



## Solution to the exam in TFY4230 STATISTICAL PHYSICS

Friday december 19, 2014

This solution consists of 10 pages.

### Problem 1. Cold Fermi gases

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

$$\ln \Theta = Vg \int \frac{d^3k}{(2\pi)^3} \ln \left[ 1 + e^{-\beta(\epsilon_{\mathbf{k}} - \mu)} \right]. \quad (1)$$

- a) What are  $\beta$  and  $\mu$ ? How is  $\Theta$  identified with thermodynamical properties?

$\beta = (k_B T)^{-1}$  is a convenient measure of temperature (with dimension inverse energy).  $\mu$  is the chemical potential (with dimension energy). The thermodynamic identification is

$$\Theta = e^{\beta PV}, \quad (2)$$

where  $P$  is pressure and  $V$  is volume.

**Remark:** It was surprising to note how many identified  $\Theta$  wrong.

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

$g$  is the degeneracy factor which counts how many internal states (typically spin states) the particle can be in for each momentum and/or position.

Since equation (1) is the partition function for gas of fermions, and all fermions must have half-integer spin (hence an even number of internal states), it becomes difficult to realize a physical system with  $g = 1$ . Hence, an accepted short answer is "no".

**Remark 1:** In principle it is physically possible to impose a system of fermions with magnetic moment to a very strong magnetic field, so that only the (say) spin-up states contribute to the partition function. For charged fermions this would at the same time distort the energy levels to a form which does not fit to equation (1), but for neutral particles the distorted levels could still fit. By finding a neutral atom with a large magnetic moment, and exerting it to a very strong magnetic field and very low temperature it *might* be possible to make a system which is well described by equation (1) with  $g = 1$ . Hence, a longer answer is "probably yes".

**Remark 2:** The above illustrates that impossibility proofs in the physical sciences may often be circumvented. In fact, the Nobel Prize in Chemistry for 2014 was given for circumventing an impossibility proof. On the other hand, countless attempts to circumvent the second law of thermodynamics have failed.

**Remark 3:** In the extension of electronics to *spintronics* one actually consider a system of electrons as consisting of two species, electrons with spin-up and electrons with spin-down. Each species can be described by a distribution corresponding to (1) with  $g = 1$ , but where both species contributes to the partition function.

**Remark 4:** Many seemed to interpret this question in a very broad sense. However, equation (1) is only valid for fermions; in addition the problem context is spelled out explicitly in the title.

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

$\varepsilon_{\mathbf{k}}$  is the energy of a particle with momentum  $\mathbf{p} = \hbar\mathbf{k}$ . For relativistic free particles

$$\varepsilon_{\mathbf{k}} = \sqrt{(\hbar c\mathbf{k})^2 + (mc^2)^2} \approx \begin{cases} mc^2 + \frac{\hbar^2}{2m}\mathbf{k}^2, & \text{for } \hbar|\mathbf{k}| \ll mc, \\ \hbar c|\mathbf{k}|, & \text{for } \hbar|\mathbf{k}| \gg mc. \end{cases} \quad (3)$$

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  $\varepsilon_{\mathbf{k}}$ . Assume that  $\mu$  is positive and large; indicate in particular the limits  $\beta(\varepsilon_{\mathbf{k}} - \mu) \ll -1$  and  $\beta(\varepsilon_{\mathbf{k}} - \mu) \gg 1$ .

$$\rho = \frac{N}{V} = \frac{1}{\beta V} \left( \frac{\partial \ln \Theta}{\partial \mu} \right)_{\beta, V} = g \int \frac{d^3k}{(2\pi)^3} \frac{1}{e^{\beta(\varepsilon_{\mathbf{k}} - \mu)} + 1} \equiv g \int \frac{d^3k}{(2\pi)^3} \langle n_{\mathbf{k}} \rangle. \quad (4)$$

Here  $0 \leq \langle n_{\mathbf{k}} \rangle \leq 1$  is the average number of particles in the one-particle mode  $\mathbf{k}$ . The integrand, which is called *the Fermi function*, is plotted in Figure 1.

