

# Mandatory assignment 1

## FYS2160

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### Task 1

#### 1.1

The internal energy of a diatomic ideal gas at a temperature  $T$  is given by

$$U = \frac{f}{2}NkT. \quad (1)$$

Since the degrees of freedom for our system is translation, rotation, but not vibration, we have  $3 + 2$  degrees of freedom. This gives us that the internal energy of our system is

$$U = \frac{5}{2}NkT. \quad (2)$$

When we have a constant volume there is no work being done. This means that, from the first law, that we have  $\Delta U = Q$ . From this we can use the definition of heat capacity to find

$$\begin{aligned} C_v &= \left( \frac{\partial Q}{\partial T} \right)_v \\ &= \left( \frac{\partial U}{\partial T} \right)_v \\ &= \frac{5}{2}Nk \left( \frac{\partial T}{\partial T} \right)_v \\ &= \frac{5}{2}Nk \end{aligned}$$

Which then is the heat capacity for our system with a constant volume.

#### 1.2

We are now studying a cycle in phase space (pressure vs volume) shown in figure [1 on the following page](#). In this figure the arrow show the direction of change for each part of the cycle, and gives us the values we will use for pressure and volume, as well as the indexes we will use for each cycle.

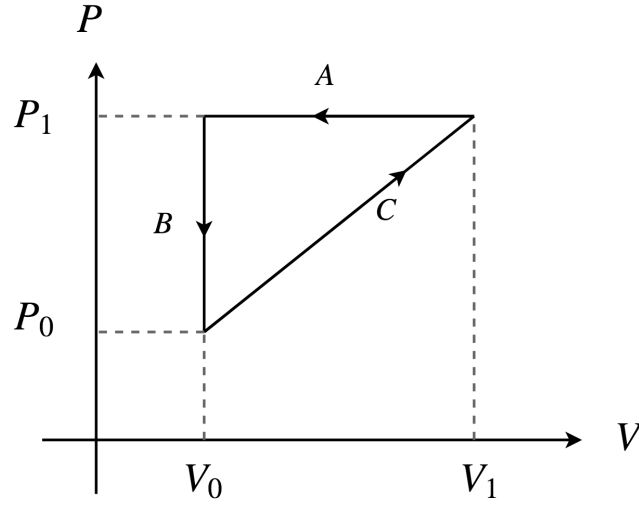


Figure 1: Phase-space diagram for the cycle we will discuss in this exercise. The arrows indicate the direction for each part of the cycle.

We are not interested in finding the change in the internal energy of the system  $\Delta U$ . We do this by the following calculations

$$\begin{aligned}
 U &= \frac{5}{2} NkT \\
 \Delta U &= \frac{5}{2} Nk\Delta T \quad (N \text{ and } k \text{ are constant}) \\
 NkT &= PV \quad (\text{ideal gas law}) \\
 T &= \frac{PV}{NkT} \quad (\text{rearranging}) \\
 \Delta U &= \frac{5}{2} Nk\Delta \left( \frac{PV}{NkT} \right) \quad (\text{Setting in for } T) \\
 &= \frac{5}{2} \Delta(PV) \quad (N \text{ and } k \text{ are constant})
 \end{aligned}$$

Now we have an expression for the change in internal energy. For each cycle can we then put in for the change in  $P$  and  $V$  to find the change in internal energy.

For cycle  $A$  the pressure is constant, while the volume changes, we then have

$$\Delta U_A = \frac{5}{2} P_1 (V_0 - V_1). \quad (3)$$

For cycle  $B$  the volume is constant, while the pressure changes, we then have

$$\Delta U_B = \frac{5}{2} V_0 (P_0 - P_1). \quad (4)$$

For cycle  $C$  both the volume and the pressure changes, we then have

$$\Delta U_C = \frac{5}{2} (P_1 V_1 - P_0 V_0). \quad (5)$$

### 1.3

To compute the work done for each part of the cycle we will use

$$W = - \int_{V_a}^{V_b} P \, dV \quad (6)$$

For the cycle we will call the largest volume for  $V_1$  and the smallest volume for  $V_0$ . The largest pressure for  $P_1$  and the smallest pressure from  $P_0$ . We call this an isobaric gas expansion.

For part  $A$  of the cycle the volume changes while the pressure is constant. We can therefore take the pressure outside of the integral. The volume goes from  $V_1$  to  $V_0$ , and the integral limits will therefor be in that order, we get

$$\begin{aligned} W_A &= -P_1 \int_{V_1}^{V_0} dV \\ &= -P_1 (V_0 - V_1) \\ &= P_1 (V_1 - V_0) \end{aligned}$$

And we have the expression for  $W_A$ , and since  $V_1 > V_0$  the work is positive.

