

## Exam stf2 Fall/Winter 2008

State clearly your name and - if available - collegekaartnummer. Tip: Read first all questions, and then start with the ones that are easiest for you. Feel free to answer in Dutch, English or both.

### 1 Paramagnetic system

Study first a single paramagnetic atom at constant temperature  $T$ . The atom can be in two spin states, spin-up and spin-down, with respect to an externally applied magnetic field  $B$ , with corresponding energies  $\epsilon = \pm\epsilon_0 = \pm mB$  where  $m$  denotes the magnetic moment of the atom (the  $+$ -sign stands for the spin up state).

- (a) Which ensemble do you use to describe such a system and why? What is the partition function  $z$  for this one-particle system?

We generalize this system now to that of  $N$  independent, identical paramagnetic atoms (that means they do not interact with each other).

- (b) What is the partition function  $Z$  for this system in terms of the one-particle partition function  $z$ ?

We calculate next the entropy  $S$ . Instead of deriving it from the partition function we use a more straightforward approach. We consider a configuration with  $n$  spins up (and thus  $N - n$  spins down).

- (c) What is the energy of this configuration? How many different configurations with this energy exist? What is the entropy of the set of configurations with that energy? (For the latter you can use Stirling's formula  $\log(M!) \approx M \log M$  for large  $M$ .)
- (d) Define by  $x \equiv n/N$  the fraction of atoms with spin up. Show that the entropy in terms of  $x$  can be written as

$$S = -Nk (x \log x + (1 - x) \log(1 - x))$$

- (e) Calculate now  $S(x)$  for  $x = 0$ ,  $x = 1/2$  and  $x = 1$ . Calculate  $dS/dx$  for those 3 values. Use this information to sketch  $S(x)$ .
- (f) Give now an expression for the energy  $E$  of the system in terms of the fraction  $x$ , and determine the minimal and maximal energy of the system. Sketch now  $S(E)$ , the entropy as a function of  $E$  and the temperature  $T$  as a function of  $E$ . (You do not have to calculate  $S(E)$  and  $T(E)$  explicitly in order to sketch them!)
- (g) Which unusual phenomenon occurs for  $x > 1/2$ ? Give at least one reason why this phenomenon is usually not observed.

## 2 Diatomic van der Waals gas

Consider the equations

$$\left(p + \frac{a}{kT} \frac{N^2}{V^2}\right) (V - V_0) = NkT$$

and

$$\lim_{v \rightarrow \infty} E = \frac{5}{2} NkT$$

that described a non-ideal diatomic gas of  $N$  molecules in a volume  $V$ .  $V_0$  and  $a$  denote positive constants. The task is to determine the entropy  $S(E, V, N)$  of this system following the below given steps.

- (a) Determine first the canonical potential  $\phi(\beta, V, N)$  using the fact that  $\partial\phi/\partial V = \beta p$  and  $\partial\phi/\partial\beta = -E$ .
- (b) Find the function  $\beta = \beta(E)$  (assume that the temperature is always positive).
- (c) Now give  $S(E, V, N)$  using  $\phi(\beta, V, N) = S(E, V, N) - \beta E$ .

## 3 Virial expansion

Consider a one-dimensional gas of  $N$  *impenetrable* particles of diameter  $D$  that are confined within a one-dimensional volume of length  $L$ . It can be shown that the equation of state of this system is given by

$$\beta p = \frac{\lambda}{1 - D\lambda}$$

Here  $\lambda = N/L$  denotes the one-dimensional number density.

- (a) Expand the above expression in terms of small densities.
- (b) Calculate the second virial coefficient

$$B_2(T) = - \int_0^\infty \left( e^{-\beta w(r)} - 1 \right) dr$$

for the above described gas. Here  $w(r)$  is the interaction potential as a function of the distance  $r$  between the particle centers (infinite for  $|r| < D$ , zero otherwise).

- (c) Check whether the  $\lambda^2$ -term in (a) corresponds to the  $\lambda^2$ -term of the virial expansion.
- (d) Assume now instead point particles,  $D = 0$ , with a power law repulsion of the form  $w(r) = Ar^{-\alpha}$  with an exponent  $\alpha > 0$  and  $A > 0$  being a constant. For which values of  $\alpha$  does the second virial coefficient exist? (Hint: The integral cannot be solved explicitly. What

you can do instead is to divide the integration domain into 2 halves, one from 0 to  $R \gg 1$  and one from  $R$  to  $\infty$  and then to estimate whether the integrals of those two parts give finite or infinite values).

- (e) Does it make sense to study the equation of state of ions in a so-called ion channel (such quasi-one-dimensional channels for ions are widespread in cell membranes) by a virial expansion?

#### 4 General questions

Give *short* answers to the following questions:

1. Does mean-field theory work better to describe a system of particles with short-range interaction or long-range interaction? And why?
2. What is the Legendre transformation? And where is it used in thermodynamics?
3. Which thermodynamic law is violated by the classical ideal gas?
4. What is the energy representation? Why is it not the most natural representation for thermodynamics?