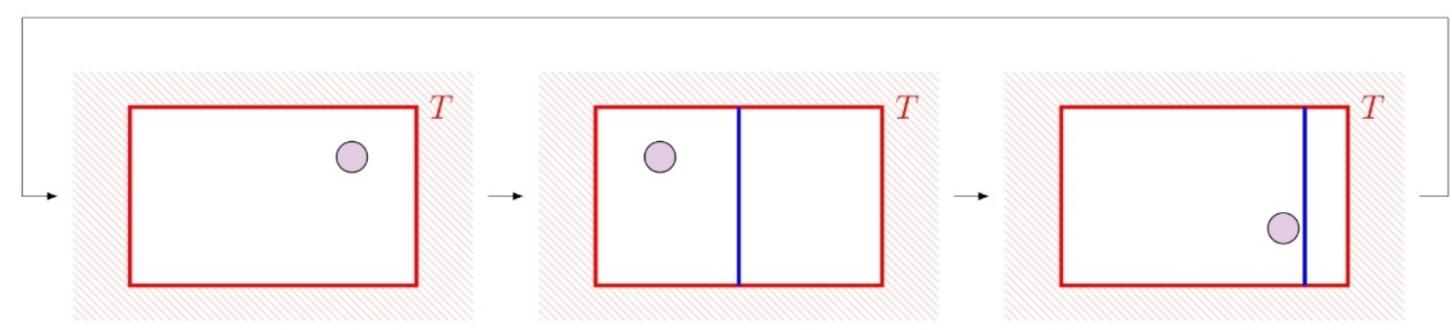


Worksheet 6. Solutions.

1 Maxwell Demon.

Consider the cycle with a single ideal gas particle: (Szilard's Engine)



No change in temperature \rightarrow Isothermal compression

» Change of Volume including the wall.
No work
isothermal.

» Expansion making work.

» Coming back to the initial config

The way you can understand this gas, is that the particle changes its temperature everytime it touches the red walls (the reservoir) to a random velocity given by the Maxwell-Boltzmann distribution.

During an isothermal expansion from V to $2V$ the work done by the molecule

$$W_{\text{by the molecule}} = \int_V^{2V} P dV = k_B T \int_V^{2V} \frac{dV}{V} = k_B T \ln(2)$$

To keep the temperature, and hence the internal energy, of the molecule constant, heat must flow into the box from the heat bath, $Q = W = k_B T \ln(2)$.

The compression, without work, adds the movable wall.

$$\Delta S_{\text{box}}^{\text{isocomp}} = k_B \ln \left(\frac{V}{2V} \right) \\ = -k_B \ln(2)$$

$\Delta S_{\text{bath}}^{\text{isocomp}} = 0 \rightarrow$ No exchange of heat nor work

During the expansion, there is work.

$$dU = dW + dQ$$

$$\Rightarrow dQ = -dW$$

$$W = k_B T \ln(2) \quad \left| \quad S_{\text{box}}^{\text{exp}} = -k_B T \ln(2) \right.$$

Then the total process

$$\left. \begin{array}{l} \Delta S_{\text{box}}^{\text{total}} = 0 \\ \Delta S_{\text{bath}}^{\text{total}} = -k_B \ln(2) \end{array} \right\} \Delta S_{\text{universe}}^{\text{total}} = k_B \ln(2)$$

→ Entropy of the universe decrease
~ work is extracted from the Bath with
"No Cost"
It took years for people to find the answers to
the question: How can this happen?

→ The solution happened to be the connection Information + Thermodynamics

look at

— Szilard's Theorem

— Landauer's principle

2 Ergodic System

No, an ideal gas cannot be considered Ergodic as it is non-interacting. The kinetic energies are conserved, so there is no way the system can explore the whole phase-space with a given initial condition. The kinetic energy "Stays" along every direction x, y and z will remain there.

3 Interstitial lattice.

We have M particles in the interstitial sites and $N-M$ in the normal sites. The internal energy goes

$$U = (N-M) \underbrace{\text{Energy Normal Site}}_0 + M \underbrace{\text{Energy inter-sites}}_{\epsilon}$$

$$U = M\epsilon$$

Now, let us write as a function of the temperature.

