Kontinuasjonseksamen 71515 Stat. mek 14.8.82

Løsninger:

I a) Hver variabel som forekommer bare i et kvadratisk ledd i Hamiltonfunksjonen, gir et bidrag $\frac{1}{2}kT$ til den indre energi for hvert molekyl.

$$H = \alpha q_1^2 + H(q_2,\dots,p,\dots)$$

$$\langle \alpha q_1^2 \rangle = \frac{\int dp\,dq\;\alpha q_1^2\, e^{-\beta H}}{\int dp\,dq\; e^{-\beta H}} = \frac{\int dq_1\,\alpha q_1^2\, e^{-\beta\alpha q_1^2}}{\int dq_1\, e^{-\beta\alpha q_1^2}} = -\frac{\partial}{\partial\beta}\ln\int_{-\infty}^{\infty} dq_1\, e^{-\beta\alpha q_1^2}$$

$$= -\frac{\partial}{\partial\beta}\ln\Big(\frac{1}{\sqrt{\beta\alpha}}\underbrace{\int_{-\infty}^{\infty} dx\, e^{-x^2}}_{\text{uavh. av }\beta}\Big) = \frac{1}{2}\frac{\partial}{\partial\beta}(\ln\beta + \ln \text{const}) = \frac{1}{2\beta} = \underline{\underline{\frac{1}{2}kT}}$$

b)

i) Enatomig molekyl:

3 kinetiske translasj. frihetsgrader $\quad U = N\frac{3}{2}kT \quad C_v = \left(\frac{\partial U}{\partial T}\right)_v = \underline{\underline{\frac{3}{2}Nk}}$

pr. mol gass $\quad C_v = \underline{\underline{\frac{3}{2}R}}$

ii) To atomig molekyl:

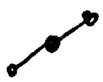
3 kin. transl. av tyngdepkt.

2 kin rotasjoner om tyngdepkt. $\quad U = N\frac{7}{2}kT \quad C_v = \underline{\underline{\frac{7}{2}Nk}}$

1 kin. og 1 pot. vibrasjons ledd $\quad$ pr. mol $\quad C_v = \underline{\underline{\frac{7}{2}R}}$

eller hvert atom 3 kin. ledd (2×3) og 1 pot. vibr. $\quad 6+1=\underline{\underline{7}}$

iii) Lineært treatomig



3 kin. transl.

2 kin rotasjon

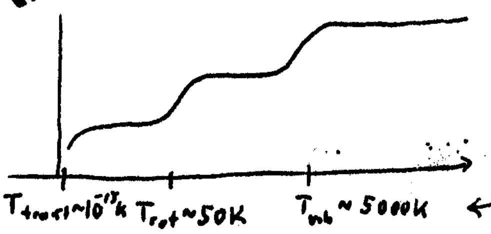
Vibrasjon: 2 longitudinale hver med kin. og pot. ledd $2\times2=4$

2 transversale — " — $2\times2=4$

eller hvert atom 3 kin ledd (3×3) og 2 longitud. og 2 transv. pot vibr. ledd $9+2+2 = \underline{\underline{13}}$ (8)

$$U = N\frac{13}{2}kT \qquad C_v = \frac{13}{2}Nk \qquad \text{pr mol} \quad C_v = \underline{\underline{\frac{12}{2}R}}$$

c)



Først over en viss temperatur nåes C_v-verdien gitt av ekvipartisjonsprins.

Ved lavere temperaturer er ikke energien høy nok til å eksitere de laveste eksiterte rotasjon og vibrasjonsnivå.

II a) Når flere ($\ell = 1, 2 \cdots N$) uavhengige delsystemer er tilstandssummen lik produktet av hvert delsystems tilstandssummer: $H = \sum_{\ell=1}^{N} H_\ell$

$$Z = \sum_{n=\{n_1, n_2, \cdots\}} e^{-\beta E_n} = \sum_{n=\{n_\ell\}} e^{-\beta \sum_\ell E_{\ell n_\ell}} = \prod_{\ell=1}^{N} \sum_{n_\ell} e^{-\beta E_{\ell n_\ell}} = \prod_{\ell=1}^{N} Z_\ell$$

Her alle delsystemene like: En partikkel med 3 mulige tilstander:

