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Tirsdag 19.januar 1982
kl.0900-1500

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

Problem 1

a) 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).

b) 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).

c) Derive a relation for the internal energy U in terms of the canonical partition function.

d) Derive relations for the internal energy U and the (average) number of particles $\langle N\rangle$ in the grand canonical ensemble.

e) 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 Ξ 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

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

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 $\chi=\frac{\partial M}{\partial \mathcal{H}}$ 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).