The number of ways in which M atoms can be placed at M interstitial sites is

$$\Omega_{\text{inter.}} = \frac{N!}{M!(N-M)!}$$

It happens that, placing the $N-M$ at the M normal sites is the same. Thus,

$$\Omega = \left(\frac{N!}{M!(N-M)!} \right)^2$$

$$\rightarrow S = k_B \ln (\Omega)$$

$$= 2k_B \ln \left[\frac{N!}{M!(N-M)!} \right]$$

$$= 2k_B \left[\ln(N!) - \ln(M!) - \ln((N-M)!) \right]$$

So, using the Stirling formula

$$\frac{S}{k_B} \approx 2[N \ln(N) - N - M \ln(M) + M - (N-M) \ln(N-M) + (N-M)]$$

$$\frac{S}{k_B} = 2 \left[N \ln(N) - M \ln(M) - (N-M) \ln(N-M) \right]$$

So, as we have

$$\frac{1}{T} = \left. \frac{\partial S}{\partial u} \right|_{N,M} \quad \text{and} \quad u = Ne.$$

$$\frac{\partial S}{\partial u} = \frac{\partial S}{\partial M} \frac{\partial M}{\partial u} = \frac{2 k_B}{e} \left[\ln(N-M)/M \right]$$

$$\frac{1}{T} = \frac{2 k_B}{e} \ln \left[\frac{N-M}{M} \right] \quad M = u/e$$

Then

$$e^{\frac{e}{2 k_B T}} = \frac{N-M}{M} = \frac{N - u/e}{u/e}$$

$$= \frac{Ne}{u} - 1$$

$$u = \frac{Ne}{e^{\frac{e}{2 k_B T}} + 1} \approx Ne e^{-\frac{e}{2 k_B T}}$$

So

$$c \approx 2 k_B N \left(\frac{e}{2 k_B T} \right)^2 e^{-e/2 k_B T}$$

$$\frac{e}{2 k_B T} = \frac{u}{\mu} \frac{1}{2 k_B T} = \frac{1}{2} \frac{u}{\mu} T \rightarrow \frac{1}{\mu}$$

3 state spin

consider each spin with magnetic moment μ .
we have

$$W = \frac{N!}{n_{+}! n_{-}! (N-n_{+}-n_{-})!}$$

With the Stirling formula.

$$\ln(W) \approx N \ln(N) - n_{+} \ln(n_{+}) - n_{-} \ln(n_{-}) \\ - (N-n_{+}-n_{-}) \ln(N-n_{+}-n_{-})$$

$$\frac{\partial \ln(W)}{\partial n_{+}} = 0 \quad \text{and} \quad \frac{\partial \ln(W)}{\partial n_{-}} = 0$$

$$n_{+} = (N - n_{+} - n_{-}) = n - 1$$

$$\rightarrow n_{+} = n_{-} = n_0 = \frac{N}{3}$$

Then the maximum entropy

$$S_{\max} = k N \ln(3).$$

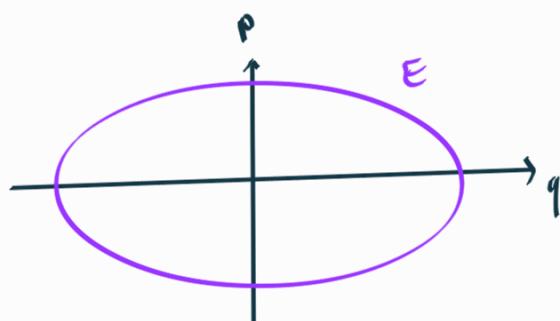
5 Classical Harmonic Oscillators.

a) The accessible volume goes as;

$$\omega = \frac{1}{h^n} \int_{H=E} dq_1 \dots dq_n dp_1 \dots dp_N \quad (5,1)$$

where in this case

$$H(\{\bar{p}, \bar{q}\}) = \sum_{i=1}^N \left[\frac{p_i^2}{2m} + \frac{m\omega^2 q_i^2}{2} \right]$$



where, we can change the variables so we have spheres instead of ellipsoids.

$$q'_i \equiv \sqrt{m\omega} q_i \quad p'_i \equiv \frac{p_i}{\sqrt{m\omega}}$$

so, the Hamiltonian goes;

$$E = H(\{\bar{q}', \bar{p}'\}) = \frac{\omega}{2} \sum_{i=1}^N (p'^2_i + q'^2_i)$$

The equation (5,1) reduces to the surface of a hypersphere of radius $R = \sqrt{2E/\omega}$

$$\omega = \frac{2\pi^N}{(N-1)!} \frac{1}{2^N} \left(\frac{2E}{\hbar\omega} \right)^N = \left(\frac{2\pi E}{\hbar\omega} \right)^N \frac{1}{N!}$$

$$S = k_B \ln (\omega) = N k_B \ln \left(\frac{2\pi E}{\hbar\omega} \right) - k_B (N \log N - N)$$

$$S = k_B N \ln \left(\frac{2\pi E}{hNw} \right) + N k_B$$

$$\approx k_B N \ln \left(\frac{2\pi E}{hNw} \right)$$

so the heat capacity

$$\frac{1}{T} \equiv \left. \frac{\partial S}{\partial E} \right|_N = \frac{N k_B}{E}$$



$$E = N k_B T \quad \xrightarrow{\qquad} \quad \frac{\partial E}{\partial T} = C = N k_B$$