For part  $B$  of the cycle we have a constant volume, while the pressure changes. Since the volume is constant, the limits for the integral are the same,  $V_0$ . We then have

$$W_B = - \int_{V_0}^{V_0} P \, dV = 0$$

Since we are integrating over a change of zero, the integral has to be zero, independent of what  $P$  is. There is therefor no work done when the pressure changes at a constant volume. We call this an Isocoric «gas expansion».

For part  $C$  of the cycle we have a change in both pressure and volume. We will then divide the area into two parts. A rectangle at the bottom, and a triangle on top. The rectangle has a *height* of  $P_0$  and a *width* of  $(V_1 - V_0)$ . This gives us an area of  $P_0 (V_1 - V_0)$ . For the triangle we have the same *width*,  $V_1 - V_0$ , and a *height* of  $(P_1 - P_0)$ . This gives us an area which is equal to half the product of the *height* and *width*, which is  $(V_1 - V_0) (P_1 - P_0) / 2$ . This gives us a total area of

$$\begin{aligned} A &= \frac{1}{2} (V_1 - V_0) (P_1 - P_0) + P_0 (V_1 - V_0) \\ &= (V_1 - V_0) \left( \frac{1}{2} (P_1 - P_0) + P_0 \right) \\ &= \frac{V_1 - V_0}{2} (P_1 + P_0) \end{aligned}$$

Which is then the area of cycle  $C$ . Since the work done by the gas is the negative area in the  $PV$ -diagram, we get the the work done on cycle  $C$  is equal to

$$W_C = - \frac{V_1 - V_0}{2} (P_1 + P_0). \quad (7)$$

### 1.4

To find the heat change along each path we will use the first law of thermodynamics

$$\Delta U = Q + W. \quad (8)$$

This can be solved for  $Q$  which gives us

$$Q = \Delta U - W. \quad (9)$$

From this equation, since we have both  $\Delta U$  and  $W$  for each cycle, we can derive the heat exchange for each cycle.

For cycle  $A$  we have

$$\begin{aligned} Q_A &= \Delta U_A - W_A \\ &= \frac{5}{2} P_1 (V_0 - V_1) - P_1 (V_1 - V_0) \\ &= P_1 \left( V_0 (5/2 + 2/2) + V_1 (5/2 - 2/2) \right) \\ &= \frac{7P_1}{2} (V_0 - V_1) \end{aligned}$$

We can then do the same for cycle  $B$

$$\begin{aligned} Q_B &= \Delta U_B - W_B \\ &= \frac{5}{2} V_0 (P_0 - P_1) - 0 \\ &= \frac{5}{2} V_0 (P_0 - P_1) \end{aligned}$$

We can then do the same for cycle  $C$

$$\begin{aligned} Q_C &= \Delta U_C - W_C \\ &= \frac{5}{2} (P_1 V_1 - P_0 V_0) + \frac{V_1 - V_0}{2} (P_1 + P_0) \\ &= P_1 \left( \frac{5}{2} V_1 + \frac{V_1 - V_0}{2} \right) + P_0 \left( \frac{-5V_0}{2} + \frac{V_1 - V_0}{2} \right) \\ &= P_1 \left( 3V_1 - \frac{V_0}{2} \right) + P_0 \left( -3V_0 + \frac{V_1}{2} \right) \end{aligned}$$

Which is then the expression for the heat flow in cycle  $C$ .

## 1.5

We now want to find the sign of  $\Delta U$ ,  $W$  and  $Q$  for each part of the cycle. We will therefor go through each phase and describe what is happening, and what the resulting sign should be for each property, based on the expressions we have found.

For cycle  $A$  we found that the change in internal energy was given by  $\frac{5}{2} P_1 (V_0 - V_1)$ , since  $V_0 < V_1$  this is a negative number. The total internal energy of the system decreases.

The work done, on the other hand, is positive and described as  $P_1 (V_1 - V_0)$ . This quantity is positive since  $V_1 > V_0$ . This means that the outside is doing work pushing inwards and reducing the volume of the box.

The heat flow during this part of the cycle is given by  $\frac{7P_1}{2} (V_0 - V_1)$ . Since  $V_0 < V_1$  this is a

negative number. The system is therefor cooling down as the outside is doing work, to be able to have the same pressure. This cycle of energy manages to cool down the system by manipulating the pressure, while holding the volume constant.