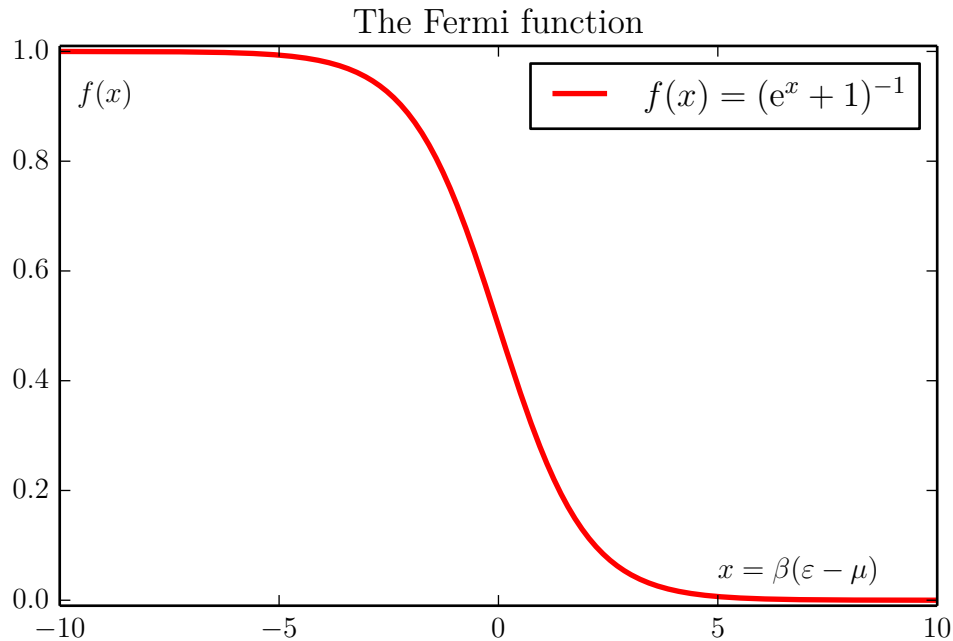


Figure 1: The Fermi function displays, in terms of scaled variables, the mean occupation of single-particle states in a system of non-interacting fermions

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

$$\frac{E}{V} = g \int \frac{d^3k}{(2\pi)^3} \varepsilon_{\mathbf{k}} \langle n_{\mathbf{k}} \rangle = g \int \frac{d^3k}{(2\pi)^3} \frac{\varepsilon_{\mathbf{k}}}{e^{\beta(\varepsilon_{\mathbf{k}} - \mu)} + 1}. \quad (5)$$

**Remark:** A common mistake here is to use an expression valid for the canonical ensemble,

$$E = -\frac{\partial}{\partial \beta} \ln Z.$$

This is not correct for the grand canonical ensemble. The brief calculation above is based on physical interpretation or intuition (which may often be a shaky foundation). A thermodynamic derivation is to start with the relation

$$PV = \mu N + TS - E \quad (6)$$

(which holds because  $\mu N = G = E + PV - TS$ ), and rewrite the thermodynamic identity as

$$VdP = Nd\mu + SdT. \quad (7)$$

It follows from this that  $TS = T \left( \frac{\partial}{\partial T} PV \right)_{\mu, V} = -\beta \left( \frac{\partial}{\partial \beta} PV \right)_{\mu, V}$  and  $\mu N = \mu \left( \frac{\partial}{\partial \mu} PV \right)_{\beta, V}$ . Hence

$$E = \mu N + TS - PV = \mu \left( \frac{\partial \beta PV}{\beta \partial \mu} \right)_{\beta, V} - \left( \frac{\partial \beta PV}{\partial \beta} \right)_{\mu, V}. \quad (8)$$

Application of this formula to  $\beta PV = \ln \Theta$  leads to the result (5), after which we may safely refer to our magnificent physical intuition.

