

FYS2160 Oblig 1

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Part 1: The Einstein Crystal

In the first part of this exercise we study an ideal crystal, often called the Einstein crystal. We can say that each atom, or particle, the crystal is made up of is in a potential similar to a harmonic oscillator.

a)

We let N describe the number of oscillators and q be the number of energy units in the system. For a system with $N = 3$ oscillators and $q = 3$, all possible microstates are

$\{1, 1, 1\}$

$\{0, 2, 1\}$

$\{0, 1, 2\}$

$\{1, 0, 2\}$

$\{1, 2, 0\}$

$\{2, 0, 1\}$

$\{2, 1, 0\}$

$\{3, 0, 0\}$

$\{0, 3, 0\}$

$\{0, 0, 3\}$

This makes the total number of microstates 10.

b)

The general formula for the number of microstates for N oscillators with q units of energy is:

$$\Omega(N, q) = \binom{q + N - 1}{q} = \frac{(q + N - 1)!}{q!(N - 1)!} \quad (1)$$

Using this equation we can calculate the number of microstates:

$$\Omega(N, q) = \frac{(q + N - 1)!}{q!(N - 1)!} = \frac{(3 + 3 - 1)!}{3!(3 - 1)!} = 10$$

which is the same answer as we found in a).

c)

We now study a system consisting of two subsystems, A and B. A has $N_A = 2$, $q_A = 5$ and B with $N_B = 2$ and $q_B = 1$. All possible microstates are then

$$\{0, 5\}\{1, 0\}$$

$$\{1, 4\}\{1, 0\}$$

$$\{2, 3\}\{1, 0\}$$

$$\{3, 2\}\{1, 0\}$$

$$\{4, 1\}\{1, 0\}$$

$$\{5, 0\}\{1, 0\}$$

$$\{0, 5\}\{0, 1\}$$

$$\{1, 4\}\{0, 1\}$$

$$\{2, 3\}\{0, 1\}$$

$$\{3, 2\}\{0, 1\}$$

$$\{4, 1\}\{0, 1\}$$

$$\{5, 0\}\{0, 1\}$$

when we let the first coloms determine subsystem A and the second determine subsystem B. This gives us a total of 12 states.

d)

If the two subsystems are in thermal contact, the energy q can be transferred between them. That means q_A and q_B can vary as long as the total energy $q = q_A + q_B$ is constant. For $N_A = 2$, $N_B = 2$ and $q = 6$, the possible values of q_A and q_B are

q_A	q_B
6	0
5	1
4	2
3	3
2	4
1	5
0	6

e)

The following program calculates the number of microstates when q_A , N_A and N_B is given. It also finds the probability for each macrostate, assuming all microstates are equally probable.

```
# Calculate the number of microstates as a function of qA, NA and NB

from math import factorial
from numpy import zeros

qTot = 6 # Total energy in the whole system
NA = 2 # Number of oscillators in subsystem A
NB = 2 # Number of oscillators in subsystem B
micro = 0 # Total number of microstates
OmegaTot = zeros(qTot+1)

# Print number of microstates for each macrostate qA:
print 'Number of microstates for each macrostate qA:'
for qA in range(0,qTot+1):
    qB = qTot - qA # Total energy in subsystem B
    OmegaA = factorial(qA + NA - 1)/(factorial(qA)*factorial(NA-1))
    OmegaB = factorial(qB + NB - 1)/(factorial(qB)*factorial(NB-1))
    OmegaTot[qA] = OmegaA * OmegaB
    print ('qA = ' + str(qA) + ': ' +str(OmegaTot[qA]))
    micro += OmegaTot[qA]
print 'The complete number of microstates is ' + str(micro)
print 'If we assume each microstate is equally probable, then the
      probability for each macrostate is'
```

```

# Make sure the sum of all probabilities is 1:
check = 0
for qA in range(0,qTot+1):
    p = OmegaTot[qA]/float(micro)
    check += p
    print ('qA = ' + str(qA) + ': P(qA) = ' + str(p))
print 'The sum of all the probabilities should be 1. We have:'
print check

