LULEÅ TEKNISKA UNIVERSITET
Avdelningen för materialvetenskap

Exam in: STATISTICAL PHYSICS AND THERMODYNAMICS 2018-03-23 (F7035T)
Suggested solutions

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1. 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 $\frac{\partial\sigma}{\partial\tau} = \gamma = constant$. 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**.

2. Also in the textbook on pages 62-63.

   (a) $Z = 1 + e^{-\epsilon_0/\tau}$ gives $U =< \epsilon >= \frac{\epsilon_0 e^{-\epsilon_0/\tau}}{1+e^{-\epsilon_0/\tau}} = \frac{\epsilon_0}{e^{\epsilon_0/\tau}+1}$

   (b)
   $$C_v = \frac{\partial}{\partial\tau}U = \frac{\partial}{\partial\tau}\frac{\epsilon_0}{e^{\epsilon_0/\tau}+1} = \frac{\epsilon_0^2}{\tau^2}\frac{e^{\epsilon_0/\tau}}{(1+e^{\epsilon_0/\tau})^2} \tag{1}$$

   (c) As $C_v > 0$ for all τ and $C_v \to 0$ as $\tau \to 0$ and $\tau \to \infty$. There has to be a maximum. Take the derivative of C_v with respect to τ and set this equal to 0.
   $\frac{\partial}{\partial\tau}\frac{\epsilon_0^2}{\tau^2}\frac{e^{\epsilon_0/\tau}}{(1+e^{\epsilon_0/\tau})^2} = \frac{1}{\epsilon_0}\left[2\frac{\epsilon_0^4}{\tau^4}\frac{e^{2\epsilon_0/\tau}}{(1+e^{\epsilon_0/\tau})^3} - 2\frac{\epsilon_0^3}{\tau^3}\frac{e^{\epsilon_0/\tau}}{(1+e^{\epsilon_0/\tau})^2} - \frac{\epsilon_0^4}{\tau^4}\frac{e^{\epsilon_0/\tau}}{(1+e^{\epsilon_0/\tau})^2}\right] = 0$
   Canceling common factors gives the following equation: $\left[2\frac{\epsilon_0}{\tau}\frac{e^{\epsilon_0/\tau}}{(1+e^{\epsilon_0/\tau})} - 2 - \frac{\epsilon_0}{\tau}\right] = 0$
   After some modifications this becomes:
   $$e^{\epsilon_0/\tau} = \frac{\frac{\epsilon_0}{\tau}+2}{\frac{\epsilon_0}{\tau}-2}. \tag{2}$$

   An equivalent result to eq. 2 is the following expression: $\frac{2\tau}{\epsilon_0} = \tanh(\frac{\epsilon_0}{2\tau})$. The equation (2) can be solved numerically or graphically (see figure 1). The maximum occurs at $\tau_{max} \approx 0.417\epsilon_0$.

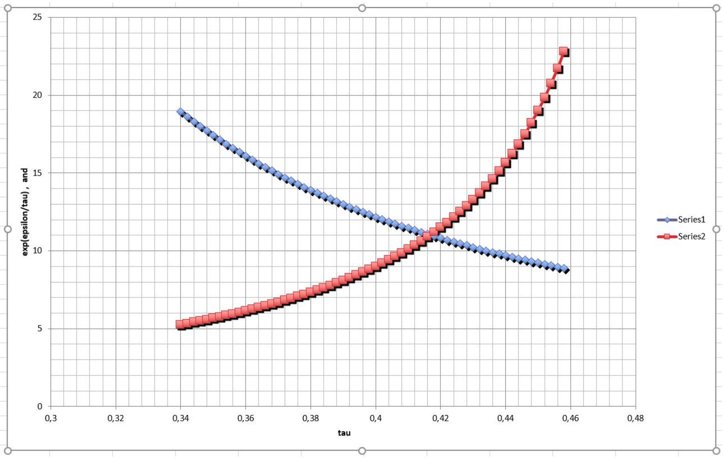

Figure 1: A graph showing the graphical solution of eq. 2. The intersection of the curves is at about $\tau_{max} \approx 0.417\epsilon_0$ where there is a maximum of the specific heat eq 1.

3. From the energy $\epsilon(j) = j(j+1)\epsilon_0$ and degeneration $g(j) = 2j+1$ we arrive at the partition function $Z_R(\tau) = \sum e^{-\epsilon_i/\tau} = \sum_{j=0}^{\infty}(2j+1)e^{-j(j+1)\epsilon_0/\tau}$. The high temperature limit $\tau >> \epsilon_0$ this becomes $Z_R(\tau) \approx \int_0^{\infty}(2j+1)e^{-j(j+1)\epsilon_0/\tau}\,\mathrm{d}j$, a change of variables ($j(j+1) = x^2$ and $\mathrm{d}j(2j+1) = 2x\,\mathrm{d}x$), $= \int_0^{\infty} 2xe^{-x^2\epsilon_0/\tau}\,\mathrm{d}x = [-\frac{\tau}{\epsilon_0}e^{-x^2\epsilon_0/\tau}]_0^{\infty} = \frac{\tau}{\epsilon_0}$

   The specific heat C_v, (high temperature) The Free energy $F = -\tau\ln Z_R \approx= -\tau\ln\frac{\tau}{\epsilon_0}$, entropy $\sigma = -\frac{\partial F}{\partial\tau} \approx \ln\frac{\tau}{\epsilon_0} + 1$, and $C_v = \tau\frac{\partial\sigma}{\partial\tau} \approx 1$. ie. $C_v = 1k_B$ per molecule in the high temperature limit.