For cycle  $B$  we have that the total change in internal energy of the system is  $\frac{5}{2}V_0(P_0 - P_1)$ . Since  $P_0 < P_1$  this change in internal energy is negative. We found that the work done during this process was zero, and is therefore neither positive nor negative. The heat flow for this cycle is given by  $\frac{5}{2}V_0(P_0 - P_1)$ . Since  $P_0 < P_1$  we have that the gas is exerting a negative work, which means that the gas is doing work, and loosing energy. The heat flow during the part of the cycle is  $\frac{5}{2}V_0(P_0 - P_1)$ . Since  $P_1 > P_0$  the heat flow is negative, the system is giving away heat to the surroundings. Therefore we have a system that is giving away all of it's energy through heat with the surroundings to decrease the pressure.

For cycle  $C$  we found that the change in internal energy was given by  $\frac{5}{2}(P_1V_1 - P_0V_0)$ . Since both  $P_1$  and  $V_1$  are larger than  $P_0$  and  $V_0$  respectively, their product has to be larger as well. Therefor the total internal energy of the system during cycle  $C$  increases.

The work during this cycle is  $-\frac{V_1 - V_0}{2}(P_1 + P_0)$ . Since  $V_1 > V_0$  we have that  $V_1 - V_0$  is a positive number. Since the pressure has to be positive, the work done during this cycle is negative. This means that the gas is doing work, and losing energy in the process.

The heat flow during the cycle is given by  $P_1\left(3V_1 - \frac{V_0}{2}\right) + P_0\left(-3V_0 + \frac{V_1}{2}\right)$ . It is harder to see of this quantity is larger or smaller than one. We can see that if  $V_0$  is very close to  $V_1$ , and  $P_0$  is very close to  $P_1$ , we will have a negative heat flow. On the other hand, if  $V_1$  and  $P_1$  are much larger than  $V_0$  and  $P_0$ , the heat is positive. Let's try to find a more clear expression for when these values are positive and negative by introducing proportionality constants;  $P_1 = aP_0$  and  $V_1 = bV_0$ , where both  $a$  and  $b > 1$ . We can then do the following calculations.

$$\begin{aligned} Q_C &= P_1\left(3V_1 - \frac{V_0}{2}\right) + P_0\left(-3V_0 + \frac{V_1}{2}\right) \\ &= aP_0(3bV_0 - V_0/2) + P_0(-3V_0 + bV_0/2) \\ &= V_0P_0(3ab - a/2 + b/2 - 3) \end{aligned}$$

We can then ask the question whether  $Q_C > 0$  or not.

We known that this since the gas is doing work, but the energy is increasing, the heat  $Q$  has to be positive for the gas to gain energy.

Adding all parts of the cycle, for each quantity, gives us

$$\begin{aligned} \Delta U_t &= \Delta U_A + \Delta U_B + \Delta U_C = 0 \\ W_t &= W_A + W_B + W_C = \frac{1}{2}(V_1 - V_0)(P_1 - P_0) > 0 \\ Q_t &= Q_A + Q_B + Q_C = \frac{1}{2}(V_0 - V_1)(P_1 - P_0) < 0 \end{aligned}$$

We know that  $Q_t$  is negative since the total change in energy is zero, and the work done is positive. The system is trading work for heat. The outside does work on the gas, and in return the outside increases it's temperature. This might be use-full for an oven, or another heating apparatus.

## Task 2

### 2.1

For a system of  $N$  independent spins, with two possible states; spin up  $s_{\uparrow} = 1$  and spin down  $s_{\downarrow} = -1$ . This gives us a total amount of micro states equal to

$$\Omega_t = 2^N. \quad (10)$$

### 2.2

To find the total spin  $S$  we have to sum over all values of  $s_i$

$$S = \sum_{i=1}^N s_i. \quad (11)$$

This is equal to the difference between number of spins pointing up  $s_{\uparrow}$  and number of spins pointing down  $s_{\downarrow}$

$$S = s_{\uparrow} - s_{\downarrow}. \quad (12)$$

Since we know that all  $N$  particles has to have either spin up or down, we can write  $s_{\uparrow} = N - s_{\downarrow}$ . Putting this into the equation we find

$$S = N - 2s_{\downarrow}. \quad (13)$$

### 2.3

We now want generate  $M$  different microstates with  $N$  spins either pointing up or down, with equal probability. We will do this numerically, and for each  $M$  we will find the the total spin  $S$ . To do this numerically we will use randomly generate numbers and find the the total spin using equation (13). In figure 2 on the next page we see the total spin  $S$  for each microstate generated. This figure does not give us that much information about the distribution of total spin  $S$ . The same data is therefore plotted in a histogram in figure 3 on the following page. To find the Gaussian distribution in the same figure we calculated the mean  $\mu$ , and the standard deviation  $\sigma$  for the measurements, and use these values in the definition of the Gaussian distribution

$$f(S) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(S-\mu)^2}{2\sigma^2}}. \quad (14)$$

