6. domácí úkol - oprava

1) Energie molekulového plynu $\qquad \hbar\omega \gg \frac{\hbar^2}{2I} \gg \alpha$

$$E_{n,l} = \hbar\omega\left(n+\frac{1}{2}\right) + \frac{\hbar^2}{2I}l(l+1) + \alpha\, l(l+1)\left(n+\frac{1}{2}\right)$$

- spočtěte E ideálního plynu, jehož teplota je v intervalu $\hbar\omega \gg T \gg \frac{\hbar^2}{2I}$

$$Z = \sum_{n,l} g_{n,l} e^{-\frac{E_{n,l}}{kT}} = \sum_{n,l}(2l+1)e^{-\frac{1}{kT}\left[\hbar\omega\left(n+\frac{1}{2}\right)+\frac{\hbar^2}{2I}l(l+1)+\alpha l(l+1)\left(n+\frac{1}{2}\right)\right]}$$

$$= \sum_l (2l+1)e^{-\frac{1}{kT}\left[\frac{\hbar^2}{2I}l(l+1)\right]} \sum_n e^{-\frac{1}{kT}\left[\left(n+\frac{1}{2}\right)\left(\hbar\omega+\alpha l(l+1)\right)\right]} =$$

$$= \sum_l (2l+1)e^{-\frac{1}{kT}\left[\frac{\hbar^2}{2I}l(l+1)\right]} \cdot \sum_n e^{-\frac{n+\frac{1}{2}}{kT}\cdot\left(\hbar\omega+\alpha l(l+1)\right)}$$

$$= \sum_l (2l+1) e^{-\frac{\frac{\hbar^2}{2I}l(l+1)}{kT}} \cdot e^{-\frac{\hbar\omega+\alpha l(l+1)}{2kT}} \cdot \underbrace{\sum_{n=0}^{\infty} e^{-\frac{n}{kT}(\hbar\omega+\alpha l(l+1))}}_{\frac{e^{\frac{\hbar\omega+\alpha l(l+1)}{kT}}}{e^{\frac{\hbar\omega+\alpha l(l+1)}{kT}}-1}}$$

$$= \sum_l (2l+1) e^{-\frac{\frac{\hbar^2}{2I}l(l+1)}{kT}} \cdot \frac{e^{+\frac{\hbar\omega+\alpha l(l+1)}{2kT}}}{e^{\frac{\hbar\omega+\alpha l(l+1)}{kT}}-1} =$$

$$= \sum_l (2l+1) \frac{e^{-\frac{\frac{\hbar^2}{2I}l(l+1)}{kT} + \frac{\hbar\omega+\alpha l(l+1)}{2kT}}}{e^{\frac{\hbar\omega+\alpha l(l+1)}{kT}} - 1} = \left| \sum_l \to \int_l \;\Big|\; \wedge \;\; \begin{matrix} l(l+1)=t \\ (2l+1)\,dl = dt \\ 0\to 0 \\ \infty\to\infty \end{matrix} \right| =$$

$$= \int e^{-\frac{\hbar^2}{2I}\frac{t}{kT}} \cdot \frac{e^{+\frac{\hbar\omega+\alpha t}{2kT}}}{e^{\frac{\hbar\omega+\alpha t}{kT}}-1}\,dt = \int \frac{e^{-\frac{\hbar^2}{2I}\frac{t}{kT}+\frac{\hbar\omega+\alpha t}{2kT}}}{\underbrace{e^{\frac{\hbar\omega+\alpha t}{kT}}-1}_{\approx e^{-\frac{\hbar\omega+\alpha t}{kT}}}}\,dt$$

- protože $\hbar\omega \gg kT$

$$= \int e^{-\frac{\hbar^2}{2I}\frac{t}{kT}-\frac{\hbar\omega+\alpha t}{2kT}}\,dt =$$

$$= e^{-\frac{\hbar\omega}{2kT}} \cdot \int_0^\infty e^{-\left(\frac{\hbar^2}{I}+\alpha\right)\frac{1}{2kT}t}\,dt = \quad \left| \begin{array}{l} -\left(\frac{\hbar^2}{I}+\alpha\right)\frac{1}{2kT}\cdot t = x \\ -\left(\frac{\hbar^2}{I}+\alpha\right)\frac{1}{2kT}\cdot dt = dx \end{array} \right|$$

$$= \frac{e^{-\frac{\hbar\omega}{2kT}}}{\left(\frac{\hbar^2}{I}+\alpha\right)\frac{1}{2kT}} = \frac{2kT}{\frac{\hbar^2}{I}+\alpha}\, e^{-\frac{\hbar\omega}{2kT}}$$

$$F = -kT \ln Z = -kT \ln\left(\frac{2kT}{\frac{\hbar^2}{I}+\alpha}\right) + \frac{\hbar\omega}{2}$$

$$S = -\left(\frac{\partial F}{\partial T}\right)_V = +k\ln\left(\frac{2kT}{\frac{\hbar^2}{I}+\alpha}\right) + kT\,\frac{\cancel{\frac{\hbar^2}{I}+\alpha}}{2\cancel{k}T}\cdot\frac{2\cancel{k}}{\cancel{\frac{\hbar^2}{I}+\alpha}}$$

$$E = F + TS = \frac{\hbar\omega}{2} + kT$$