FYS2160 Termodynamikk og statistisk fysikk
Oblig 3

Ole Gunnar Johansen

19. september 2015

Denne obligen inneholder 4 sider.

Exercise 1

a) In a crystal with N atoms and n vacancies, there are in total $N + n$ spots where the atoms can take place. The multiplicity is therefore

$$\Omega(N, n) = \binom{N+n}{n} = \frac{(N+n)!}{n!N!} \tag{1}$$

b) The entropy can then be written using the Boltzmann formula:

$$\begin{aligned} S &= k \ln \Omega \\ &= k \ln \binom{N+n}{n} \\ &= k \ln \left(\frac{(n+N)!}{n!N!} \right) \\ &= k \left[\ln((N+n)!) - \ln(n!) - \ln(N!) \right] \end{aligned} \tag{2}$$

c) Using Stirling's approximation:

$$\ln(x!) \approx \ln \sqrt{2\pi x} + x \ln x - x \approx x \ln x - x, \tag{3}$$

where in the last transition the assumption of large x were made (OK since we are assuming $N >> 1$), we can rewrite eq. (2):

$$\begin{aligned} S &\approx k \left[(N+n) \ln(N+n) - (N+n) - n \ln n + n - N \ln N + N \right] \\ &= k \left[(N+n) \ln(N+n) - n \ln n - N \ln N \right] \\ &= k \left[(N+n) \ln \left(N \left(1 + \frac{n}{N} \right) \right) - n \ln n - N \ln N \right] \\ &= k \left[(N+n) \left(\ln N + \ln \left(1 + \frac{n}{N} \right) \right) - n \ln n - N \ln N \right] \end{aligned} \tag{4}$$

Using Taylor expansion we get, for small x:

$$\ln(1+x) = x + O(x^2)$$

Using this under the assumption $n << N$, we can simplify eq. (4) to

$$S \approx kn\left[\ln\left(\frac{N}{n}\right) + \frac{n}{N} + 1\right] \tag{5}$$

d) From the definition of temperature, we have that

$$\frac{1}{T} = \left(\frac{\partial S}{\partial U}\right)_{N,V} \tag{6}$$

when the number of particles N and the volume V is held constant. To free atoms in the crystal so that there are n vacancies, requires energy equal to

$$U = n\Delta\epsilon \Rightarrow n = \frac{U}{\Delta\epsilon}$$

Plugging this back into eq. (5) and using eq. (6), we get

$$\begin{aligned}
\frac{1}{T} &= \frac{\partial}{\partial U}\left(k\frac{U}{\Delta\epsilon}\left(\ln\left(\frac{N\Delta\epsilon}{U}\right) + \frac{U}{N\Delta\epsilon} + 1\right)\right) \\
&= \frac{k}{\Delta\epsilon}\left(\ln\frac{N}{n} + \frac{2n}{N}\right) \\
\Rightarrow T &= \frac{\Delta\epsilon}{k}\left(\ln\frac{N}{n} + \frac{2n}{N}\right)^{-1}
\end{aligned}$$

e) From the previous task, we have

$$T = \frac{\Delta\epsilon}{k}\left(\ln\frac{N}{n} + \frac{2n}{N}\right)^{-1}$$

In the limit when $N >> n$ (i.e. small temperatures), $\ln\frac{N}{n} >> \frac{2n}{N}$. In this limit, the temperature is

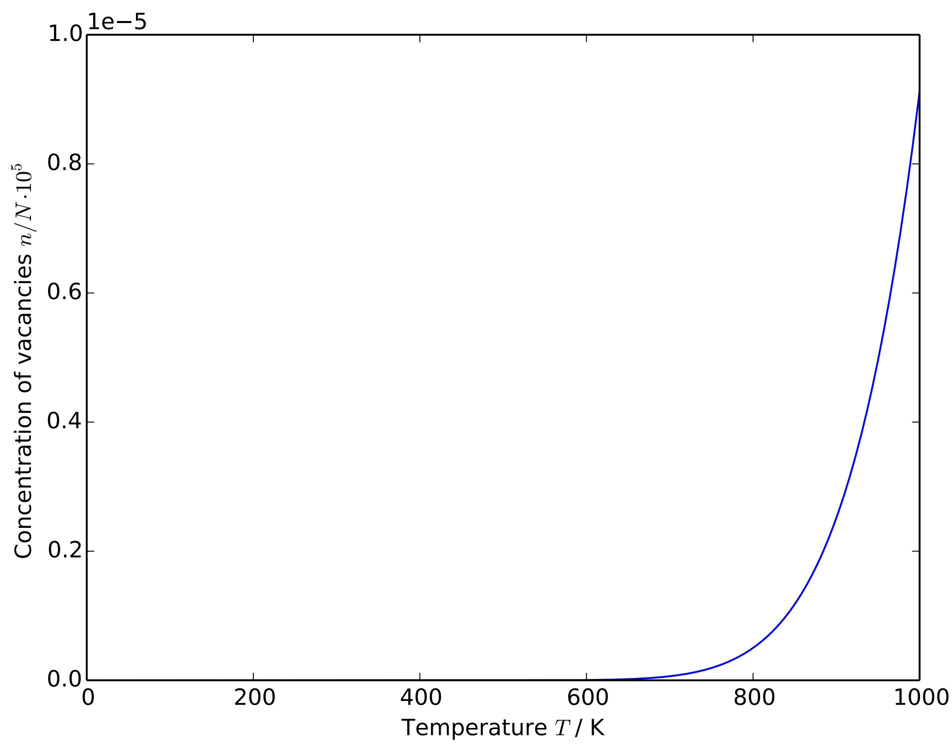
$$\begin{aligned}
T &\approx \frac{\Delta\epsilon}{k}\left(\ln\frac{n}{N}\right)^{-1} \\
\Rightarrow n &\approx Ne^{-\Delta\epsilon/(kT)}
\end{aligned} \tag{7}$$