```

When running this program, the following output is given:

```

'''
Number of microstates for each macrostate qA:
qA = 0: 7.0
qA = 1: 12.0
qA = 2: 15.0
qA = 3: 16.0
qA = 4: 15.0
qA = 5: 12.0
qA = 6: 7.0
The complete number of microstates is 84.0
If we assume each microstate is equally probable, then the probability
    for each macrostate is
qA = 0: P(qA) = 0.0833333333333
qA = 1: P(qA) = 0.142857142857
qA = 2: P(qA) = 0.178571428571
qA = 3: P(qA) = 0.190476190476
qA = 4: P(qA) = 0.178571428571
qA = 5: P(qA) = 0.142857142857
qA = 6: P(qA) = 0.0833333333333
The sum of all the probabilities should be 1. We have:
1.0
'''

```

f)

In subsection c) we do not have thermal contact between the two subsystems. There, we found the total number of microstates to be 12. In e) however, we do have thermal contact and the total number of microstates is raised to be 84, which is seven times greater. Generally we can say that if subsystems are in thermal contact, the total number of microstates must increase compared to when they are not in thermal contact.

g)

The following program plots the probability $P(q_A)$ as a function of q_A for all possible values of q_A . We study the system where $N_A = 50$, $N_B = 50$ and

$q = q_A + q_B = 100$. It also calculates the most probable macrostate and how probable this state is.

```

from numpy import zeros
from math import factorial
import matplotlib.pyplot as plt

NA = 50
NB = 50
qTot = 100
OmegaTot = zeros(qTot+1)
qAvec = zeros(qTot+1)
micro = 0

# Calculate the probability for each macrostate qA
for qA in range(0,qTot+1):
    qB = qTot - qA # Total energy in subsystem B
    OmegaA = factorial(qA + NA - 1)/(factorial(qA)*factorial(NA-1))
    OmegaB = factorial(qB + NB - 1)/(factorial(qB)*factorial(NB-1))
    OmegaTot[qA] = OmegaA * OmegaB
    qAvec[qA] = qA
    micro += OmegaTot[qA]
print 'The total number of microstates is ' + str(micro)

# Make sure the sum of all probabilities is 1:
check = 0
p = zeros(qTot+1)
for qA in range(0,qTot+1):
    p[qA] = float(OmegaTot[qA])/float(micro)
    check += p[qA]
eps = 0.1
if 1-eps < check < 1+eps:
    print 'The sum of all probabilities is ' + str(check)
else:
    print 'Something went wrong. The sum of all probabilities is ' +
        str(check)

# Most probable macrostate:
print 'The most probable macrostate is qA = ' + str(qAvec[p.argmax()]) +
    ', with probability ' + str(max(p))

# Plotting the probability P(qA)
font = {'size' : 18}
plt.rc('font', **font)
plt.plot(qAvec,p,linewidth=2.0)
plt.xlabel('qA')
plt.ylabel('P(qA)')
plt.show()

```

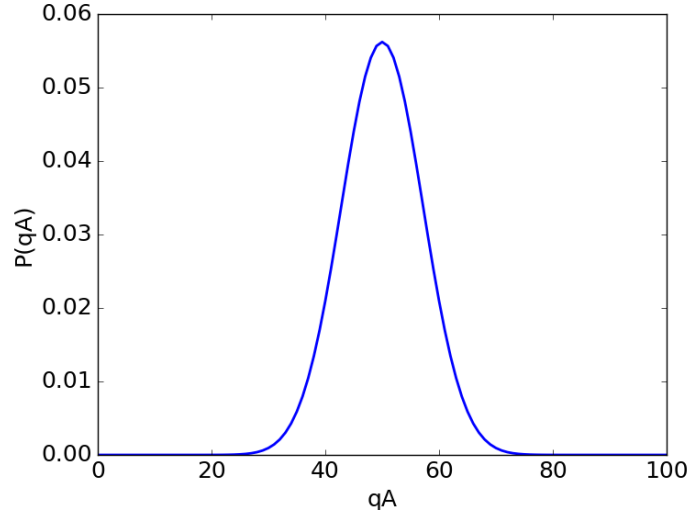


Figure 1: The probability for each macrostate as a function of q_A . We see that the most probable macrostate is 50, and macrostates far from this value is extremely unlikely. For systems with more particles, the spike gets thinner and higher.

