

UNIVERSITETET I TRONDHEIM
 NORGES TEKNISKE HØGSKOLE
 INSTITUTT FOR TEORETISK FYSIKK

Faglig kontakt under eksamen:
 Professor P.C.Hemmer
 Tlf.(9)3648

Eksamen i
 fag 71561 Klassiske mangepartikkelsystemer
 Tirsdag 19.januar 1982
 kl.0900-1500

Tillatte hjelpemidler: Regnestav, lommekalkulator og matematisk formelsamling (Rottmann).

Problem 1

- Give the ensemble distributions in the microcanonical ensemble, the canonical ensemble and the grand canonical ensemble for a fluid (the positions and momenta of the particles are indicated by \vec{r}_i and \vec{p}_i respectively).
- Define the canonical partition function $Z_N(T,V)$ and the grand canonical partition function $\Xi(\mu,T,V)$. What is the physical meaning of quantities N, T, V and μ (Do not give a derivation of this, just give their names like: N is number of particles in the system).
- Derive a relation for the internal energy U in terms of the canonical partition function.
- Derive relations for the internal energy U and the (average) number of particles $\langle N \rangle$ in the grand canonical ensemble.
- Show that in the canonical ensemble

$$\frac{\partial^2}{\partial \beta^2} \ln Z_N = \langle (H - \langle H \rangle)^2 \rangle .$$

Show that in the grand canonical ensemble

$$(kT)^2 \frac{\partial^2}{\partial \mu^2} \ln \Xi = \langle (N - \langle N \rangle)^2 \rangle .$$

Which thermodynamic quantities correspond with these averages ?

- f. Calculate Z_N and E for an ideal gas. What are the resulting values for U and $\langle (H - \langle H \rangle)^2 \rangle$ in the canonical ensemble and for $\langle N \rangle$ and $\langle (N - \langle N \rangle)^2 \rangle$ in the grand canonical ensemble? Comment on the relative size of the fluctuations.

Problem 2

Consider the Ising model. The energy is given by

$$H = J \sum_{(i,j)} \sigma_i \sigma_j - m \mathcal{H} \sum_i \sigma_i .$$

Here σ_i may have values ± 1 while $i=1, \dots, N$. The sum in the first term is over all nearest neighbouring pairs.

- a) Calculate the partition function, the average magnetic moment per spin $M = m \langle \sigma_i \rangle$ and the magnetic susceptibility per spin

$$\chi = \frac{\partial M}{\partial \mathcal{H}} \quad \text{for the special case that } J=0 .$$

One may now calculate the partition for $J \neq 0$ using the mean field approximation:

$$\sum_{(i,j)} \sigma_i \sigma_j \Rightarrow \sum_{(i,j)} \sigma_i \langle \sigma_j \rangle = M \frac{n}{m} \sum_i \sigma_i$$

where n is the number of nearest neighbours.

- b) Show that in this approximation

$$M = \tanh[\beta(m\mathcal{H} - \frac{n}{m} J M)] .$$

- c) Give an expression for the susceptibility χ .
 d) Discuss the behaviour of M and χ in the mean field approximation for $\mathcal{H}=0$.

For the one dimensional case the energy is

$$H = J \sum_{i=1}^N \sigma_i \sigma_{i+1} - m \mathcal{H} \sum_{i=1}^N \sigma_i$$

where we take $\sigma_{N+1} = \sigma_1$ in this case.

- e) Calculate the partition function for the one dimensional case.
 f) Calculate the resulting magnetic moment and the susceptibility per spin for the one dimensional case.

Problem 3

- a) Define the reduced distribution functions $n_2(\vec{r}_1, \vec{r}_2)$, $n_2^S(\vec{r}_1, \vec{r}_2)$ and the pair correlation function $g_2(\vec{r}_1, \vec{r}_2)$ in a fluid.
- b) Derive an expression for the pressure in terms of the pair correlation function. (Use the fact that the potential energy is the sum of pair potentials).
- c) Derive an expression for $n_2(\vec{r}_1, \vec{r}_2)$ to the second order in the activity z . Give the corresponding expression for $g_2(\vec{r}_1, \vec{r}_2)$ to the zeroth order in the density.
- d) What is the resulting formula for the second virial coefficient? For what purpose is this formula useful?

The molecular density is defined as

$$\rho(\vec{r}) = \sum_i \delta(\vec{r} - \vec{r}_i)$$

The fluctuation around the average value in equilibrium $\rho = \langle \rho(\vec{r}) \rangle$ is defined by

$$\Delta\rho(\vec{r}) = \rho(\vec{r}) - \rho$$

- e) Derive the relation between the auto correlation function of the density fluctuation

$$S_2(\vec{r}, \vec{r}') = \langle \Delta\rho(\vec{r}) \Delta\rho(\vec{r}') \rangle$$

and the pair correlation function (using the canonical ensemble).