TKJ4215 Statistisk termodynamikk i kjemi og biologi
Eksamen 08.06.2016, 09.00-13.00

Norges Teknisk-Naturvitenskapelige Universitet
Hjelpemiddelkode A. (Alle trykte og håndskrevne hjelpemidler tillatt. Alle kalkulatorer tillatt.)
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NB: Oppgavene teller ikke like mye. Totalt er 100 poeng fordelt på to oppgaver. Se parentes etter oppgavenummer for antall poeng per deloppgave.

Exercise 1 (15, 20, 10, 10)

a) We have a condensed system with two types of relatively heavy particles, A and B, in a solvent of S molecules. We disregard interactions between the particles, but the A and B particles are so heavy that they are affected by a gravitational force, e.g. $f_A = m_A g$ acting in the z-direction. Derive equilibrium conditions in terms of the chemical potentials μ_A and μ_B, respectively, including also the gravitational force.

b) Derive relations for the concentration dependencies, $c_A(z)$ and $c_B(z)$, relative to their respective concentration at the top of the container, $c_A(0)$ and $c_B(0)$. In a container of height h, how big differences in mass is required to have ten times more A particles than B particles at the bottom of the container? Here it can be assumed that the concentrations on the top of the container are equal, $c_A(0) = c_B(0)$. Which particles have the largest mass, A or B? What is the role of entropy here and what happens in the limit of a high temperature T?

c) We will briefly also consider the interactions between A and B particles, w_{AA}, w_{BB} and w_{AB}, within the Bragg-Williams model. Discuss (not derive) how the interactions may affect the result in b). If we in addition include particle-solvent interactions, w_{As} and w_{Bs}, how can they affect the result?

d) Finally, what are the basic approximations in a lattice model for a liquid as well as for the Bragg-Williams approximation?

Exercise 2 (15, 10, 15, 5)

a) Derive an extended version of the Boltzmann distribution law in the canonical ensemble with the extra constraint that the kinetic energy, K is conserved. In this case, it can be assumed that all particles on energy level j has the same kinetic energy K_j.

b) What is an ensemble and which are the three common ensembles mainly used in this course?

c) How is the partition function modified in a)? In general, what is the interpretation of the partition function and why is it useful? Why is the numerical value of the partition function in most cases not meaningful?

d) We derive the Boltzmann distribution for $F(T, V, N)$ by minimizing F. It can instead be done by maximizing the entropy of the system also for $F(T, V, N)$. Briefly sketch how that can be done to obtain the identical result as by minimizing $F(T, V, N)$.