Oblig 1

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1 First law of thermodynamics

1.1

Since only the translational and rotational degrees of freedom are active, and it is a diatomic gas, we only have $\frac{1}{2}mv_x^2$, $\frac{1}{2}mv_y^2$, $\frac{1}{2}mv_z^2$, $\frac{1}{2}I\omega_x^2$ and $\frac{1}{2}I\omega_y^2$. This means that $f = 5$. The internal energy is then

$$U = \frac{1}{2}NfkT \tag{1}$$

Heat capacity at constant volume is given by

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V \tag{2}$$

$$C_V = \frac{\mathrm{d}}{\mathrm{dT}}\left(\frac{1}{2}NfkT\right) \tag{3}$$

$$C_V = \frac{1}{2}Nfk \tag{4}$$

1.2

The change in internal energy for each step in the process and for the full cycle can be found by

$$\Delta U = \frac{1}{2}Nfk\Delta T \tag{5}$$

And using the ideal gas law we get

$$T = \frac{PV}{Nk} \tag{6}$$

$$\Delta T = \frac{1}{Nk}\Delta P\Delta V \tag{7}$$

which for path A in the cyclic process with constant pressure gives

$$\Delta U_A = \frac{1}{2}Nfk(\frac{1}{Nk}P\Delta V) \tag{8}$$

$$\Delta U_A = \frac{f}{2}P\Delta V = \frac{5}{2}P\Delta V \tag{9}$$

Path B maintains constant volume which means we get

$$\Delta U_B = \frac{5}{2}\Delta P V \tag{10}$$

and for path C

$$\Delta U_C = \frac{5}{2}\Delta P \Delta V \tag{11}$$

Lastly the net change in energy after going around the whole cycle is

$$\Delta U = 0 \tag{12}$$

since we are back in the original state.

1.3

Work is given by

$$W = -\int_{V_i}^{V_f} P(V) dV \tag{13}$$

Path A(Constant pressure)

$$W_A = -\int_{V_i}^{V_f} P dV = -P \cdot (V_f - V_i) = -P\Delta V \tag{14}$$

Path B(Constant volume)

$$W_B = -\int_a^a P(V) dV = 0 \tag{15}$$

and path C is the line $P(V) = P_1 + a(V - V_1)$ where $a = \frac{P_f - P_i}{V_f - V_i}$.

$$\begin{aligned} W_C &= -\int_{V_f}^{V_i} P(V) dV \\ &= -\int_{V_f}^{V_i} P_i + a(V - V_i) dV \\ &= -P_i(V_i - V_f) - a\int_{V_f}^{V_i} (V - V_i) dV \\ &= -P_i(V_i - V_f) - a\int_{V_f - V_i}^{0} V dV \\ &= -P_i(V_i - V_f) + \frac{a}{2}(V_f - V_i)^2 \\ &= -P_i(V_i - V_f) + \frac{1}{2}(V_f - V_i)(P_f - P_i) \\ &= (V_f - V_i)(P_i + \frac{1}{2}P_f - \frac{1}{2}P_i) \\ &= \frac{1}{2}(V_f - V_i)(P_f + P_i) \\ &= \frac{1}{2}\Delta V(P_f + P_i) \end{aligned} \tag{16}$$

For the whole cycle we have

$$
\begin{aligned}
W = W_A + W_B + W_C &= \frac{1}{2}\Delta V(P_f + P_i) - P_i\Delta V \\
&= \frac{1}{2}\Delta V P_f + \frac{1}{2}\Delta V P_i - P_i\Delta V \\
&= \frac{1}{2}\Delta V(P_f - P_i) \\
&= \frac{1}{2}\Delta P\Delta V
\end{aligned}
\tag{17}
$$

1.4

Now that we know ΔU and W for each step and for the cyle, we can calculate the heat exchange Q by using $\Delta U = Q + W$.

$$Q_A = \frac{5}{2}P\Delta V + P\Delta V = \frac{7}{2}P\Delta V \tag{18}$$

$$Q_B = \frac{5}{2}\Delta PV \tag{19}$$

$$
\begin{aligned}
Q_C &= \frac{5}{2}\Delta P\Delta V - \frac{1}{2}\Delta V(P_f + P_i) \\
&= \frac{5}{2}\Delta V P_f - \frac{5}{2}\Delta V P_i - \frac{1}{2}\Delta V P_f - \frac{1}{2}\Delta V P_i \\
&= 2\Delta V P_f - 3\Delta V P_i
\end{aligned}
\tag{20}
$$

The total heat exchange is equal to negative the work put in.

$$Q = -W = -\frac{1}{2}\Delta P\Delta V \tag{21}$$

1.5

For the whole cycle, ΔU is 0, W is positive(work has been put in), and Q is negative(Heat was emitted in exchange for work).
In path A ΔU_A is negative, W_A is positive and Q_A is negative. Path B has $\Delta U_B < 0$, $W_B = 0$ and $Q_B = U_B < 0$(No work was put in, so all emitted heat was taken from the internal energy). And finally for path C we have $\Delta U_C > 0$ and $W_C > 0$. So what this accomplishes is that the cycle lowers the temperature of the gas using work being put in from an outside source.