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

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

It may be instructive to first plot the Fermi function as function of  $\varepsilon$  for a fixed temperature  $T$ , and investigate how the shape changes as we vary  $T$ . This is shown in figure 2.

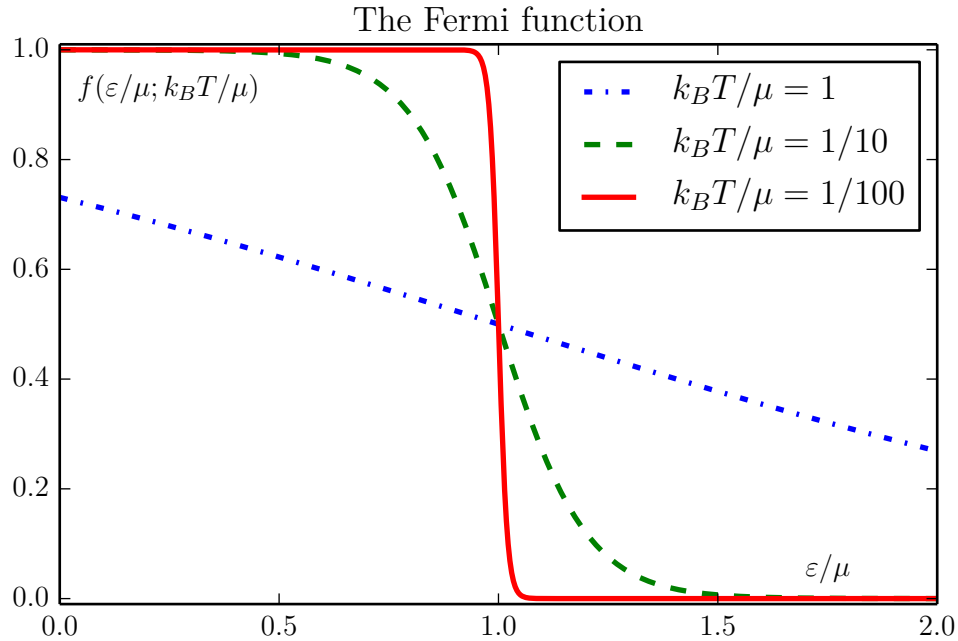


Figure 2: The Fermi function, as function of scaled energy for various values of scaled temperature. It becomes a step function at zero temperature.

We see that when  $k_B T/\mu \ll 1$  we may set  $f = 1$  when  $\varepsilon < \mu$ , and  $f = 0$  when  $\varepsilon > \mu$ . Mathematically this can be expressed as

$$f = \theta(k_F - |\mathbf{k}|), \quad \text{where} \quad \frac{\hbar^2 k_F^2}{2m} = \mu_{\text{NR}}. \quad (9)$$

It follows that

$$\rho = \frac{4\pi g}{(2\pi)^3} \int_0^{k_F} k^2 dk = \frac{g}{6\pi^2} k_F^3 = \frac{g}{6\pi^2} \left( \frac{2m\mu_{\text{NR}}}{\hbar^2} \right)^{3/2}. \quad (10)$$

This is an acceptable answer, but it may be more instructive to find  $E_F$  in terms of  $\rho$ :

$$E_F = \mu_{\text{NR}}(T = 0) = \left(\frac{6\pi^2}{g}\right)^{2/3} \frac{\hbar^2}{2m} \rho^{2/3}. \quad (11)$$

- 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?

At  $T = 0$  the only available parameters are the density  $\rho$  (with dimension  $[\rho] = \text{m}^{-3}$ ) and the combination  $\hbar^2/m$  (with dimension  $[\hbar^2/m] = \text{kg m}^2/\text{s}^2$ ). Thus, we must have

$$E_F \propto \rho^x \left(\frac{\hbar^2}{m}\right)^y$$

for some numerical constants  $x$  and  $y$ . Since  $E_F$  is an energy with dimension  $[E_F] = \text{kg m}^2/\text{s}^2$ , the only solution is  $x = 2/3$  and  $y = 1$ . I.e.,

$$E_F = c(g) \frac{\hbar^2}{m} \rho^{2/3}, \quad (12)$$

for some numerical factor  $c(g)$ . Comparison with equation (11) shows that  $c(g) \approx 4.785$  for electrons ( $g = 2$ ).