   For low temperatures, $\tau << \epsilon_0$ we get $Z_R(\tau) \approx 1 + 3e^{-2\epsilon_0/\tau}$ and the free energy $F = -\tau\ln(1 + 3e^{-2\epsilon_0/\tau})$ and the entropy

$$\sigma = -\frac{\partial F}{\partial\tau} = \ln(1+3e^{-2\epsilon_0/\tau}) + \frac{1}{(1+3e^{-2\epsilon_0/\tau})}\cdot\frac{6\epsilon_0}{\tau}e^{-2\epsilon_0/\tau}. \tag{3}$$

   This leads to

$$C_v = \tau\frac{\partial\sigma}{\partial\tau} = \frac{1}{(1+3e^{-2\epsilon_0/\tau})}\cdot\frac{6\epsilon_0}{\tau}e^{-2\epsilon_0/\tau} - \frac{1}{(1+3e^{-2\epsilon_0/\tau})}\cdot\frac{6\epsilon_0}{\tau}e^{-2\epsilon_0/\tau} + \tag{4}$$

$$\frac{1}{(1+3e^{-2\epsilon_0/\tau})^2}\cdot\frac{6\epsilon_0^2}{\tau^2}e^{-4\epsilon_0/\tau} + \frac{1}{(1+3e^{-2\epsilon_0/\tau})}\cdot\frac{12\epsilon_0^2}{\tau^2}e^{-2\epsilon_0/\tau} = \tag{5}$$

$$\frac{12\epsilon_0^2 e^{-2\epsilon_0/\tau}}{\tau^2(1+3e^{-2\epsilon_0/\tau})}\left[1 + \frac{e^{-2\epsilon_0/\tau}}{2(1+3e^{-2\epsilon_0/\tau})}\right] \tag{6}$$

   and approximating for small x, $\frac{1}{1+x} \approx 1 - x$ gives

$$C_v \approx \frac{12\epsilon_0^2 e^{-2\epsilon_0/\tau}}{\tau^2}(1 - 3e^{-2\epsilon_0/\tau})(1 + \frac{e^{-2\epsilon_0/\tau}}{2}(1 - 3e^{-2\epsilon_0/\tau})) \approx \frac{12\epsilon_0^2 e^{-2\epsilon_0/\tau}}{\tau^2}. \tag{7}$$

   There is a second route to this result.

$$U = \tau^2\frac{\partial}{\partial\tau}\ln Z = \tau^2\frac{1}{(1+3e^{-2\epsilon_0/\tau})}\frac{6\epsilon_0 e^{-2\epsilon_0/\tau}}{\tau^2} = \frac{6\epsilon_0 e^{-2\epsilon_0/\tau}}{(1+3e^{-2\epsilon_0/\tau})}$$

Next step is

$$C_v = \frac{\partial}{\partial\tau}\frac{6\epsilon_0 e^{-2\epsilon_0/\tau}}{(1+3e^{-2\epsilon_0/\tau})} = \frac{6\epsilon_0\frac{2\epsilon_0}{\tau^2}e^{-2\epsilon_0/\tau}}{(1+3e^{-2\epsilon_0/\tau})} - \frac{6\epsilon_0 e^{-2\epsilon_0/\tau}}{(1+3e^{-2\epsilon_0/\tau})^2}\frac{2\epsilon_0}{\tau^2}e^{-2\epsilon_0/\tau} =$$

$$\frac{12\frac{\epsilon_0^2}{\tau^2}e^{-2\epsilon_0/\tau}}{(1+3e^{-2\epsilon_0/\tau})}\left(1-\frac{e^{-2\epsilon_0/\tau}}{(1+3e^{-2\epsilon_0/\tau})}\right) \approx \frac{12\epsilon_0^2 e^{-2\epsilon_0/\tau}}{\tau^2}$$

which is the same result as previous.

Answer: For $\tau >> \epsilon_0 : C_v = 1$, and $Z_R(\tau) = \frac{\tau}{\epsilon_0}$.
For $\tau << \epsilon_0 : C_v = \frac{12\epsilon_0^2 e^{-2\epsilon_0/\tau}}{\tau^2}$, and $Z_R(\tau) = 1 + 3e^{-2\epsilon_0/\tau}$.

4. DNA, tillstånden är: **0** brutna energin $= 0\epsilon$ antal tillstånd $=g^0 = 1$, **1** bruten energin $= 1\epsilon$ och antal tillstånd $=g$, **2** brutna energin $= 2\epsilon$ och antal tillstånd $=g^2$, **3** brutna energin $= 3\epsilon$ 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.

5. 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)