The output is then:

```
'''
The total number of microstates is 4.52742573281e+58
The sum of all probabilities is 1.0
The most probable macrostate is qA = 50.0, with probability
0.056207787852
'''
```

As running the program tells us, the most probable macrostate is $q_A = 50$, which has the probability $P(50) = 0.056$. The distribution of probabilities for the different macrostates is plotted in figure 1. The graph clearly shows that the most likely macrostates are those where q_A and q_B are

h)

The multiplicity of the Einstein crystal can be expressed as

$$\Omega(N, q) = \binom{q + N - 1}{q} = \frac{(q + N - 1)!}{q!(N - 1)!} \quad (2)$$

This can be simplified to a smaller number which is easier to represent on a computer by using Sterling's approximation:

$$\ln \Omega(N, q) \approx N \left(\ln \left(\frac{q}{N} \right) + 1 \right) \quad (3)$$

and assuming that $N/q \ll 1$ and $N \gg 1$.

$$\begin{aligned} \Omega(N, q) &= \frac{(q + N - 1)!}{q!(N - 1)!} \\ \ln(\Omega(N, q)) &= \ln \left(\frac{(q + N - 1)!}{q!(N - 1)!} \right) \\ &= \ln(q + N - 1)! - \ln q! - \ln(N - 1)! \\ &= (q + N - 1) \ln(q + N - 1) - (q + N - 1) - (q \ln q - q) \\ &\quad - ((N - 1) \ln(N - 1) - (N - 1)) \\ &= (q + N - 1) \ln(q + N - 1) - q \ln q - (N - 1) \ln(N - 1) \end{aligned}$$

If we then use our approximation $N \gg 1$ we get

$$\begin{aligned} &\approx (q + N) \ln(q + N) - q \ln q - N \ln N \\ &= q \left(\ln \left(\frac{q + N}{q} \right) \right) + N \left(\ln + \left(\frac{q + N}{N} \right) \right) \end{aligned}$$

By further using the approximations $N/q \ll 1$ and $q \gg N$ we can rewrite our equation to

$$= q \left(\ln \left(1 + \frac{N}{q} \right) \right) + N \left(\ln \left(\frac{q}{N} \right) \right)$$

First degree Taylor expansion then gives

$$\begin{aligned} &= q \left(\frac{N}{q} \right) + N \ln \left(\frac{q}{N} \right) \\ &= N + N \ln \left(\frac{q}{N} \right) \\ &= N \left(\ln \left(\frac{q}{N} \right) + 1 \right) \end{aligned}$$

which is the expression we wanted.

i)

The entropy of an isolated system with given number of particles N , energy E in a confined volume V is

$$S = k \ln \Omega(N, V, E). \quad (4)$$

As we in this exercise do not study a changing volume and use energy E given by ϵq , the entropy of our Einstein crystal is given as

$$S = k \ln \Omega(N, V, E) = k \ln \Omega(N, q) \approx kN \left(\ln \left(\frac{q}{N} \right) + 1 \right)$$

when we use the approximation we found in part h).

j)

The inverse of the temperature is given as

$$\begin{aligned}
\frac{1}{T} &= \left(\frac{\partial S}{\partial E} \right)_{N,V} \\
&= \frac{1}{\epsilon} \left(\frac{\partial S}{\partial q} \right)_N \\
&= \frac{\partial}{\partial q} \frac{1}{\epsilon} kN \left(\ln \left(\frac{q}{N} + 1 \right) \right) \\
&= \frac{kN}{\epsilon} \frac{\partial}{\partial q} \left(\ln \left(\frac{q}{N} + 1 \right) \right) \\
&= \frac{kn}{\epsilon q}
\end{aligned}$$

which means the temperature is given by

$$T = \frac{\epsilon q}{kN}.$$

By remembering that $\epsilon q = E$, we find our known expression

$$E = NkT$$

which is a good sign.

Part 2: The Spin System

In this second part we will study a spin system. The system is made of particles which have spin either up or down. As our only interest in these particles are about their spin, we will refer to them as spins.

k)

As each particle has spin either $+1$ or -1 , we can enumerate each microsystem by defining each spin as either $+1$ or -1 . An example would be

$$\{1, 1, -1, 1, -1, -1, -1, 1\}$$

which is a random microstate for an $N = 8$ system.