- h) The number density of free electrons in aluminium is  $\rho = 2.1 \cdot 10^{29} \text{ m}^{-3}$ . 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:**

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

Here the information about  $m_{\text{Al}}$  is irrelevant. Insertion of the other parameters into (11) gives

$$T_F = 149\,307 \text{ K}. \quad (13)$$

That means that  $T/T_F \approx 1/50$  at room temperature. Like other metals it is not a bad approximation to consider aluminium at room temperature as a zero temperature system.

**Remark:** Here the information about  $m_{\text{Al}}$  is not needed; it was included as a distraction — just like real life is filled with distractions and false clues.

## 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

$$H = J(s_0 s_1 + s_1 s_2 + s_2 s_0), \quad (14)$$

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

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

There are  $2^3 = 8$  possible configurations in all

Configurations	Energy
↑↑↑	$3J$
↓↓↓	$3J$
↓↑↑, ↑↓↑, ↑↑↓	$-J$
↑↓↓, ↓↓↑, ↓↑↑	$-J$

I.e., there are 6 configurations with energy  $-J$ , and 2 configurations with energy  $3J$ .

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

At zero temperature only the 6 states of energy  $-J$  are equally probable, while the last two or frozen out:

$$S = k_B \ln 6. \quad (15)$$

At infinite temperature all 8 states are equally probable:

$$S = k_B \ln 8. \quad (16)$$

**Remarks:** Here candidates were expected to remember the famous formula of Boltzmann,  $S = k_B \ln \Omega$ . And know how to use it: (i) At zero temperature only the ground state is available, and  $\Omega$  becomes the degeneracy of the ground state, (ii) at infinite temperature all states of the system are available with equal probability, and  $\Omega$  becomes the total number of states (a common misunderstanding is to believe that only the states of highest energy should be counted at infinite temperature).

Some identify the wrong states with the ground states. Some use the general formula  $S = (E - F)/T$ , treating  $F$  and  $E$  as temperature independent, to conclude that  $S = \infty$  at  $T = 0$ , and  $S = 0$  at  $T = \infty$  (which is qualitatively exactly the opposite of physical behavior).

Those who calculated the complete entropy expression first, and next took the appropriate limits (and got these right) were given full score. However, this is a dangerous (hence wrong) and complicated procedure, with no security net for catching algebraic errors. The limiting behaviors should be computed independently, and used to check the general expression.

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

$$Z = e^{\beta J} (6 + 2 e^{-4\beta J}), \quad (17a)$$

or

$$\ln Z = \beta J + \ln 2 + \ln (3 + e^{-4\beta J}) \quad (17b)$$

- d) Calculate the mean energy  $E$  as function of the temperature parameter  $\beta$ .

$$E = -\frac{\partial}{\partial \beta} \ln Z = -J + \frac{4J}{3e^{4\beta J} + 1}. \quad (18)$$

**Remark:** Some mathematically equivalent expressions are

$$E = 3J \left( \frac{e^{-3\beta J} - e^{\beta J}}{e^{-3\beta J} + 3e^{\beta J}} \right) = -3J \left( \frac{1 - e^{-4\beta J}}{3 + e^{-4\beta J}} \right).$$

However, since these expressions contain (many) more  $\beta$ -dependent terms, they lead to more cumbersome calculations of the heat capacity  $C$ . It is a good advice to simplify  $\ln Z$  as much as possible *before* taking any derivatives.