As we can see in figure 3 on the next page the histogram over total spin  $S$  follows a Gaussian distribution.

### 2.4

The multiplicity for  $N$  spins where  $s_{\downarrow}$  is given by

$$\Omega(N, s_{\downarrow}) = \frac{N!}{s_{\downarrow}! (N - s_{\downarrow})!}. \quad (15)$$

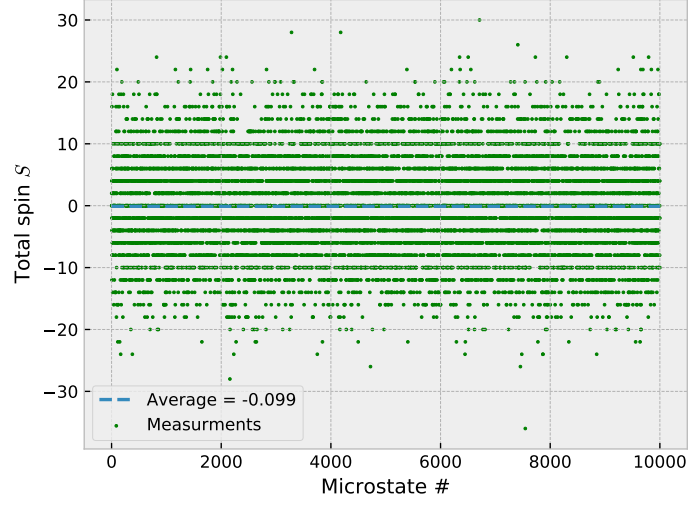


Figure 2: Total spin  $S$  for each microstate generated randomly on computer for  $M = 10^4$  and  $N = 60$  using [1 on page 11](#).

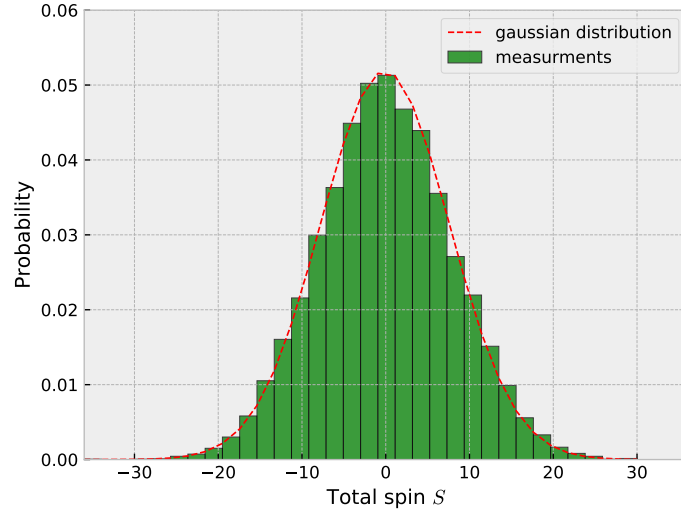


Figure 3: Histogram over total spin  $S$  for  $10^4$  microstates generated randomly on computer for  $N = 60$  using [1 on page 11](#).

We want this expression as a function of the total spin  $S$  instead. To find this we use [\(13\)](#) to find

$$\begin{aligned}
 S &= N - 2s_{\downarrow} \\
 S - N &= -2s_{\downarrow} \\
 \frac{N - S}{2} &= s_{\downarrow}
 \end{aligned}$$

By inserting this in equation (15) we find

$$\begin{aligned}\Omega(N, S) &= \frac{N!}{\left(\frac{N-S}{2}\right)! \left(N - \frac{N-S}{2}\right)!} \\ &= \frac{N!}{\left(\frac{N-S}{2}\right)! \left(\frac{2N}{2} - \frac{N-S}{2}\right)!}\end{aligned}$$

Which gives us

$$\Omega(N, S) = \frac{N!}{\left(\frac{N-S}{2}\right)! \left(\frac{N+S}{2}\right)!} \quad (16)$$