f) From eq. (7), it is evident that in the limit when $T \to 0$, $n \to 0$ which was the behaviour we wanted.

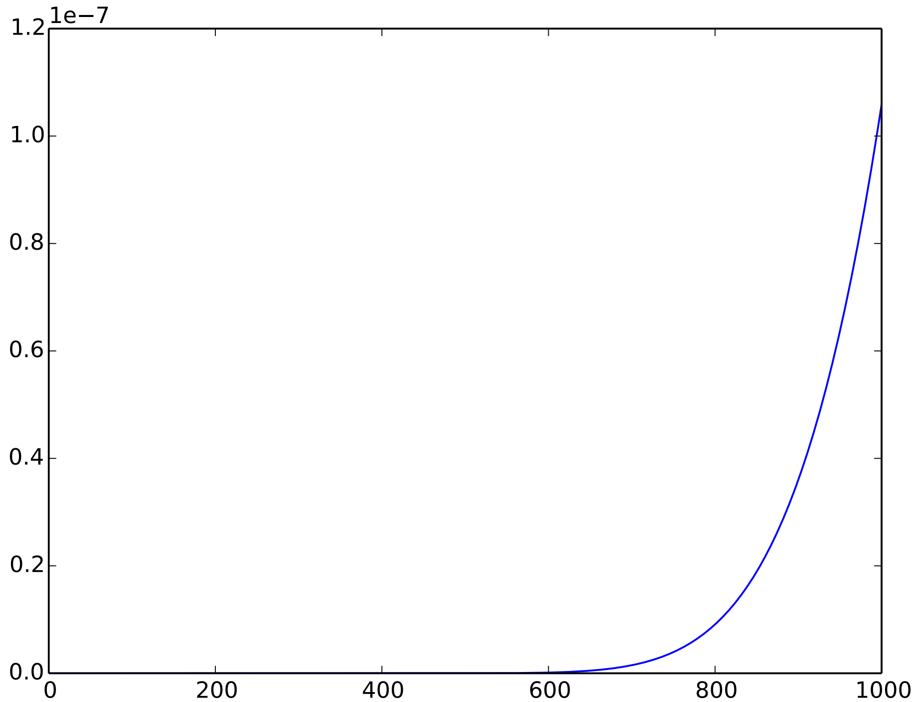
g) Assuming $\Delta\epsilon = 1$ eV, the concentration of vacancies n/N is plotted in fig. 1

h) The heat capacity is defined as

$$C_V = \left(\frac{\partial U}{\partial T}\right)_{N,V}$$



Figur 1: Concentration of vacancies n/N in the crystal as a function of temperature.



Figur 2: Specific heat capacity of the crystal as a function of temperature

Again, using that the total energy needed to make n vacancies is U. Then $n = U/\Delta\epsilon$ as above. Eq. (7) then becomes

$$\frac{U}{\Delta\epsilon} = Ne^{-\Delta\epsilon/(kT)}$$
$$U = \Delta\epsilon N e^{-\Delta\epsilon/(kT)}$$

so the expression for the specific heat capacity is

$$\begin{aligned} C_V &= \Delta\epsilon N e^{-\Delta\epsilon/(kT)} \cdot \frac{\Delta\epsilon}{kT^2} \\ &= \frac{\Delta\epsilon^2 N}{kT^2} e^{-\Delta\epsilon/(kT)} \end{aligned}$$

A plot of this in the temperature range from $T = 0$ to $T = 1000$ K is found in fig. 2.

Oblig 3 slutt