- e) Calculate the heat capacity  $C$  as function of the temperature parameter  $\beta$ .

$$\frac{C}{k_B} = \beta^2 \frac{\partial^2 \ln Z}{\partial \beta^2} = -\beta^2 \frac{\partial E}{\partial \beta} = \frac{48 \cdot (\beta J)^2 e^{4\beta J}}{(3e^{4\beta J} + 1)^2}. \quad (19)$$

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

$$\frac{C}{k_B} \approx \frac{1}{3} (4J/k_B T)^2 e^{-4J/k_B T} \quad \text{as } T \rightarrow 0, \tag{20a}$$

$$\frac{C}{k_B} \approx 3 (J/k_B T)^2 \quad \text{as } T \rightarrow \infty. \tag{20b}$$

**Remark 1:** With *behavior* is ment more that just the limiting values (here zero). *How* these limits are approached are important aspects of the behavior.

**Remark 2:** It is a general feature of systems with a lowest energy gap  $\Delta E$  that the low temperature heat capacity has the behavior

$$\frac{C}{k_B} \propto \left( \frac{\Delta E}{k_B T} \right)^2 e^{-\Delta E/k_B T}.$$

The exact prefactor is  $g_1/g_0$ , where  $g_0$  is the degeneracy of the ground state, and  $g_1$  the degeneracy of the first excited state. In this case  $g_0 = 6$  and  $g_1 = 2$ .

**Remark 3:** It is a general feature of systems whose energies are restricted to a finite range that the high temperature heat capacity has the behavior

$$\frac{C}{k_b} \propto \frac{1}{(k_B T)^2}.$$

The exact prefactor is

$$\text{Var}(E) = \int dE \rho(E) (E - \bar{E})^2, \quad \text{where } \bar{E} = \int dE \rho(E) E,$$

and  $\rho(E)$  is the normalized density of states per energy. In this case  $\rho(E) = \frac{3}{4} \delta(E + J) + \frac{1}{4} \delta(E - 3J)$ .

**Remark 4:** The full temperature behavior of equation (19) is illustrated in figure 3.

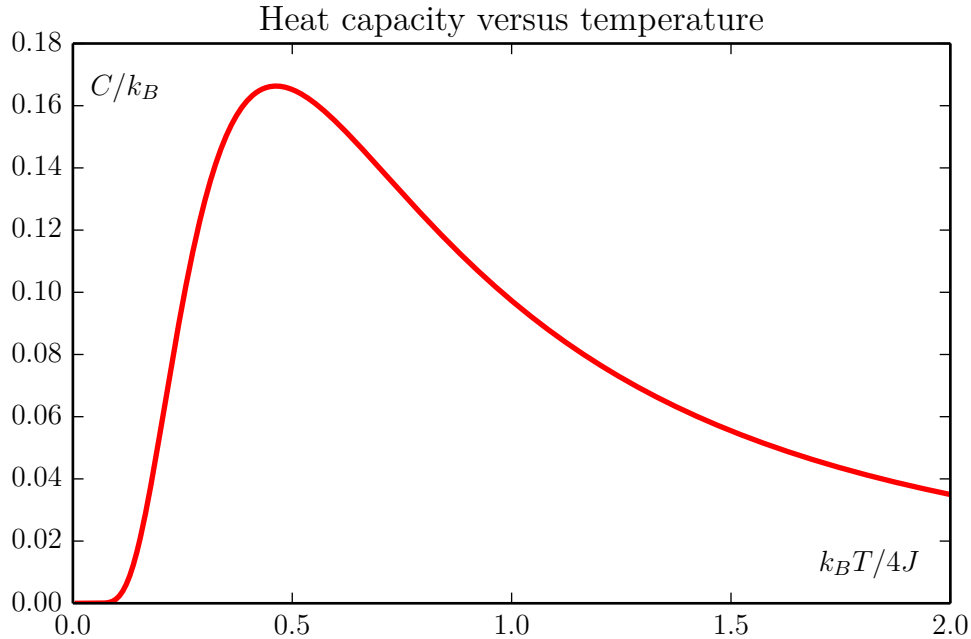


Figure 3: The heat capacity of a 3-site frustrated Ising chain as function of temperature.

g) Calculate the entropy  $S$  of this chain as function of the temperature parameter  $\beta$ .