## 2.5

Since working with factorials can lead to very large numbers, and trouble numerically, we will use Stirlings Approximation for factorials

$$\ln N! \approx N \ln N - N \quad (17)$$

on the multiplicity of our system of  $N$  spins (16). Using properties of the logarithm and Taylor approximations we can simplify (16) by a great deal, lets begin.

$$\begin{aligned}\ln \Omega &= \ln \left( \frac{N!}{\left(\frac{N-S}{2}\right)! \left(\frac{N+S}{2}\right)!} \right) \\ &= \ln N! - \ln \left( \left(\frac{N-S}{2}\right)! \right) - \ln \left( \left(\frac{N+S}{2}\right)! \right) \\ &\approx N \ln N - N + \frac{N+S}{2} + \frac{N-S}{2} - \left(\frac{N-S}{2}\right) \ln \left(\frac{N-S}{2}\right) - \left(\frac{N+S}{2}\right) \ln \left(\frac{N+S}{2}\right) \\ &= N \ln N - N + N - \left(\frac{N-S}{2}\right) \ln \left(\frac{N}{2} \left(1 - \frac{S}{N}\right)\right) - \left(\frac{N+S}{2}\right) \ln \left(\frac{N}{2} \left(1 + \frac{S}{N}\right)\right) \\ &= N \ln N - \left(\frac{N-S}{2}\right) \left( \ln \frac{N}{2} + \ln \left(1 - \frac{S}{N}\right) \right) - \left(\frac{N+S}{2}\right) \left( \ln \frac{N}{2} + \ln \left(1 + \frac{S}{N}\right) \right)\end{aligned}$$

On our last term here we will use the Taylor expansion of  $\ln 1 + x$  which is approximately equal to  $x - x^2/2$  when  $x$  is small. We will therefore assume that  $S/N$  as a very small number. This is a very safe approximation when looking at systems in thermal equilibrium. The small fluctuations around  $S = 0$  is absurdly small compared to the total number of spins  $N$ . This is even more true



for larger systems when  $N > 10^{23}$ . Lets use this taylor expansion and see what we find

$$\begin{aligned}
\ln \Omega &= N \ln N - \left( \frac{N-S}{2} \right) \left( \ln \frac{N}{2} + \frac{S}{N} - \frac{S^2}{N^2} \right) - \left( \frac{N+S}{2} \right) \left( \ln \frac{N}{2} - \frac{S}{N} - \frac{S^2}{N^2} \right) \\
&= N \ln N - \frac{N}{2} \left( 2 \ln \frac{N}{2} - \frac{S^2}{N^2} \right) + \frac{S}{2} \left( -\frac{2S}{N} \right) \\
&= N \ln N - N \ln \frac{N}{2} + \frac{S^2}{2N} - \frac{S^2}{N} \\
&= N \ln N - N (\ln N - \ln 2) - \frac{S^2}{2N} \\
&= N \ln N - N \ln N + N \ln 2 - \frac{S^2}{2N} \\
&= N \ln 2 - \frac{S^2}{2N}
\end{aligned}$$

The expression has become a lot more simple to work with. Since this is the logarithm of  $\Omega$  we will now find  $\Omega$

$$\begin{aligned}
\ln \Omega &= N \ln 2 - \frac{S^2}{2N} \\
\Omega &= e^{N \ln 2 - \frac{S^2}{2N}} \\
&= e^{N \ln 2} e^{-\frac{S^2}{2N}}
\end{aligned}$$

Which can be written as

$$\Omega(N, S) = 2^N e^{-\frac{S^2}{2N}} \quad (18)$$

To arrive at this answer have used some assumptions. For using Stirling's Approximation we have to assume that  $N$  is large. By large we mean bigger than around 15, which is easy to achieve in thermal systems. When using the Taylor expansion of  $\ln(1+x)$  we assumed that  $S/N$  is a small number. For systems in thermal equilibrium this is true, since in these systems the fluctuations around  $S=0$  is incredibly small compared to the total number of spinners.

