## LULEÅ TEKNISKA UNIVERSITET

Avdelningen för materialvetenskap
Exam in: Statistical Physics and Thermodynamics 2019-03-30 (F7035T)
Suggested solutions

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 $\tau=200 \mathrm{~K}$ to 800 K the entropy $\sigma$ will increase by a factor 4 .
b: In the case of the electro magnetic field we have that the energy density is $u \propto \tau^{4}$ (StefanBoltzmann $T^{4}$ 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 500 K to 2000 K the entropy $\sigma$ will increase by a factor of $\left(\frac{2000}{500}\right)^{3}=64$ that is a factor of $\mathbf{6 4}$.
2. Use the relation $\frac{1}{\tau}=\frac{\partial \sigma}{\partial E} . \sigma=\frac{c^{3} A}{4 G \hbar}=\frac{c^{3} 4 \pi R_{s}^{2}}{4 G \hbar}=\frac{c^{3} 4 \pi}{4 G \hbar} \frac{4 G^{2} M^{2}}{c^{4}}=\frac{4 \pi G E^{2}}{\hbar c^{5}}$. Now we can evaluate for the temperature. $\frac{1}{\tau}=\frac{\partial \sigma}{\partial E}=\frac{8 \pi G M}{\hbar c^{3}}$, an alternative route is to use $\tau=\frac{\partial E}{\partial \sigma}$ this will give the same result.
b) $U=\frac{3}{2} \tau=1 \mathrm{eV}$ will give ratio $\frac{18 e^{13.6 / 3^{2} \tau}}{8 e^{13.6 / 2^{2} \tau}}=\frac{18}{8} e^{20.4(1 / 9-1 / 4)}=\frac{18}{8} e^{-2.833}=0.1323 \approx 0.13$
3. For a molecule the heat capacity $C_{v}$ is given by $C_{v}=\left(\frac{\partial U}{\partial T}\right)_{V}$. The partition function is $Z=$ $1+3 e^{-\epsilon / \tau}$. The energy is $U=\frac{3 \epsilon e^{-\epsilon / \tau}}{Z}$

$$
\begin{equation*}
C_{v}=\left(\frac{\partial U}{\partial \tau}\right)_{V}=\frac{3\left(\frac{\epsilon}{\tau}\right)^{2} e^{\epsilon / \tau}}{\left(3+e^{\epsilon / \tau}\right)^{2}} \tag{1}
\end{equation*}
$$

Now let $x=\epsilon / \tau$

$$
\begin{equation*}
C_{v}=\frac{3 x^{2} e^{x}}{\left(3+e^{x}\right)^{2}} \tag{2}
\end{equation*}
$$

Taking the derivative $\frac{\partial C_{v}}{\partial x}$ we arrive at an equation for the maximum of $C_{v}$ as $3(2+x)+(2-$ $x) e^{x}=0$. The maximum is at about $x \approx 2.845$, which gives $C_{v}=1.023$ and using the correct units $C_{v}=1.023 k_{B}$.
4. a) The partition sum is given by: $Z=\sum_{n_{1}=0, n_{2}=0}^{\infty} e^{-\left(n_{1}+n_{2}+1.0\right) \hbar \omega / k_{B} T}=$ $\sum_{n=0}^{\infty} g(n) e^{-(n+1.0) \hbar \omega / k_{B} T}$, where $g(n)$ is the degeneracy of the energy levels and $n=n_{1}+n_{2}$. There are two ways to evaluate this sum. One simple and one more elaborate. Only the simple solution is presented here. The sum for $Z$ can be done as a product of two separate independent geometric sums.
$Z=\sum_{n_{1}=0, n_{2}=0}^{\infty} e^{-\left(n_{1}+n_{2}+1.0\right) \hbar \omega / k_{B} T}=\sum_{n_{1}=0}^{\infty} e^{-\left(n_{1}+0.5\right) \hbar \omega / k_{B} T} \cdot \sum_{n_{2}=0}^{\infty} e^{-\left(n_{2}+0.5\right) \hbar \omega / k_{B} T}=$ $\left(\sum_{n=0}^{\infty} e^{-(n+0.5) \hbar \omega / k_{B} T}\right)^{2}=e^{-\hbar \omega / k_{B} T}\left(\sum_{n=0}^{\infty} e^{-n \hbar \omega / k_{B} T}\right)^{2}=e^{-\hbar \omega / k_{B} T}\left(\frac{1}{1-e^{-\hbar \omega / k_{B} T}}\right)^{2}=$ and we arrive at the following for the partition function $Z$ :

$$
Z=\left(\frac{1}{e^{+\hbar \omega / 2 k_{B} T}-e^{-\hbar \omega / 2 k_{B} T}}\right)^{2}=\text { or }=e^{-\hbar \omega / k_{B} T}\left(\frac{1}{1-e^{-\hbar \omega / k_{B} T}}\right)^{2} .
$$

b) There is one state of the lower energy and two states with the next higher energy. The probability to find the oscillator in a state of energy is proportional to the Boltzmann factor, we arrive at the following equation. $1 e^{-1,0 \hbar \omega / k_{B} T}=2 e^{-2,0 \hbar \omega / k_{B} T}$ and $e^{1 \hbar \omega / k_{B} T}=2$ which evaluates to $T=\frac{1 \hbar \omega}{k_{B} \ln 2}$ or if you prefer $\tau, \tau=\frac{1 \hbar \omega}{\ln 2}$, which is equally correct.
c) The partition sum at this specific temperature is given by: $\left(k_{B} T=\tau=\frac{1 \hbar \omega}{\ln 2}\right)$ we arrive at the following

$$
Z=\left(\frac{1}{e^{+\frac{\ln 2}{2}}-e^{-\frac{\ln 2}{2}}}\right)^{2}=\left(\frac{1}{\sqrt{2}-\frac{1}{\sqrt{2}}}\right)^{2}
$$

We continue with the calculation of the probability: (we may choose any of the two energies as their probabilities will be equal at the temperature in question: $\left(1 e^{-1,0 \hbar \omega / k_{B} T}=\right.$ $\left.2 e^{-2,0 \hbar \omega / k_{B} T}\right)$

$$
\begin{gathered}
P=e^{-\hbar \omega / k_{B} T} /\left(\frac{1}{\sqrt{2}-\frac{1}{\sqrt{2}}}\right)^{2}=2^{-1}\left(\sqrt{2}-\frac{1}{\sqrt{2}}\right)^{2}=\left(\frac{1}{\sqrt{2}}\right)^{2}\left(\sqrt{2}-\frac{1}{\sqrt{2}}\right)^{2}= \\
\left(1-\frac{1}{2}\right)^{2}=\frac{1}{4}=0.25
\end{gathered}
$$

The probability to be in a state of one of these energys is $P=\frac{1}{4}=0.25$
5. See also problem 10.5 in Kittel and Kroemer a: $F=-N_{f} \epsilon_{0}+N_{g} \tau\left(\ln \frac{N_{g}}{V n_{Q}}-1\right)$ b: $N_{g}=$ $V n_{Q} e^{-\epsilon_{0} / \tau}$ c: Make a figure of $\ln p$ as a function of $1 / T$. The slope of the straight line is $-\frac{\epsilon_{0}}{k_{B}}$ which gives an energy $\epsilon_{0}=0.53 \mathrm{eV}$.