2

2.1

Since we have N spins with only 2 directions each, this is just like flipping a coin and we get

$$\Omega_{max} = 2^N \tag{22}$$

2.2

The total net spin is given by

$$S = \sum_i s_i = N_+ - N_- \tag{23}$$

2.3

While looping through an array of length M we can generate N numbers which are either -1 or 1 randomly, add them all together, and the resulting number will be the net spin for that microstate. This number is added to the array each loop and we end up with a list with the net spin of all the microstates. The distribution is here plotted in a histogram and we can easily see that it closely resembles a gaussian distribution.

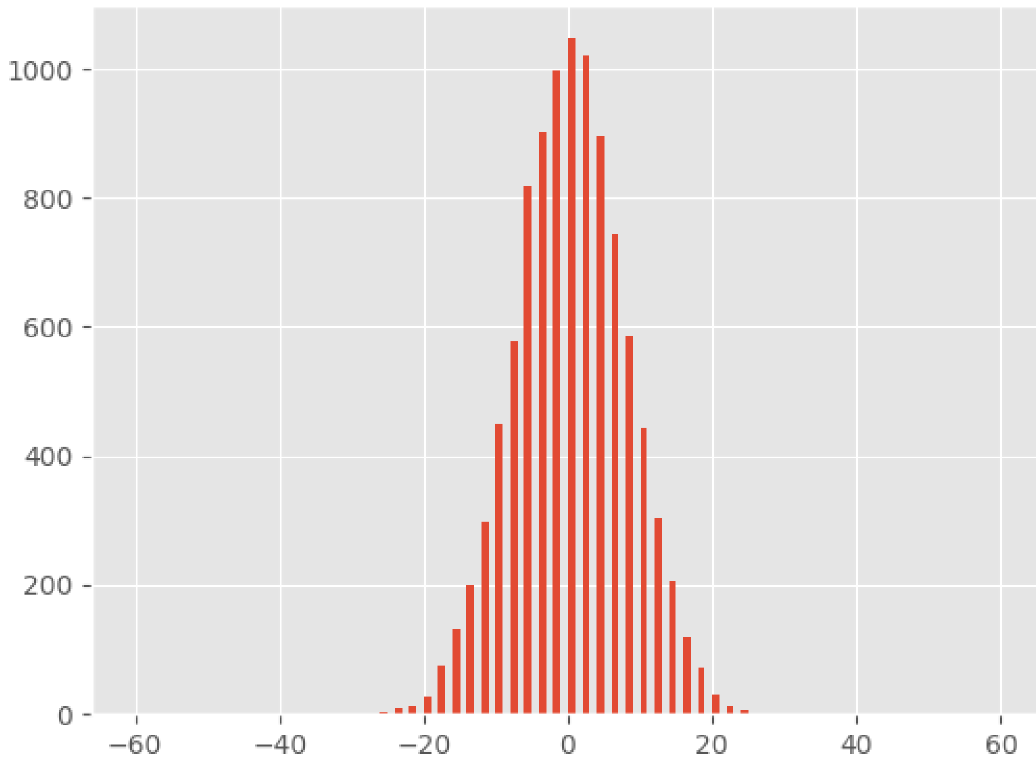

Figure 1: Caption

2.4

We have

$$\Omega(N, n) = \frac{N!}{n! \cdot (N-n)!} \tag{24}$$

We also know that $N = N_+ + N_-$ and from 2.2 that $S = N_+ - N_-$.
If we now set

$$N + S = N_+ + N_- + N_+ - N_- = 2N_+ \tag{25}$$

we see that

$$N_+ = \frac{N+S}{2} \tag{26}$$

If we do the same with $N - S$ we get

$$N_- = \frac{N-S}{2} \tag{27}$$

From task 2.1 we know that

$$\Omega = \binom{N}{N_+} = \frac{N!}{N_+! \cdot (N - N_+)!} \tag{28}$$

We put in $N = N_+ + N_-$ and get

$$\frac{N!}{N_+! \cdot N_-} \tag{29}$$

If we put in our definitions for N_+ and N_- swe are left with

$$\Omega(N,S) = \frac{N!}{(\frac{N+S}{2})! \cdot (\frac{N-S}{2})!} \tag{30}$$

which is what we were supposed to show.