The maximum multiplicity is at equilibrium, which in our case is  $S=0$ . By using  $S=0$  in equation (16) we find

$$\Omega(N, S) = \frac{N!}{\frac{N}{2}! \frac{N}{2}!} \quad (19)$$

Using Stirling's approximation

$$N! \approx N^N e^{-N} \sqrt{2\pi N}, \quad (20)$$

we can write the state of maximum multiplicity as

$$\begin{aligned}
\Omega(N, S=0) &= \frac{N^N e^{-N} \sqrt{2\pi N}}{\left( \left( \frac{N}{2} \right)^{N/2} e^{-N/2 \sqrt{\pi N}} \right)^2} \\
&= \frac{N^N e^{-N} \sqrt{2\pi N}}{\left( \frac{N}{2} \right)^N e^{-N \pi N}} \\
&= 2^N \sqrt{\frac{2}{\pi N}}
\end{aligned}$$

The factor  $\sqrt{2/\pi N}$  was ignored when using Stirling's approximation for the logarithm of a factorial, when we calculated the multiplicity as a function of total spin  $S$ . For the answer we got the factor  $2^N$  is much larger, and we can safely ignore the factor  $\sqrt{2/\pi N}$ . This is true up until the point where you calculate the probability for macrostate  $S$ . When you divide by  $2^N$  you need the factor  $\sqrt{2/\pi N}$  to normalize the answer. Therefore it is more correct to include the factor  $\sqrt{2/\pi N}$  when showing the multiplicity for each macrostate, but can safely be ignored when we want to calculate the multiplicity for each macrostate. This means that we can write the multiplicity as

$$\Omega(N, S) = \sqrt{\frac{2}{\pi N}} 2^N e^{-\frac{S^2}{2N}} = \Omega_{max} e^{-\frac{S^2}{2N}} \quad (21)$$

## 2.6

We found an expression for the multiplicity of our system as a function of the total spin  $S$  (18). We can compare this equation to the simulation done earlier, and see if the theory fits the simulation. This is shown in figure 4 on the following page. As we can see, the analytical expression for the distribution which we have found fits perfectly. The analytical work we did is in compliance with the numerical simulation.

## 2.7

The entropy of a system is equal to the logarithm of the multiplicity function, times a constant. For our case (21) this will result in

$$\text{entropy} = k_b \left[ N \ln 2 - \frac{S^2}{2N} + \ln(2\pi N) \right] \quad (22)$$

We find that the largest entropy is with  $S = 0$ , as we would assume, since it has the largest multiplicity.

The entropy as a function of total spin  $S$  for  $N = 60$  is shown in figure 5 on the next page.

The entropy as a function of both  $N$  and  $S$  is shown in figure 6 on page 12. As we can see from the figure, for every possible value of  $N$  the state with the largest entropy is for  $S = 0$ . As we would assume, since it is the state with the largest multiplicity.

As you see from the figure it makes no sense that a system of, for example,  $N = 20$  spinners, can have more than 20 total spin  $S$ , and that is true. These had to be included for the plot to work, but should be ignored since they have no physical meaning. Since they had no physical meaning they were set to zero in the plot.

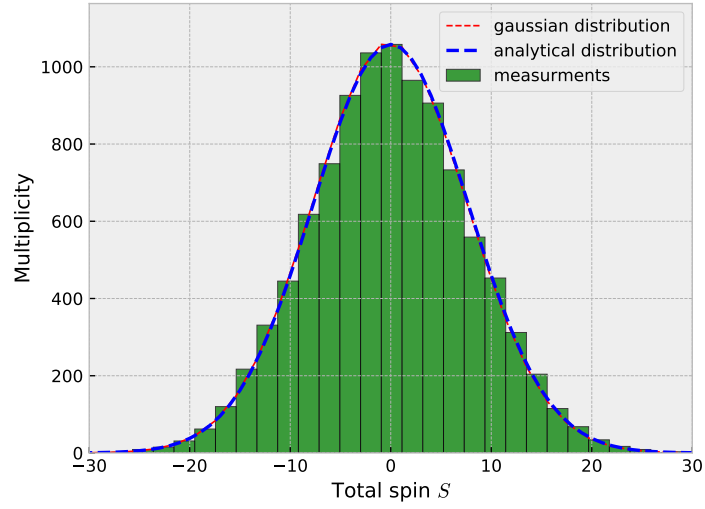


Figure 4: Histogram over total spin  $S$  for  $10^4$  microstates generated randomly on computer for  $N = 60$  using 1. This is shown side by side with prediction from equation (18).