ε_3, ε_2, ε_1

$$Z_\ell = \sum_{i=1}^{3} e^{-\beta \varepsilon_i} = e^{-\beta\varepsilon_1} + e^{-\beta\varepsilon_2} + e^{-\beta\varepsilon_3} \qquad \beta = \frac{1}{kT}$$

$$\underline{Z = \left(e^{-\beta\varepsilon_1} + e^{-\beta\varepsilon_2} + e^{-\beta\varepsilon_3}\right)^N}$$

$$e^{-\frac{F}{kT}} = Z \qquad F = -kT\ln Z = \underline{-NkT\ln\left(e^{-\beta\varepsilon_1} + e^{-\beta\varepsilon_2} + e^{-\beta\varepsilon_3}\right)} = \underline{N\varepsilon_1 - NkT\ln\left(1 + e^{-\beta(\varepsilon_2-\varepsilon_1)} + e^{-\beta(\varepsilon_3-\varepsilon_1)}\right)}$$

$$S = -\left(\frac{\partial F}{\partial T}\right)_V = Nk\ln\left(e^{-\beta\varepsilon_1} + e^{-\beta\varepsilon_2} + e^{-\beta\varepsilon_3}\right) + \frac{N}{T}\,\frac{\varepsilon_1 e^{-\beta\varepsilon_1} + \varepsilon_2 e^{-\beta\varepsilon_2} + \varepsilon_3 e^{-\beta\varepsilon_3}}{e^{-\beta\varepsilon_1} + e^{-\beta\varepsilon_2} + e^{-\beta 3}}$$

$$= Nk\ln\left(1 + e^{-\beta(\varepsilon_2-\varepsilon_1)} + e^{-\beta(\varepsilon_3-\varepsilon_1)}\right) + \frac{N}{T}\,\frac{(\varepsilon_2-\varepsilon_1)e^{-\beta(\varepsilon_2-\varepsilon_1)} + (\varepsilon_3-\varepsilon_1)e^{-\beta(\varepsilon_3-\varepsilon_1)}}{1 + e^{-\beta(\varepsilon_2-\varepsilon_1)} + e^{-\beta(\varepsilon_3-\varepsilon_1)}}$$

$$U = \left(\sum_i \varepsilon_i \frac{e^{-\beta\varepsilon_i}}{Z}\right) N = N\,\frac{\varepsilon_1 e^{-\beta\varepsilon_1} + \varepsilon_2 e^{-\beta\varepsilon_2} + \varepsilon_3 e^{-\beta\varepsilon_3}}{e^{-\beta\varepsilon_1} + e^{-\beta\varepsilon_2} + e^{-\beta\varepsilon_3}}$$

b) $\underline{T \ll T_{s1} = \frac{\varepsilon_2 - \varepsilon_1}{k}}$, $\quad e^{-\beta(\varepsilon_3-\varepsilon_1)} < e^{-\beta(\varepsilon_2-\varepsilon_1)} \ll 1.$

$$\frac{U}{N} = \varepsilon_1 + \frac{(\varepsilon_2-\varepsilon_1)e^{-\beta(\varepsilon_2-\varepsilon_1)} + (\varepsilon_3-\varepsilon_1)e^{-\beta(\varepsilon_3-\varepsilon_1)}}{1 + e^{-\beta(\varepsilon_2-\varepsilon_1)} + e^{-\beta(\varepsilon_3-\varepsilon_1)}} \xrightarrow[T\to 0]{} \underline{\underline{\varepsilon_1}}$$

$U = N\varepsilon_1$ Alle elektronene i grunntilstandene

Bruker $\ln(1+\delta) = \delta - \frac{1}{2}\delta^2 + \cdots$ og får:

$$\frac{S}{N} \to k\left(e^{-\beta(\varepsilon_2-\varepsilon_1)} + e^{-\beta(\varepsilon_3-\varepsilon_1)} - \cdots\right) + \frac{1}{T}\left((\varepsilon_2-\varepsilon_1)e^{-\beta(\varepsilon_2-\varepsilon_1)} + (\varepsilon_3-\varepsilon_1)e^{-\beta(\varepsilon_3-\varepsilon_1)} + \cdots\right)$$

$$\to \frac{\varepsilon_2-\varepsilon_1}{T} e^{-\beta(\varepsilon_2-\varepsilon_1)} = \frac{kT_{s1}}{T} e^{-T_{s1}/T} \to \underline{\underline{0}}$$ ($\sim \ln 1$ Bare 1 mulig tilstand)

$$T \gg T_{s2} = \frac{\varepsilon_3 - \varepsilon_1}{k}, \quad e^{-\beta(\varepsilon_2-\varepsilon_1)} \approx e^{-\beta(\varepsilon_3-\varepsilon_1)} \approx e^0 = 1.$$

$$\frac{U}{N} \longrightarrow \underline{\underline{\frac{\varepsilon_1+\varepsilon_2+\varepsilon_3}{3}}}$$ Jevnt fordelt på nivåene

$$\frac{S}{N} \to k\ln 3 + \frac{1}{T}\,\frac{\varepsilon_1+\varepsilon_2+\varepsilon_3}{3} \to \underline{\underline{k\ln 3}}$$ 3 like fordelingsmuligheter for hvert elektron

stat. mek. 14.8.82

III
$$\varepsilon = \sqrt{p^2c^2 + (mc^2)^2} \to pc = \hbar c k \qquad \text{for} \qquad pc \gg mc^2$$

