LULEÅ TEKNISKA UNIVERSITET
Avdelningen för materialvetenskap

Exam in: STATISTICAL PHYSICS AND THERMODYNAMICS 2014-03-28 (F7035T)
Suggested solutions

---

1. The partition function is $Z_{\text{rot}} = \sum_{j=0}^{\infty}(2j+1)e^{-j(j+1)\frac{\hbar^2}{2I\tau}} \approx 1 + 3e^{-\frac{\hbar^2}{I\tau}} = 1 + 3e^{-x}$ where $x = \frac{\hbar^2}{I\tau} >> 1$. Truncation only possible for low τ. For N identical molecules the rotational part of the partition function is $Z_{\text{rot}}^{(N)} = \frac{1}{N!}Z_{\text{rot}}^N$.

   And hence the free energy evaluates to ($\ln(1+x) \approx x$ for small x) $F_{\text{rot}} = -N\tau \ln Z_{\text{rot}} + \tau \ln N! = -N\tau \ln(1+3e^{-x}) + \tau \ln N! \approx -3N\tau e^{-x} + \tau \ln N!$. For the entropy we get $\sigma_{\text{rot}} = -\frac{\partial F}{\partial \tau}_V \approx 3N(1+x)e^{-x} + \ln N!$ and now we can calculate the specific heat as $(C_v)_{\text{rot}} = \tau \frac{\partial \sigma}{\partial \tau}_V \approx 3Nx^2e^{-x} = 3N\left(\frac{\hbar^2}{I\tau}\right)^2 e^{-\frac{\hbar^2}{I\tau}}$

2. a) Energi tätheten ges av (efter en del räknande enligt KK93-94) $\frac{U}{V} = \frac{\pi^2\tau^4}{15\hbar^3c^3}$

   b+c) $d\sigma = dU/\tau$ ger efter integrering (KK95) $\sigma = \frac{4\pi^2\tau^3V}{45\hbar^3c^3}$ sedan $\frac{p}{\tau} = \left(\frac{\partial\sigma}{\partial V}\right)_U$. Först måste dock τ elimineras ur uttrycket för σ med hjälp av uttrycket för energitätheten enligt uppgift a. $\tau^3 = \left(\frac{U}{V}\right)^{3/4}\left(\frac{15\hbar^3c^3}{\pi^2}\right)^{3/4}$ vilket ger för entropin $\sigma = \frac{4\pi^2}{45\hbar^3c^3}(U)^{3/4}\left(\frac{15\hbar^3c^3}{\pi^2}\right)^{3/4}(V)^{1/4}$. Detta uttryck innehåler inte variablerna U eller V via variabeln τ.

   Nu ges trycket av $\frac{p}{\tau} = \left(\frac{\partial\sigma}{\partial V}\right)_U$ vilket ger $\frac{p}{\tau} = \frac{4\pi^2}{45\hbar^3c^3}(U)^{3/4}\left(\frac{15\hbar^3c^3}{\pi^2}\right)^{3/4}\frac{1}{4}(V)^{-3/4}$ = byt tillbaka till τ igen $= \frac{4\pi^2}{45\hbar^3c^3}\left(\frac{15\hbar^3c^3}{\pi^2}\right)^{3/4}\frac{1}{4}\left(\frac{15\hbar^3c^3}{\pi^2}\right)^{-3/4}\tau^3 = \frac{\pi^2}{45\hbar^3c^3}\tau^3$. Vilket ger $p = \frac{\pi^2}{45\hbar^3c^3}\tau^4$ och med utrycket för energitätheten ger detta: $pV = \frac{1}{3}U$

3. The general relation for the specific heat is $C_v = \tau\left(\frac{\partial\sigma}{\partial\tau}\right)_v$

   a: in case of the conduction electrons we have $C_v = \gamma\tau$ these two relations combine to give $\gamma\tau = \tau\left(\frac{\partial\sigma}{\partial\tau}\right)_v$ leading to $\frac{\partial\sigma}{\partial\tau} = \gamma = \textit{constant}$. and hence integrating to $\sigma \propto \tau +$'new constant' where the 'new constant' is zero as the the entropy is zero at temperature absolute zero. If the temperature increases from $\tau = 300$K to 800 K the entropy σ will increase by a factor of $\mathbf{\frac{8}{3} \approx 2.67}$.

   b: In the case of the electro magnetic field we have that the energy density is $u \propto \tau^4$ (Stefan–Boltzmann T^4 law) and hence we have for the specific heat $C_v \propto \tau^3$ (Note the similarity to phonons at low temperature the Debye T^3 law). As in a) we arrive at $\frac{\partial\sigma}{\partial\tau} \propto \tau^2$ and hence $\sigma \propto \tau^3$. If the temperature is raised from 500K to 1200K the entropy σ will increase by a factor of $(\frac{1200}{500})^3 = 13.824$ that is a factor of **13.8**.