As each particle can have 2 different states, we have a binomial distribution, and an N -spin system can therefore have 2^N microstates.

l)

When we define s_+ as the number of spins with value $+1$, S_- as the number of spins with value -1 and $2s = S_+ + S_-$ is the net spin, an expression for the total energy E is then

$$E(s) = -2s\mu B.$$

m)

This program generates $M = 10000$ microstates for an $N = 50$ system randomly. It also plots the energies E of the system. We have assumed that all microstates are equally likely.

```
from random import randint
from numpy import zeros, histogram, linspace
import matplotlib.pyplot as plt

N = 50
M = 10000
M_values = zeros(M)

# Create random integers and make s = +/- 1
# Store final values in array M_values
print "Looping..."
for j in range(0,M):
    i = 0
    s = 0
    while i < N+1:
        rand = randint(0,1)
        i += 1
        if rand == 1:
            s += 1
        elif rand == 0:
            s -= 1
        else:
            print 'Error: random integer not 1 or 0'
    M_values[j] = s
print 'Done!' # It might take some time to run
M_values = - M_values
# Fun loop to check the average value:
sums = 0
for i in range(0,M):
    sums += M_values[i]
print "Average value: " + str(sums/M)

# Making a histogram
b = linspace(-29,30,60)-0.5 # Make it beautiful
font = {'size' : 18}
plt.rc('font', **font)
plt.hist(M_values, bins = b)
plt.xlabel('Energy [ $\mu$ B]')
plt.ylabel('Counts')
plt.show()
```

The energies are plotted in the histogram presented in figure 2. The figure shows that microstates close to 0 (equilibrium state) are most common, and hence also most probable. The data is generated by adding or subtracting 1,

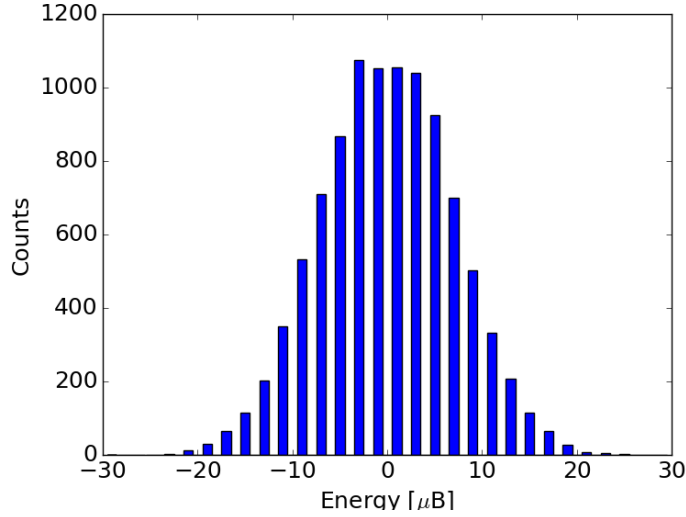


Figure 2: Histogram of the energies found in m). This is a run with $M = 10000$ microstates. It is clear that the middle values around zero are the most probable as they are the microstates in equilibrium state. For this specific run, we found the middle value of all states to be -0.0238 , which is close to zero.

according to the state of the spins in the system. As we for every macrosystem do this N times, we are bound to get energies that are either even or odd, depending on the value of N .

n)

The multiplicity of a macrostate S_+ is given by

$$\Omega(N, S_+) = \binom{N}{S_+} = \frac{N!}{S_+!(N - S_+)!} = \frac{N!}{S_+!S_-!}.$$

o)

By using $2s = S_+ - S_-$ and $N = S_+ + S_-$ we can insert $S_+ = N/2 + s$ and $S_- = N/2 - s$ into our answer in n) to find that

$$\Omega(N, s) = \frac{N!}{(\frac{N}{2} + s)!(\frac{N}{2} - s)!}.$$

p)

In the lecture notes under chapter 4.5 "The binomial distribution" equation 4.88 says

$$P(N, n) = \frac{N!}{(\frac{N}{2} - n)! (\frac{N}{2} + n)!} 2^{-N}$$

which is the same as in our case. The only difference is that this equation finds the probability P , instead of the multiplicity Ω . Luckily, the probability is just the multiplicity divided by the total number of outcomes, which here is 2^N . This means that our equation found in o) is the same as the one presented in the lecture notes. By mapping our problem onto the one found in the lecture notes, we can use the solution found in equation 4.91:

$$P(N, n) = C(N) e^{-\frac{u^2}{n/2}} = C(N) e^{-\frac{2u^2}{N}}$$

Here, the factor 2^{-N} is hidden in $C(N)$. As $C(N)$ is a constant (for constant N), we can use our constant $\Omega(N, 0)$ and find

$$\Omega(N, S) = \Omega(N, 0) e^{-\frac{2s^2}{N}}$$

q)

The analytical result from p) is plotted in figure 3 together with the numerically generated histogram. We can see that they fit well together and that our analytical approach seems right. To make the overlap even better, we need a higher value of N .

r)

We now go back to using the exact multiplicity

$$\Omega(N, S_+) = \frac{N!}{S_+! S_-!}$$

The entropy is given as $S = k \ln \Omega$, where k is Boltzmann's constant. The entropy for our spin system is then

$$\begin{aligned} S &= k \ln \Omega \\ &= k \ln \frac{N!}{S_+! S_-!} \\ &= k(\ln N! - \ln S_+! - \ln S_-!) \end{aligned}$$

Numerically, this might be difficult to calculate for large values of N . For $N = 50$, as we have used in this exercise, it works fine. For very large N (realistic systems), we need to use approximations, such as Sterling's approximation.

