

2)

a) The energy levels are $0, \epsilon,$ and 2ϵ .

- if all particles are in the $i=1$ state, then the average energy per particle is zero.

- if all particles are in the $i=3$ state, then

The avg. energy per particle is $U = \frac{E_{TOT}}{EN} = \frac{N(2\epsilon)}{EN} = 2$.

So $U_{min} = 0, U_{max} = 2$

Gives U units of ϵ

b)

let $n_i =$ the number of particles in the i^{th} state.

denote a configuration of the whole system by $\{n_i\}, i=1,2,3$

The number of ways of realizing that configuration is

$$W = \frac{N!}{\prod_{i=1}^3 n_i!}$$

The most probable configuration is that configuration that maximizes W .

So let's find it.

$$\ln W = \ln N! - \sum_{j=1}^3 \ln(n_j!)$$

use Stirling's approximation.

$$\ln W \approx N \ln N - N - \sum_{j=1}^3 (n_j \ln n_j - n_j) = N \ln N - \sum_{j=1}^3 n_j \ln n_j - N + \sum_{j=1}^3 n_j$$

cancel

This is to be maximized subject to the constraints:

$$n_1 + n_2 + n_3 = N$$

$$0(n_1) + \epsilon n_2 + 2\epsilon n_3 = U = N\epsilon$$

There are only three states, so using Lagrange multipliers is overkill.

lets do it by brute force.

$$d \ln W = - \sum_{j=1}^N n_j \frac{dn_j}{n_j} + \ln n_j dn_j$$

$$d \ln W = - \sum_{j=1}^N (1 + \ln n_j) dn_j$$

Set $d \ln W = 0$, so that

$$0 = (1 + \ln n_1) dn_1 + (1 + \ln n_2) dn_2 + (1 + \ln n_3) dn_3$$

Now use the constraints, which reduce to:

$$0 = dn_1 + dn_2 + dn_3 \rightarrow dn_1 = -dn_2 - dn_3$$

$$0 = \epsilon dn_2 + 2\epsilon dn_3 \rightarrow dn_2 = -2 dn_3$$

Therefore

$$0 = (1 + \ln n_1) (-dn_2 - dn_3) + (1 + \ln n_2) (-2 dn_3) + (1 + \ln n_3) dn_3$$

$$0 = -(1 + \ln n_1) dn_2 + \left[-(1 + \ln n_1) - 2(1 + \ln n_2) + (1 + \ln n_3) \right] dn_3$$

$$0 = \left[2(1 + \ln n_1) - (1 + \ln n_1) - 2(1 + \ln n_2) + (1 + \ln n_3) \right] dn_3$$

$$0 = 2 \ln n_1 - \ln n_1 - 2 \ln n_2 + \ln n_3$$

$$0 = \ln \left(\frac{n_1 n_3}{n_2^2} \right)$$

$$\frac{n_1 n_3}{n_2^2} = 1$$

\rightarrow

$$\frac{n_1}{n_2} = \frac{n_2}{n_3}$$

(inserting the * notation)

c)

$$x \equiv \frac{n_3}{n_2} = \frac{n_2}{n_1}$$

$$\text{So, } n_2 = x n_1 \quad \text{and} \quad n_3 = x^2 n_1$$

combine these with the constraints.

$$\left. \begin{aligned} n_1 + n_2 + n_3 &= N \\ n_1 + x n_1 + x^2 n_1 &= N \\ n_1(1 + x + x^2) &= N \end{aligned} \right\} \begin{aligned} n_2 + 2n_3 &= Nu \\ x n_1 + 2x^2 n_1 &= Nu \\ n_1(x)(1 + 2x) &= Nu \end{aligned}$$

dividing one by the other,

$$\frac{Nu}{N} = \frac{n_1(x)(1+2x)}{n_1(1+x+x^2)} \Rightarrow u = \frac{(x)(1+2x)}{1+x+x^2}$$

$$u(1+x+x^2) = x+2x^2$$

$$(u-2)x^2 + (u-1)x + u = 0$$

so

$$x = \frac{-(u-1) \pm \sqrt{(u-1)^2 - 4(u-2)u}}{2(u-2)}$$

Since x is a ratio of positive numbers (or zeros), choose the $-$ sign.

Then, as u goes from $0 \rightarrow 1 \rightarrow 2$, x goes from $0 \rightarrow 1 \rightarrow \infty$.

d) entropy $S = k \ln W$ where W is evaluated at n_1^x, n_2^x, n_3^x .