2.5

With this in hand we can use Sterling's approximation $\ln N! \approx N\ln N - N$ on all three factorials(using $N = N$, $N = \frac{1}{\frac{N+S}{2}}$ and $N = \frac{1}{\frac{N-S}{2}}$, and taking the logarithm of both sides using logarithm rules) to get

$$\begin{aligned} \ln\Omega &= N\ln N - N - \Big((\frac{N+S}{2})\ln(\frac{N+S}{2}) - (\frac{N+S}{2}) + (\frac{N-S}{2})\ln(\frac{N-S}{2}) - (\frac{N-S}{2}) \Big) \\ &= N\ln N - N - (\frac{N+S}{2})\ln(\frac{N+S}{2}) + (\frac{N+S}{2}) - (\frac{N-S}{2})\ln(\frac{N-S}{2}) + (\frac{N-S}{2}) \end{aligned} \tag{31}$$

More logarithmic rules and lots of algebra later we have

$$\ln\Omega = N\ln 2 - \frac{S^2}{2N} \tag{32}$$

By raising e to the power of both sides we get

$$\begin{aligned} \Omega &= e^{N\ln 2 - \frac{S^2}{2N}} \\ &= e^{N\ln 2} \cdot e^{-\frac{S^2}{2N}} \\ &= 2^N \cdot e^{-\frac{S^2}{2N}} \end{aligned} \tag{33}$$

and as we know from task 2.1, we have $\Omega_{max} = 2^N$ which means we have what we wanted

$$\Omega(N,S) = \Omega_{max} \cdot e^{-\frac{S^2}{2N}} \tag{34}$$

This formula is valid when $N >> S$.

2.6

Our formula for $\Omega(N, S)$ produces a gaussian curve. So does our histogram from 2.3. Running the program with $M = 2^N$ should give about the same curve and this seems reasonable.

2.7

When plotting the analytic solution using boltzmann's formula I got something that looks like it's trying to resemble a gaussian distribution, but flips around the x-axis after passing 0 for some reason. Could not figure this one out.

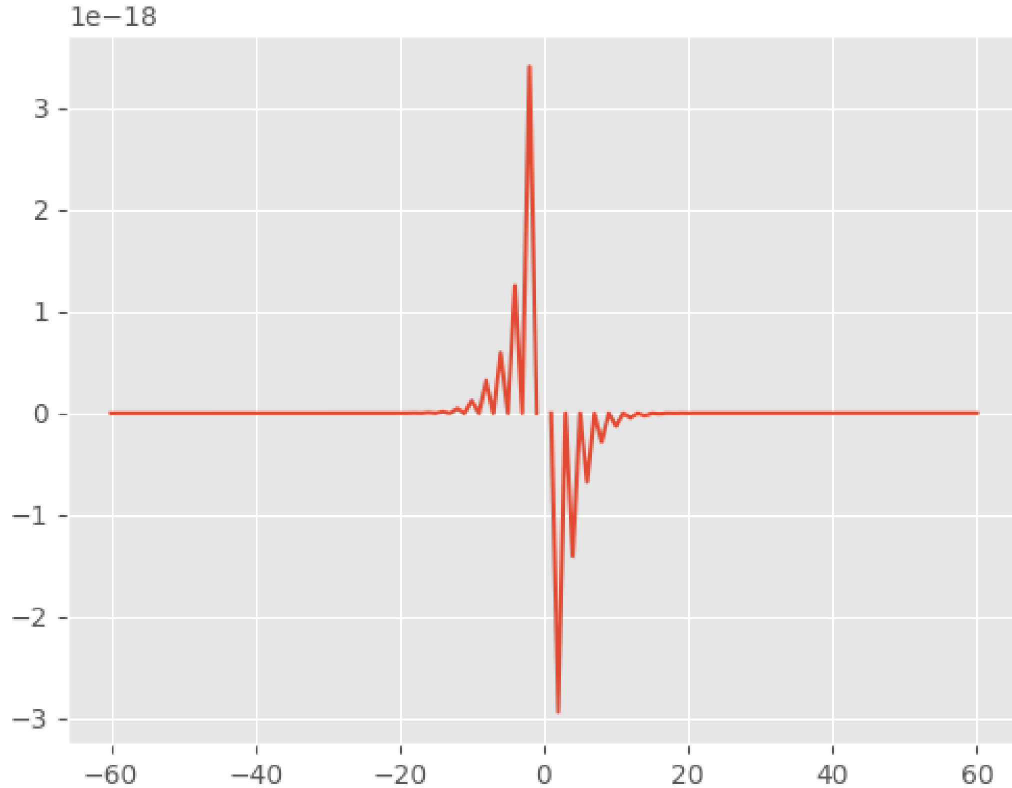

Figure 2: Caption