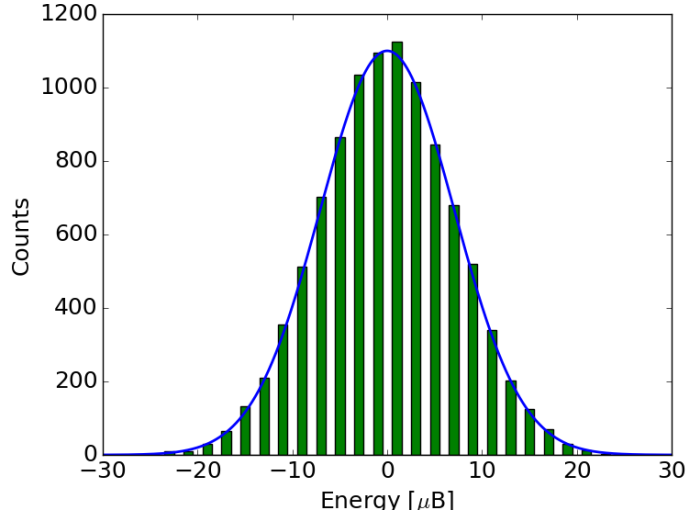


Figure 3: The analytical probability (scaled to match the numerical result) plotted with the histogram of our results. We see that the outline seems to match the histogram, although we have not taken into considerations even and odd numbers in our plot of the analytical result.

s)

The temperature is given as

$$\frac{1}{T} = \frac{\partial S}{\partial U} = \frac{\partial S}{\partial S_+} \frac{\partial S_+}{\partial U}$$

In l) we found the energy to be $U = -2s\mu B$. This gives us an expression for S_+ and its derivative

$$S_+ = \frac{N}{2} - \frac{U}{2\mu B}$$

$$\Rightarrow \frac{\partial S_+}{\partial U} = -\frac{1}{2\mu B}$$

Using the expression for the entropy found in r), the first derivative of S is

$$\begin{aligned}
\frac{\partial S}{\partial S_+} &= \frac{\partial}{\partial S_+} k(\ln N! - \ln S_+! - \ln(N - S_+)!) \\
&= -k \left[\frac{\partial}{\partial S_+} \ln S_+! + \frac{\partial}{\partial S_+} \ln(N - S_+)! \right] \\
&\approx -k \left[\frac{\partial}{\partial S_+} (S_+ \ln S_+ - S_+) + \frac{\partial}{\partial S_+} ((N - S_+) \ln(N - S_+) - (N - S_+)) \right] \\
&= -k \left[1 \cdot \ln S_+ + S_+ \frac{1}{S_+} - 1 + \frac{\partial}{\partial S_+} N \ln(N - S_+) - \frac{\partial}{\partial S_+} \ln(N - S_+) - \frac{\partial}{\partial S_+} (N - S_+) \right] \\
&= -k \left[\ln S_+ + \frac{N}{N - S_+} (-1) - 1 \cdot \ln(N - S_+) + S_+ \frac{1}{N - S_+} (-1) + 1 \right] \\
&= -k \left[\ln S_+ - \frac{N}{N - S_+} - \ln(N - S_+) + \frac{S_+}{N - S_+} + 1 \right] \\
&= -k \left[\ln \left(\frac{S_+}{N - S_+} \right) - \frac{N - S_+}{N - S_+} + 1 \right] \\
&= -k \ln \left(\frac{S_+}{N - S_+} \right)
\end{aligned}$$

where we in the third step have used Sterling's approximation. The inverse of the temperature is then given as

$$\frac{1}{T} = \frac{k}{2\mu B} \ln \left(\frac{S_+}{N - S_+} \right)$$

which means that the temperature is

$$T = \frac{2\mu B}{k} \ln \left(\frac{N - S_+}{S_+} \right).$$