Solution exam stf2 Fall/Winter 2011

1 Adiabatic curve

(a) We have

$$\beta = \frac{KN}{E} \quad \text{and} \quad \gamma = \frac{N}{V}.$$

Hence along an adiabatic curve one has

$$dS = \frac{KN}{E} dE + \frac{N}{V} dV = 0.$$

This means

$$\frac{dE}{dV} = -\frac{E}{KV}$$

which is solved by

$$E = cV^{-1/K}$$

with c being a constant. This can be rewritten as $VE^K = C_2$. From $p = Nk_B T/V = E/(VK)$ follows then

$$p = \frac{cV^{-1/K}}{VK} = \frac{c}{K} \frac{1}{V^{(K+1)/K}}.$$

i.e. $pV^{(K+1)/K} = C_1$. *(3 points)*

(b) Adiabatic curves go like $p \sim 1/V^{5/3}$ and decrease therefore faster than isothermes, $p \sim 1/V$. *(1 point)*

2 Entropy of spin system

(a) Energy:

$$E(n) = mBn - mB(N-n) = (2n - N)mB$$

Number of configurations:

$$\mathcal{N}(n) = \frac{N!}{n!(N-n)!}$$

Entropy:

$$\frac{S(n)}{k_B} = \ln \mathcal{N}(n) = \ln N! - \ln n! - \ln (N-n)!$$

(1 point)

(b) Use of Stirling's formula leads to

$$\frac{S(n)}{k_B} \approx N \ln N - n \ln n - (N-n) \ln (N-n).$$

Add and subtract $n \ln N$:

$$\frac{S(n)}{k_B} \approx N \ln N - n \ln n - (N-n) \ln (N-n) + n \ln N - n \ln N$$

leading to

$$\frac{S(n)}{k_B} \approx -n \ln \frac{n}{N} - (N-n) \ln \left(\frac{N-n}{N} \right)$$

or

$$S(x) \approx -k_B N \left(x \ln x + (1-x) \ln (1-x) \right).$$

(*1 point*)

(c) $S(0) = 0$, $S(1/2) = k_B N \ln(2) > 0$ and $S(1) = 0$. From

$$\frac{dS(x)}{dx} = S'(x) = -k_B N \left(\ln x - \ln (1-x) \right)$$

one finds $S'(0) = +\infty$, $S'(1/2) = 0$ and $S'(1) = -\infty$. $S(x)$ has thus a shape similar to the upper half of a circle. (*1 point*)

(d) energy:

$$E(x) = (2x-1)\, mBN$$

minimal energy $-mBN$ for $x = 0$, maximal energy $+mBN$ for $x = 1$. $S(E)$ is an even function and $T(E)$ an odd function with a singularity at $E = 0$. (*1 point*)

(e) Negative temperature, i.e. $\beta < 0$. Usually not observed because spins have kinetic energy or – if not – system equilibrates with surroundings at a common positive temperature. (*2 point*)

3 Virial expansion

(a) The second virial coefficient is given by

$$B_2 = -2\pi \int_0^D \left(e^{-\beta W} - 1 \right) r^2 dr - 2\pi \int_D^A \left(e^{\beta U} - 1 \right) r^2 dr$$

leading to

$$B_2 = \frac{2\pi}{3} D^3 \left(1 - e^{-\beta W} \right) + \frac{2\pi}{3} \left(A^3 - D^3 \right) \left(1 - e^{\beta U} \right).$$

(*1 point*)

(b) We now search for values of $\beta > 0$ for which $B_2 = 0$. This leads to the condition

$$D^3 \left(1 - e^{-\beta W} \right) = \left(D^3 - A^3 \right) \left(1 - e^{\beta U} \right)$$

that can be rewritten as

$$e^{-\beta W} = \left(1 - \frac{A^3}{D^3}\right) e^{\beta U} + \frac{A^3}{D^3}.$$

This is always solved for $\beta = 0$ but we search here for a finite temperature solution. On both sides of this equation we have monotonously decaying functions, both have the value 1 for $\beta = 0$. The function on the lhs is concave and goes asymptotically towards 0 for $\beta \to \infty$, the one on the rhs is convex and goes to $-\infty$ for $\beta \to \infty$. The functions on the lhs and rhs thus only cross at a finite value of β, if the slope at $\beta = 0$ of the function on the lhs is more negative than the one on the rhs. This leads to the condition

$$-We^{-\beta W} < \left(1 - \frac{A^3}{D^3}\right) Ue^{\beta U}$$

and thus

$$\beta < -\frac{1}{U+W} \ln \left(\left(\frac{A^3}{D^3} - 1 \right) \frac{U}{W} \right).$$

Since such a system must have a positive temperature, one has only to a solution with a finite value of β if

$$\frac{1}{U+W} \ln \left(\left(\frac{A^3}{D^3} - 1 \right) \frac{U}{W} \right) < 0.$$

(*2.5 points*)

(c) Even if $\beta = 0$ this system does not behave like an ideal gas since most of the higher order virial coefficients (e.g. B_3) are in general not vanishing. (*1.5 point*)

4 Ferromagnetism

(a) The partition function is given by:

$$Z = \sum_{\{s_i = \pm 1\}} e^{-\beta H(\{s_i\})} = \sum_{\{s_i = \pm 1\}} \prod_i e^{\beta m B s_i} = \left(e^{\beta m B} + e^{-\beta m B}\right)^N$$

In short

$$Z = \left[2 \cosh\left(\beta m B\right)\right]^N$$

The free energy is thus

$$F = -k_B T \ln Z = -k_B T N \ln\left(2 \cosh\left(\beta m B\right)\right)$$

Mean magnetization per spin:

$$m \langle s \rangle = -\frac{1}{N} \frac{\partial F}{\partial B} = m \tanh\left(\beta m B\right).$$

(*2 points*)

(b) Mean-field Hamiltonian

$$H_{MF} = -\left(mB + Jz\left\langle s\right\rangle\right)\sum_i s_i.$$

(1 point)

(c) Comparision between the Hamiltonian from (a) and the mean-field Hamiltonian shows that one just has to replace mB by $mB + Jz\langle s\rangle$. Hence

$$Z = \left[2\cosh\left(\beta\left(mB + Jz\left\langle s\right\rangle\right)\right)\right]^N$$

and

$$\left\langle s\right\rangle = \tanh\left(\beta\left(mB + Jz\left\langle s\right\rangle\right)\right).$$

(*2 point*)