4. The distribution inside the box is: $P(v) = 4\pi(\frac{M}{2\pi\tau})^{3/2}v^2e^{-Mv^2/2\tau}$ in the exiting beam from the oven the distribution is $\propto vP(v)$ (sid 395 CK). The most probable velocity is given by the maximum of $\propto vP(v)$. $\frac{\mathrm{d}}{\mathrm{d}v}(v^3e^{-Mv^2/2\tau} = ... = e^{-Mv^2/2\tau}(3v^2 - v^4M/\tau) = 0$. Which gives the most probable velocity $v_{ms} = \sqrt{\frac{3\tau}{M}}$. The time for the drum to rotate half a turn is the same as the it takes for a Sodium (Na) with the v_{ms} to travel through the drum the distance d, denote this time as $t_{1/2}$. The equation to solve is $t_{1/2} \cdot v_{ms} = d$. For the angular velocity $\omega = \frac{2\pi}{2t_{1/2}} = \frac{\pi}{d}\sqrt{\frac{3\tau}{M}} = \frac{\pi}{d}\sqrt{\frac{3k_BT}{M}} = \frac{\pi}{0.10}\sqrt{\frac{3\cdot 1.3807\cdot 10^{-23}\cdot 553.1}{22.9898\cdot 1.661\cdot 10^{-27}}} = 24333.78 \approx 2.43\cdot 10^4$rad/s (=3872,84 revolutions per second)

5. DNA, tillstånden är: **0** brutna energin = 0ϵ antal tillstånd $=g^0 = 1$, **1** bruten energin = 1ϵ och antal tillstånd $=g$, **2** brutna energin = 2ϵ och antal tillstånd $=g^2$, **3** brutna energin = 3ϵ och antal tillstånd $=g^3$ osv. För N länkar blir tillståndsumman en geometrisk summa. $Z^{(N)} = \sum_{N_b=0}^{N} g^{N_b}e^{-N_b\epsilon/\tau}$, som kan räknas ut explicit till $Z^{(N)} = \frac{1-(ge^{-\epsilon/\tau})^{N+1}}{1-ge^{-\epsilon/\tau}}$ För konvergens av serien (då $N \to \infty$ krävs att $ge^{-\epsilon/\tau} < 1$.

   Börja med fallet $ge^{-\epsilon/\tau} < 1$ och låt $N \to \infty$ sannolikheten för ett tillstånd med N_b brutna bindningar blir då $f_b = \frac{g^{N_b}e^{-N_b\epsilon/\tau}}{Z} = \frac{g^{N_b}e^{-N_b\epsilon/\tau}(1-ge^{-\epsilon/\tau})}{1-(ge^{-\epsilon/\tau})^{N+1}} \approx \frac{g^{N_b}e^{-N_b\epsilon/\tau}(1-ge^{-\epsilon/\tau})}{1} = g^{N_b}e^{-N_b\epsilon/\tau}(1 - ge^{-\epsilon/\tau})$ och detta är noll för tillstånde med stort antal brutna bindningar.

   Fallet $ge^{-\epsilon/\tau} > 1$ och låt N vara ett stort tal. sannolikheten för ett tillstånd med N_b brutna bindningar blir då $f_b = \frac{g^{N_b}e^{-N_b\epsilon/\tau}}{Z} = \frac{g^{N_b}e^{-N_b\epsilon/\tau}(ge^{-\epsilon/\tau}-1)}{(ge^{-\epsilon/\tau})^{N+1}-1} \approx \frac{g^{N_b}e^{-N_b\epsilon/\tau}(ge^{-\epsilon/\tau}-1)}{(ge^{-\epsilon/\tau})^{N+1}}$

   Sannolikheten för att $N_b = N$: $f_b = \frac{(ge^{-\epsilon/\tau}-1)}{(ge^{-\epsilon/\tau})^1} = 1 - \frac{1}{ge^{-\epsilon/\tau}}$
   Sannolikheten för att $N_b = N - 1$: $f_b = \frac{(ge^{-\epsilon/\tau}-1)}{(ge^{-\epsilon/\tau})^2} = \frac{1}{ge^{-\epsilon/\tau}} - \frac{1}{(ge^{-\epsilon/\tau})^2}$
   Sannolikheten för att $N_b = N - 2$: $f_b = \frac{(ge^{-\epsilon/\tau}-1)}{(ge^{-\epsilon/\tau})^3} = \frac{1}{(ge^{-\epsilon/\tau})^2} - \frac{1}{(ge^{-\epsilon/\tau})^3}$
   Sannolikheten för att $N_b = N - 2$: $f_b = \frac{(ge^{-\epsilon/\tau}-1)}{(ge^{-\epsilon/\tau})^4} = \frac{1}{(ge^{-\epsilon/\tau})^3} - \frac{1}{(ge^{-\epsilon/\tau})^4}$ osv.
   Bilda nu väntevärdet av antalet andelen brutna bindningar: $F_b = \frac{N}{N}(1 - \frac{1}{ge^{-\epsilon/\tau}}) + \frac{N-1}{N}(\frac{1}{ge^{-\epsilon/\tau}} - \frac{1}{(ge^{-\epsilon/\tau})^2}) + \frac{N-2}{N}(\frac{1}{(ge^{-\epsilon/\tau})^2} - \frac{1}{(ge^{-\epsilon/\tau})^3}) + \frac{N-3}{N}(\frac{1}{(ge^{-\epsilon/\tau})^3} - \frac{1}{(ge^{-\epsilon/\tau})^4}) + ... = 1 - \frac{1}{N}\frac{1}{ge^{-\epsilon/\tau}} - \frac{1}{N}\frac{1}{(ge^{-\epsilon/\tau})^2} - \frac{1}{N}\frac{1}{(ge^{-\epsilon/\tau})^3} - \frac{1}{N}\frac{1}{(ge^{-\epsilon/\tau})^3} - \frac{1}{N}\frac{1}{(ge^{-\epsilon/\tau})^4} - ... = 1 - \frac{1}{N}(\text{konvergerande geometrisk summa}) \to 1$ då $N \to \infty$. Antingen är andelen brutna bindningar 0 (betyder väldigt få brutna) eller så är andelen 1 dvs hela DNA molekylen är öppnad.