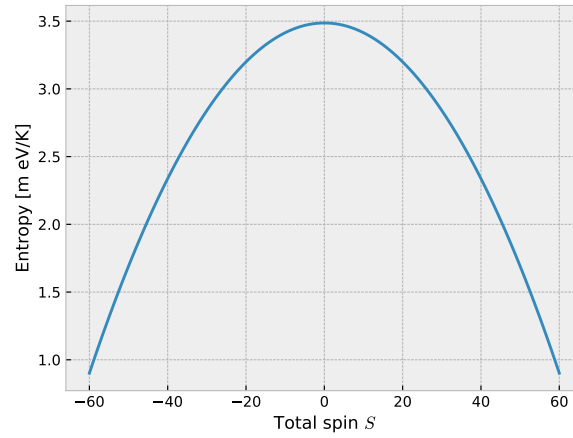


Figure 5: Entropy as a function of total spin  $S$  for  $N = 60$ .

## Plotting bins

Listing 1: Code for simulating random spins and plotting results vs theory

```
1 import numpy as np
2 import matplotlib.pyplot as plt
3 import matplotlib.mlab as mlab
4 import seaborn as sns
```

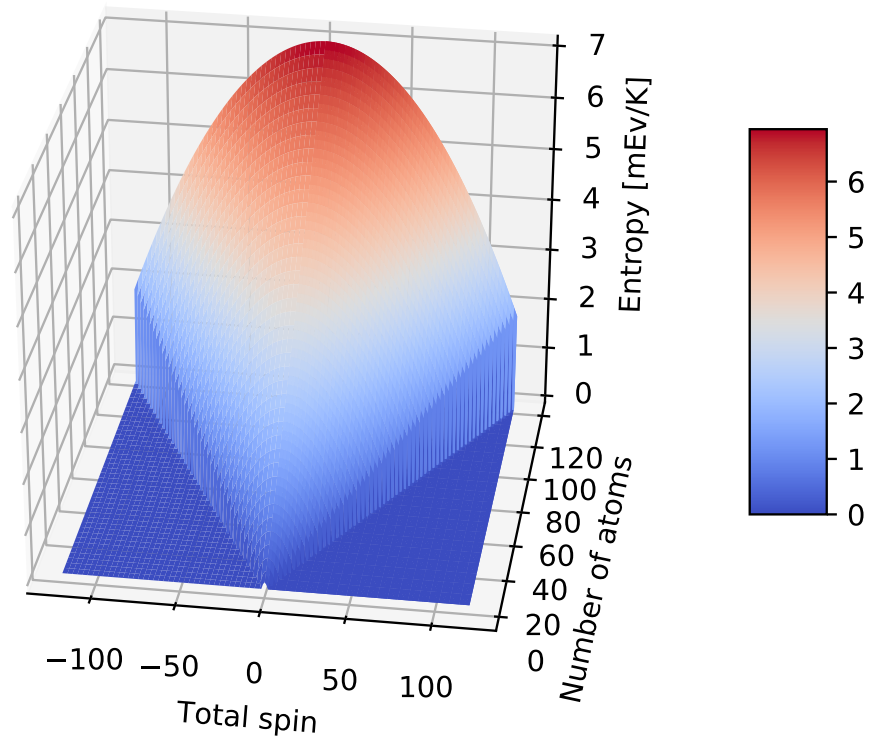


Figure 6: Entropy as a function of number of spinners and total spin.

```

5 plt.style.use("bmh")
6 sns.color_palette("hls", 1)
7
8 def find_total_spin(M, number):
9     array = number - 2*np.sum(np.random.randint(0, 2, (M, number)), axis=1)
10    return array
11
12 def analytical_distribution(S, N):
13     return np.exp(-S**2.0/(2.0*N))*np.sqrt(2.0/(np.pi*N))
14
15 M = int(1e4)
16 N = int(60)
17 M_array = np.linspace(1, M, M)
18 answer = find_total_spin(M, N)
19
20 plt.scatter(np.linspace(1, M, M), answer, s=2.5, c="green", label="Measurments")
21 plt.xlabel(r"Microstate #")
22 plt.ylabel(r"Total spin $$$")
23 plt.plot(M_array, np.mean(answer)*np.ones(M), "--", label=r"Average = %4.3f" % (np.←
    mean(answer)))
24 plt.legend(loc="best")