Since  $\ln Z = -\beta F = -\beta(E - TS)$ , we find

$$\frac{S}{k_B} = \ln Z + \beta E = \ln 2 + \ln(3 + e^{-4\beta J}) + \frac{4\beta J}{3e^{4\beta J} + 1}. \tag{21}$$

**Remark 1:** We see from equation (21) that  $S/k_B = \ln 6$  when  $T = 0$ , and  $S/k_B = \ln 8$  when  $\beta = 0$ , in agreement with point **b**).

**Remark 2:** The full temperature behavior of equation (21) is illustrated in the figure 4.

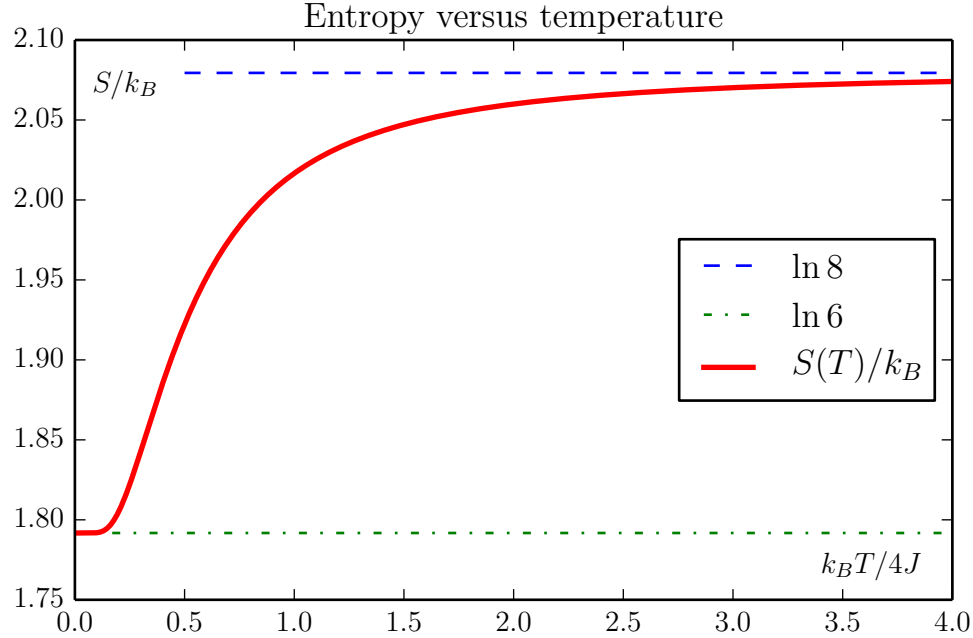


Figure 4: The entropy of a 3-site frustrated Ising chain as function of temperature.

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

$$\Delta H = -\mu B(s_0 + s_1 + s_2). \tag{22}$$

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

Configurations	Energy
↑↑↑	$3J - 3\mu B$
↓↓↓	$3J + 3\mu B$
↓↑↑, ↑↓↑, ↑↑↓	$-J - \mu B$
↑↓↓, ↓↑↓, ↓↓↑	$-J + \mu B$

There are 3 configurations with energy  $-J - \mu B$ , 3 configurations with energy  $-J + \mu B$ , one configuration with energy  $3J - 3\mu B$ , and one configuration with energy  $3J + 3\mu B$ .

**Remark:** Note that the configuration of lowest energy depends on the ratio between  $J$  and  $\mu B$ . For  $J/(\mu B) > 1/2$  there are 3 lowest energy configurations:  $\downarrow\uparrow\uparrow$ ,  $\uparrow\downarrow\uparrow$ , and  $\uparrow\uparrow\downarrow$ . For  $J/(\mu B) < 1/2$  there is one lowest energy configuration:  $\uparrow\uparrow\uparrow$ . For  $J/(\mu B) = 1$  these two possibilities have the same energy, and the lowest energy configuration is 4-fold degenerate. I.e., there is a zero-temperature phase transition in the system at  $\mu B = 2J$ .