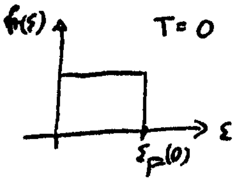
Fermioner
$$N = \sum_k \frac{1}{e^{\frac{\varepsilon-\varepsilon_F}{kT}}+1} \approx \int_0^\infty \frac{1}{e^{\frac{\varepsilon-\varepsilon_F}{kT}}+1} \frac{V}{(2\pi)^3}\, 2\cdot 4\pi k^2 dk$$

når integralet over $\vec{k}$'s retninger er utført (har isotropi)

$$= \frac{8\pi V}{(2\pi)^3}\left(\frac{1}{\hbar c}\right)^3 \int_0^\infty \frac{\varepsilon^2 d\varepsilon}{e^{\frac{\varepsilon-\varepsilon_F}{kT}}+1} \equiv \zeta \int_0^\infty f(\varepsilon)\frac{d}{d\varepsilon}F(\varepsilon)\,d\varepsilon$$

med $\frac{d}{d\varepsilon}F(\varepsilon) = \varepsilon^2$ $\qquad F(\varepsilon) = \frac{1}{3}\varepsilon^3$ (+ konst)

a) $\underline{T=0}$
$$f(\varepsilon) = \frac{1}{e^{\frac{\varepsilon-\varepsilon_F}{kT}}+1} \to \begin{cases} 1 & \varepsilon < \varepsilon_F(0) \\ 0 & \varepsilon > \varepsilon_F(0) \end{cases}$$



$$\rho = \frac{N}{V} = \frac{1}{\pi^2}\left(\frac{1}{\hbar c}\right)^3 \int_0^{\varepsilon_F(0)} \varepsilon^2 d\varepsilon = \frac{1}{3\pi^2}\left(\frac{1}{\hbar c}\right)^3 (\varepsilon_F(0))^3$$

$$\Rightarrow \qquad \underline{\varepsilon_F(0) = (3\pi^2\rho)^{1/3}\hbar c}$$

$$\frac{U}{N} = \frac{\int_0^\infty \varepsilon(k) f(k)\,dk}{\int_0^\infty f(k)\,dk} \xrightarrow{T\to 0} \frac{\int_0^{\varepsilon_F(0)} \varepsilon^3 d\varepsilon}{\int_0^{\varepsilon_F(0)} \varepsilon^2 d\varepsilon} = \frac{\frac{1}{4}\varepsilon_F^4(0)}{\frac{1}{3}\varepsilon_F^3(0)} = \underline{\frac{3}{4}\varepsilon_F(0)}$$

b) $\underline{0 \le T \ll T_F = \frac{\varepsilon_F(0)}{k}}$

$$N = \zeta \int_0^\infty f(\varepsilon)\frac{d}{d\varepsilon}F(\varepsilon)\,d\varepsilon = \zeta\left(F(\varepsilon_F(T)) + \frac{\pi^2}{6}(kT)^2 F''(\varepsilon_F(T)) + \cdots\right)$$
$$= \zeta\left(\frac{1}{3}\varepsilon_F^3(T) + \frac{\pi^2}{6}(kT)^2\, 2\varepsilon_F(T) + \cdots\right)$$

$$\rho = \frac{N}{V} = \frac{1}{3}\frac{1}{\pi^2(\hbar c)^3}\varepsilon_F^3(T)\left[1 + \pi^2\left(\frac{kT}{\varepsilon_F(T)}\right)^2 + \cdots\right]$$

$$\varepsilon_F(T) = (3\pi^2\rho)^{1/3}\hbar c\left[1 + \pi\left(\frac{kT}{\varepsilon_F(T)}\right)^2 + \cdots\right]^{-1/3} = \underline{\varepsilon_F(0)\left[1 - \frac{\pi^2}{3}\left(\frac{kT}{\varepsilon_F(0)}\right)^2 + \cdots\right]}$$

Gir T-avhengigheten når $\rho = \text{konst} = \frac{1}{3\pi^2}\left(\frac{\varepsilon_F(0)}{\hbar c}\right)^3$