```

```

25 plt.savefig("figure/task_2.3.pdf")
26 plt.show()
27
28 bin_array = np.arange(int(min(answer)), int(max(answer)))-0.5
29 number_of_bins = max(answer)-min(answer)
30
31 n, bins, patches = plt.hist(answer, int(number_of_bins/2.0)-1, normed=1, facecolor='↵
    green', alpha=0.75, edgecolor = 'black', label="measurments")
32 mu, sigma = np.mean(answer), np.std(answer)
33 y = mlab.normpdf(bins, mu, sigma)
34 l = plt.plot(bins, y, 'r—', linewidth=1, label="gaussian distribution")
35
36 plt.ylabel(r"Probability")
37 plt.xlabel(r"Total spin $$$")
38 plt.axis([-np.max(abs(answer)), np.max(abs(answer)), 0, 0.06])
39 plt.legend(loc="best")
40 plt.savefig("figure/histogram.pdf")
41 plt.show()
42
43 n, bins, patches = plt.hist(answer, int((int(max(answer))-min(answer))/2.0)-1, ↵
    facecolor='green', alpha=0.75, edgecolor = 'black', label="measurments")
44
45 mu = np.mean(answer)
46 sigma = np.std(answer)
47 y = mlab.normpdf(bins, mu, sigma)*np.count_nonzero(answer==0)/max(mlab.normpdf(bins, ↵
    mu, sigma))
48 plt.plot(bins, y, 'r—', linewidth=1, label="gaussian distribution")
49
50 S_array = np.linspace(-N, N, N*2+1)
51 analytical = analytical_distribution(S_array, N=60)
52 plt.plot(S_array, analytical*(max(analytical)*np.count_nonzero(answer==0), "b—", ↵
    label="analytical distribution")
53
54 plt.ylabel(r"Multiplicity")
55 plt.xlabel(r"Total spin $$$")
56 plt.axis([-30, 30, 0, 1.1*np.count_nonzero(answer==0)])
57 plt.legend(loc="best")
58 plt.savefig("figure/task_2.6.pdf")
59 plt.show()

```

## Plotting entropy

Listing 2: Code for calculating the entropy as a function of  $S$  and  $N$  and plotting the result.  
language

```

1 import numpy as np
2 import matplotlib.pyplot as plt
3 import scipy.misc as scm
4 from mpl_toolkits.mplot3d import Axes3D
5 from matplotlib import cm
6 from matplotlib.ticker import LinearLocator, FormatStrFormatter
7 import seaborn as sns
8 plt.style.use("bmh")
9 sns.color_palette("hls", 1)
10
11 def get_entropy(N, S):
12     kb = 8.6173303*1e-5 #Ev/K
13     return kb*(np.log(2)*N-S**2/(2*N)+np.log(np.sqrt(2*np.pi/N)))
14
15 number_of_particles = 60
16 number_of_Ns = number_of_particles+1
17 N = np.linspace(1, number_of_particles, number_of_Ns)
18 sigma = np.zeros((number_of_Ns, number_of_particles+1))
19
20 for i in range(number_of_Ns):
21     S = np.linspace(0, N[i], N[i]+1)

```

```

22     sigma[i, :int(N[i]+1)] = get_entropy(N[i], S)
23
24 S = np.linspace(0, number_of_particles, number_of_particles+1)
25
26
27 S_both = np.linspace(-number_of_particles, number_of_particles, 2*number_of_particles+1)
28 Ent_both = get_entropy(number_of_particles, S_both)
29 plt.plot(S_both, Ent_both*1e3)
30 plt.xlabel(r"Total spin $$$")
31 plt.ylabel(r"Entropy [m eV/K]")
32 plt.savefig("figure/task_2.7.1.pdf")
33 plt.show()
34
35
36 fig = plt.figure()
37 ax = fig.gca(projection='3d')
38
39 # Make data.
40 X, Y = np.meshgrid(S, N)
41 Z = sigma*1e3
42
43 # Plot the surface.
44 surf = ax.plot_surface(X, Y, Z, cmap=cm.coolwarm)#linewidth=0, antialiased=False)
45 surf = ax.plot_surface(-X, Y, Z, cmap=cm.coolwarm)#linewidth=0, antialiased=False)
46 fig.colorbar(surf, shrink=0.5, aspect=5)
47
48 plt.ylabel("Number of atoms")
49 plt.xlabel("Total spin")
50 ax.set_zlabel("Entropy [mEv/K]")
51 wframe = None
52
53 print("Largest entropy           :      %5.4f Ev/K" % np.max(np.max(Z)*1e-3))
54
55 for phi in np.linspace(45, 45+180, 100):
56     # If a line collection is already remove it before drawing.
57     if wframe:
58         ax.collections.remove(wframe)
59
60     wframe = ax.plot_surface(X, Y, Z, rstride=2, cstride=2, cmap=cm.coolwarm)
61     ax.view_init(30, -phi)
62     plt.savefig("figure/%06d.pdf" % phi)
63     plt.pause(.001)
64 plt.show()

```