-1+\frac{2\,e^{2Bm\beta}}{\left(1+e^{2Bm\beta}\right)}\right)m \;\texttt{// FullSimplify}$$

Out[286]=

$m\,\mathrm{Tanh}[B\,m\,\beta]$

Wir erhalten für J=0 das Ergebnis aus dem 1D spin system ohne kopplung, und für T=0 sehen wir, dass das mittlere magnetische Moment dem magnetischen Moment gleicht.

4) $H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - mB \sum_i \sigma_i$

a) Nein, geht nicht wegen dem zweiten Term, trafo ins „Schwerpunktsystem" nicht möglich

b) $$mB \sum_i \sigma_i = \frac{mB}{2} \sum_i \sigma_i + \sigma_i = \frac{mB}{2}\left(\sum_i \sigma_i + \sum_j \sigma_j\right) = \frac{mB}{2} \sum_{\langle i,j \rangle} \sigma_i + \sigma_j$$

$$\Rightarrow H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - \frac{mB}{2} \sum_{\langle i,j \rangle} \sigma_i + \sigma_j$$

c) $$\hat{T} = \begin{pmatrix} e^{\beta J + \beta m B} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J - \beta m B} \end{pmatrix} \qquad \langle S_i | \hat{T}_\pm | S_j \rangle_\pm$$

$$\cancel{Z_i = \exp(-\beta H_i) = \exp\left(+\beta J \sum_{\langle i,j \rangle} \sigma_i \sigma_j + \frac{mB}{2} \sum_{\langle i,j \rangle} \sigma_i + \sigma_j\right) =}$$

$$\left.\begin{array}{l} \text{For } i=j: \ \langle S_i | \hat{T}_\pm | S_i \rangle_\pm = \hat{T}_{i,i\pm} = e^{\beta J \pm \beta m B} \\ \text{For } i \neq j \ \langle S_i | \hat{T}_\pm | S_j \rangle = \hat{T}_{i,j} = e^{-\beta J} \end{array}\right\} = e^{-\beta H_{i,j}}$$

Sum over $\sigma_i = \pm$

d) $$Z = \sum e^{-\beta H} = e^{-\beta \sum_i H_i} = \prod_{i=0}^{N} e^{-\beta H_i} = \prod_{i=0}^{N} \langle S_i | \pm \hat{T} | S_i \rangle_\pm = \langle S_i | \pm \hat{T}^N | S_i \rangle_\pm =$$

$$= \underline{\underline{Tr(\hat{T}^N)}}$$

$\alpha = \beta J \quad \gamma = mB\beta$

$\big(\beta J \quad \alpha + \gamma$