NTNU

Institutt for fysikk

Contact during the exam:
Professor Kåre Olaussen
Telephone: 9 36 52 eller 45 43 71 70

Exam in TFY4230 STATISTICAL PHYSICS

Friday december 19, 2014
09:00–13:00

Allowed help: Alternativ **C**
Standard calculator (according to the NTNU list).
One A4 formula sheet; personal handwritten notes are allowed on this.
K. Rottman: *Matematisk formelsamling* (all languages).
Barnett & Cronin: *Mathematical Formulae*.

This problemset consists of 3 pages.

Problem 1. Cold Fermi gases

The grand canonical partition function Θ for an ideal Fermi gas can be expressed in the form

$$\ln\Theta = Vg\int\frac{d^3k}{(2\pi)^3}\,\ln\left[1+\mathrm{e}^{-\beta(\varepsilon_{\boldsymbol{k}}-\mu)}\right]. \tag{1}$$

a) What are β and μ? How is Θ identified with thermodynamical properties?

b) What is g? Does there exist physical systems where one may set $g=1$?

c) What is $\varepsilon_{\boldsymbol{k}}$? What is the form of $\varepsilon_{\boldsymbol{k}}$ for relativistic particles with mass?

d) Find (or write down) an integral expression for the particle density $\rho = N/V$ of this system.
Sketch how the integrand of this expression varies with $\varepsilon_{\boldsymbol{k}}$. Assume that μ is positive and large; indicate in particular the limits $\beta(\varepsilon_{\boldsymbol{k}}-\mu) \ll -1$ and $\beta(\varepsilon_{\boldsymbol{k}}-\mu) \gg 1$.

e) Find (or write down) an integral expression for the energy density E/V of this system.

Assume now that we may make the approximation $\varepsilon_{\boldsymbol{k}}-\mu \approx \frac{\hbar^2}{2m}\boldsymbol{k}^2 - \mu_{\rm NR}$, and that the temperature may be set to zero.

f) Find the connection between $\mu_{\rm NR}$ (in this case also denoted the Fermi energy E_F) and the particle density ρ.

g) Show that the answer of the previous point essentially can be found by dimensional analysis (apart for a numerical factor which must be of order 1):
(i) Which physical parameters can the answer depend on?
(ii) How must these parameters be combined to give an expression of dimension energy?

h) The number density of free electrons in aluminium is $\rho = 2.1 \cdot 10^{29}$ m^{-3}. Assume that these electrons can be treated as an ideal Fermi gas.

What is the Fermi temperature T_F (defined by $k_B T_F = E_F$) for this material?

Given:

$$\begin{aligned} \hbar &= 1.054 \cdot 10^{-34}\ \text{kg m}^2\,\text{s}^{-1}, \\ k_B &= 1.381 \cdot 10^{-23}\ \text{kg m}^2\,\text{s}^{-2}\,\text{K}^{-1}, \\ m_e &= 9.109 \cdot 10^{-31}\ \text{kg}, \\ m_{\text{Al}} &\approx 4.482 \cdot 10^{-26}\ \text{kg}. \end{aligned}$$

Problem 2. Frustrated Ising chain

In this problem we consider a closed Ising chain with antiferromagnetic interactions, with an odd number of spins. We first simplify to the case of three spins. The Hamilton function then becomes

$$H = J\,(s_0 s_1 + s_1 s_2 + s_2 s_0)\,, \tag{2}$$

where each Ising spin s_i takes the values ± 1, and $J > 0$.

a) What are the possible energies of this chain, and how many configurations are there for each of these energies?

b) What is the entropy S of this chain at (i) zero temperature, and (ii) infinite temperature?

c) Write down the canonical partition function for this chain.

d) Calculate the mean energy E as function of the temperature parameter β.

e) Calculate the heat capacity C as function of the temperature parameter β.

f) What is the behavior of C as (i) $T \to 0$, and (ii) as $T \to \infty$?

g) Calculate the entropy S of this chain as function of the temperature parameter β.

Now add a magnetic field, such that the Hamilton function acquires an additional contribution,

$$\Delta H = -\mu B (s_0 + s_1 + s_2). \tag{3}$$

h) What are the possible energies of this chain now; and how many configurations are there for each of these energies?

Finally consider the general case of a chain with $2N + 1$ spins.

i) What is the *lowest* possible energy of the chain, and how many configurations have this energy?

Problem 3. Lattice vibrations

A slightly simplified model for linear lattice vibrations is given by the Hamilton function

$$H = \frac{1}{2M} \sum_m p_m^2 + \frac{1}{2} \sum_{mn} q_m K_{m,n} q_n, \tag{4}$$

where $K_{m,n}$ is a symmetric $N \times N$ matrix with all eigenvalues positive, $\lambda_j = M\,\omega_j^2$.

a) What is the classical heat capacity C for this system according to the equipartition principle?

Quantum mechanically the system constitutes a collection of N harmonic oscillators, with frequencies ω_j defined by the eigenvalues

$$\mathcal{S} = \left\{ \lambda_j = M\omega_j^2 \,|\, j = 0, \ldots, N-1 \right\}. \tag{5}$$

To find $\mathcal{S}$ numerically for a large system one may use a routine from **scipy.sparse.linalg**. This requires one to make a function which performs the operation $\psi_m \to \sum_n K_{mn}\psi_n$. The code below shows a one-dimensional example of such an operation.

```
def K(psi):
    """Return␣(-1)␣times␣the␣1D␣lattice␣laplacian␣of␣psi"""
    Kpsi  = 2*psi
    Kpsi -= numpy.roll(psi, 1, axis=0)
    Kpsi -= numpy.roll(psi,-1, axis=0)
    return Kpsi/2
```

b) From the code above one may read out what the explicit expression for $\sum_{mn} q_m K_{m,n} q_n$ is in this case. Write down this expression.

c) Generalize the code above to two- and three-dimensional lattices with corresponding nearest-neighbor interactions.

For a large lattice the frequencies will be very close, and are best described by a function $\rho(\omega)$, the density of states.
Numerically we may construct such a density through a histogram. The code below is an example of how this can be done (taken from a slightly different situation).

```
def makeHistogram(data, min, max, nbins):
    """Return␣a␣histogram␣of␣the␣contents␣in␣data"""
    bins  = numpy.linspace(min, max, nbins+1)
    return numpy.histogram(data, bins=bins)
```

d) Modify the code above to the calculation of $\rho(\omega)$, under the assumption that `data` contains the set $\mathcal{S}$ of eigenvalues.

e) Assume that $\mathcal{S}$ consists of 10 000 eigenvalues in the interval between 0 and 10. Which values would you choose for the parameters `min`, `max` and `nbins`?