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?

Consider first the case that  $\mu B = 0$ . The lowest energy is obtained when all neighboring pairs have anti-parallel spins. Unfortunately, for a chain with an odd number  $2N + 1$  of spins this is not possible. There must always be at least one neighboring pair with parallel spins. This is why we call the chain *frustrated*.

Only one parallel pair lead to the lowest energy. There are  $2N + 1$  different choices for this pair. In addition, the net spin of the chain may be either  $+1$  or  $-1$ . Hence, in this case the lowest energy is

$$(1 - 2N)J, \quad \text{with a degeneracy of } 2(2N + 1).$$

Consider next a small  $\mu B > 0$ . The configurations of lowest energy will now have a net spin of  $+1$ . In this case the lowest energy is

$$(1 - 2N)J - \mu B, \quad \text{with a degeneracy of } (2N + 1).$$

However, if  $\mu B$  becomes large enough the lowest energy will occur when all spins are pointing upwards. This unique configuration will have the lowest energy of

$$(2N + 1)(J - \mu B).$$

The (zero temperature phase) transition between the two cases occurs when  $\mu B = 2J$ .

### Problem 3. Lattice vibrations

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

$$H = \frac{1}{2M} \sum_m p_m^2 + \frac{1}{2} \sum_{mn} q_m K_{m,n} q_n, \quad (23)$$

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?

There are  $N$  momentum and  $N$  position degrees of freedom which are coupled quadratically. This implies a classical heat capacity

$$C = \left(\frac{1}{2}N + \frac{1}{2}N\right) k_B = Nk_B. \quad (24)$$

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

$$S = \{\lambda_j = M\omega_j^2 \mid j = 0, \dots, N-1\}. \quad (25)$$

To find  $S$  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  $\psi_m \rightarrow \sum_n K_{m,n} \psi_n$ . The code below shows a one-dimensional example of such an operation.

```
1 def K(psi):
2     """Return_{(-1)}_times_the_1D_lattice_laplacian_of_psi."""
3     Kpsi = 2*psi
4     Kpsi -= numpy.roll(psi, 1, axis=0)
5     Kpsi -= numpy.roll(psi,-1, axis=0)
6     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.

Line 3 in the code initializes  $(K\psi)_m = 2\psi_m$ , line 4 subtracts  $\psi_{m-1}$  from  $(K\psi)_m$ , and line 5 subtracts  $\psi_{m+1}$  from  $(K\psi)_m$ . Finally in line 6 the result is reduced by a factor  $\frac{1}{2}$ .

This means that

$$(K\psi)_m = \frac{1}{2} (2\psi_m - \psi_{m-1} - \psi_{m+1}),$$

a lattice version of the second derivative of  $\psi$  (it is called the second difference). Therefore,

$$K_{m,n} = \delta_{m,n} - \frac{1}{2}\delta_{m-1,n} - \frac{1}{2}\delta_{m+1,n},$$

and

$$\frac{1}{2} \sum_{mn} q_m K_{m,n} q_n = \sum_{m=0}^{N-1} q_m (q_m - q_{m+1}). \quad (26)$$

In all expressions above we count indices modulo  $N$ . I.e.,  $\psi_{N+m} \equiv \psi_m$ , and  $\psi_{-m} \equiv \psi_{N-m}$ .



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

In two (three) dimensions the components of  $\psi$  and  $q$  are naturally described by two (three) indices, and we should take the second difference in both (all) directions. I.e.,

$$(K\psi)_{m,n} = \frac{1}{2} (4\psi_{m,n} - \psi_{m-1,n} - \psi_{m+1,n} - \psi_{m,n-1} - \psi_{m,n+1})$$

in two dimensions, and

$$(K\psi)_{m,n,p} = \frac{1}{2} \left( 6\psi_{m,n,p} - \psi_{m-1,n,p} - \psi_{m+1,n,p} - \psi_{m,n-1,p} - \psi_{m,n+1,p} - \psi_{m,n,p-1} - \psi_{m,n,p+1} \right)$$

in three dimensions. A routine which works in all dimensions is listed below:

```
1 def K(psi):
2     """Return (-1) times the lattice laplacian of psi."""
3     Kpsi = numpy.zeros_like(psi) # Allocate space of correct shape
4     for d in range(len(psi.shape)):
5         Kpsi += 2*psi
6         Kpsi -= numpy.roll(psi, 1, axis=d)
7         Kpsi -= numpy.roll(psi,-1, axis=d)
8     return Kpsi/2
```

**Remark 1:** In the real world there is an additional complication, due to the fact that a LinearOperator routine must accept and return one-dimensional arrays. To handle this we must modify the code above

```
1 def K(psi):
2     """Return (-1) times the lattice laplacian of psi."""
3     psi = numpy.reshape(psi, shape)
4     # Insert previous lines 3-7
5     return numpy.ravel(Kpsi/2)
```

Here the parameter shape must be defined outside the K-routine.

**Remark 2:** There are many applications where a routine for the lattice laplacian is needed, but the example given here is somewhat artificial. The analytic eigenvalues of  $K$  is easy to find: If shape = (n0, n1, n2),

$$\lambda_{j_0,j_1,j_2} = 2 \sin^2 \left( \frac{\pi j_0}{n_0} \right) + 2 \sin^2 \left( \frac{\pi j_1}{n_1} \right) + 2 \sin^2 \left( \frac{\pi j_2}{n_2} \right), \quad (27)$$

where  $j_0 = 0, 1, \dots, n_0 - 1$  etc.

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).

```
1 def makeHistogram(data, dmin, dmax, nbins):
2     """Return a histogram of the contents in data."""
3     bins = numpy.linspace(dmin, dmax, nbins+1)
4     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  $S$  of eigenvalues.

Since data is assumed to consist of the eigenvalues of  $K$ , we must first convert this information to frequencies. This requires knowledge of  $M$ , which can be given as a parameter to the routine (or a global variable). We take it to be a parameter with a default value, leading to the code

```
1 def makeHistogram(data, fmin, fmax, nbins, M=1):
2     """Return a histogram of the frequency distribution."""
3     freqs = numpy.sqrt(data/M)
4     bins = numpy.linspace(fmin, fmax, nbins+1)
5     return numpy.histogram(freqs, bins=bins)
```

**Remark:** For comparison with f.i. analytic estimates it can be useful to scale the histogram so that it resembles the continuum distribution  $\rho(\omega)$ , normalized to  $\int d\omega \rho(\omega) = 1$ . This is achieved by an addition after line 3 above:

```
freqs /= numpy.sum(freqs) * (bins[1] - bins[0])
```

Here the division by  $\Delta\omega = (\text{bins}[1] - \text{bins}[0])$  takes into account that the relative number  $h(\omega)$  of frequencies in a bin of width  $\Delta\omega$  around  $\omega$  is related to the frequency distribution by  $h(\omega) = \rho(\omega)\Delta\omega$ .

- 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 `fmin`, `fmax` and `nbins`?

We could choose `fmin = 0` and `fmax = numpy.sqrt(10/M)`. An optimal choice of `nbins` may require some amount of experimentation before obtaining a smooth curve, but `nbins = 200` is a reasonable first choice.

**Remark:** In some cases, when f.i. running simulations or finding computing eigenvalues of a very large sparse matrix, it may be very time and memory consuming to produce data for a histogram, while manipulation of the histogram itself will require few resources. In such cases it is better to err on the safe side by covering a larger interval than the expected outcomes, and using many more bins than expected necessary. It is simple to throw away unpopulated bins, and to combine results from several bins into one. It is difficult to go the other way.