$$\text{So } \frac{S}{k} = \ln W \approx N \ln N - N - n_1 \ln n_1 + n_1 - n_2 \ln n_2 + n_2 - n_3 \ln n_3 + n_3$$

$$\frac{S}{Nk} = \ln N - \left(\frac{n_1}{N}\right) \ln n_1 - \left(\frac{n_2}{N}\right) \ln n_2 - \left(\frac{n_3}{N}\right) \ln n_3.$$

recall: $n_2 = x n_1$, $n_3 = x^2 n_1$. So,

$$\frac{S}{Nk} = \ln N - \left(\frac{n_1}{N}\right) \ln n_1 - x \left(\frac{n_1}{N}\right) \ln(x n_1) - x^2 \left(\frac{n_1}{N}\right) \ln(x^2 n_1)$$

$$\frac{S}{Nk} = \ln N - \ln n_1 \left[\frac{n_1}{N} + \frac{x n_1}{N} + \frac{x^2 n_1}{N} \right] - x \left(\frac{n_1}{N}\right) \ln x - x^2 \left(\frac{n_1}{N}\right) \ln(x^2)$$

$$\frac{S}{Nk} = \ln N - \ln n_1 \left(\frac{N}{N}\right) - \ln x \left[\frac{x n_1}{N} + \frac{2 x^2 n_1}{N} \right]$$

$$\frac{S}{Nk} = \ln N - \ln n_1 - \ln x \left[\frac{(n_1)(x)(1+2x)}{N} \right]$$

recall from constraint #2 that $(n_1)(x)(1+2x) = Nu$.

So

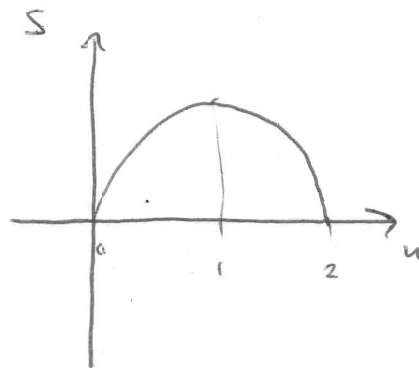
$$\frac{S}{N} = k \left[\ln \left(\frac{N}{n_1}\right) - u \ln x \right]$$

recall from constraint #1 that

$$(1+x+x^2) = \frac{N}{n_1}.$$

$$\frac{S}{N} = k \left[\ln(1+x+x^2) - u \ln x \right]$$

u	x	S
0	0	0
1	1	$k \ln 3$
2	∞	$\approx \ln \left(\frac{x^2}{x^2}\right) \rightarrow 0$



e) use $\frac{1}{T} = \left. \frac{\partial S}{\partial U} \right|_V$ where $U = Nu \epsilon$.

so $\frac{1}{T} = \frac{\partial S}{\partial u} \frac{\partial u}{\partial U} = \frac{\partial S}{\partial u} \left(\frac{1}{N\epsilon} \right)$.

$$\frac{N\epsilon}{T} = \frac{\partial S}{\partial u} = \frac{\partial}{\partial u} \left[Nk \left(\ln(1+x+x^2) - u \ln x \right) \right]$$

$$\frac{N\epsilon}{T} = Nk \left[\left(\frac{1+2x}{1+x+x^2} \right) \frac{dx}{du} - \frac{u}{x} \frac{dx}{du} - \ln x \right]$$

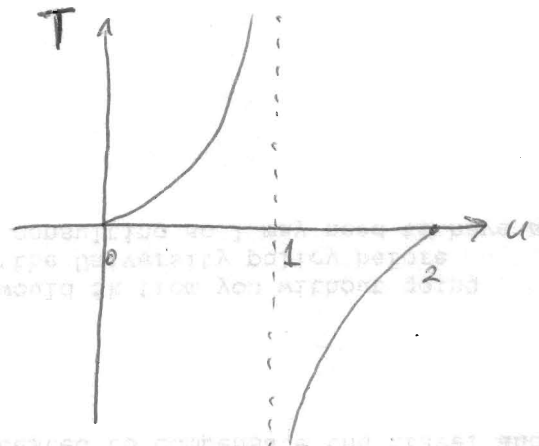
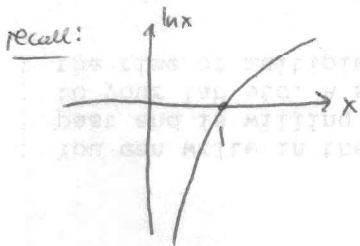
again, use $1+x+x^2 = \frac{N}{n_1}$ & $(n_1)(x)(1+x) = N$.

$$\frac{\epsilon}{kT} = \left(\frac{Nu}{n_1 x} \right) \left(\frac{1}{N/n_1} \right) - \frac{u}{x} \frac{dx}{du} - \ln x$$

$$\frac{\epsilon}{kT} = \left(\frac{u}{x} - \frac{u}{x} \right) \frac{dx}{du} - \ln x \quad \rightarrow \quad T = - \frac{\epsilon}{k \ln x}$$

f)

u	x	T
0	0	0
1	1	∞
2	+∞	0



g) From $T = -\frac{\epsilon}{k \ln x}$, get $x = e^{-\epsilon/kT}$.

recall constraints; and recall $\epsilon_i = (i-1)\epsilon$.

$$\frac{n_1}{N} = \frac{1}{1+x+x^2} = \frac{1}{1+e^{-\epsilon/kT} + e^{-2\epsilon/kT}} = \frac{1}{\sum_{j=1}^3 e^{-\epsilon_j/kT}} \quad \checkmark$$

$n_2 = x n_1$, so

$$\frac{n_2}{N} = \frac{e^{-\epsilon/kT}}{\sum_{j=1}^3 e^{-\epsilon_j/kT}} = \frac{e^{-\epsilon_2/kT}}{\sum_{j=1}^3 e^{-\epsilon_j/kT}} \quad \checkmark$$

$n_3 = x^2 n_1$, so

$$\frac{n_3}{N} = \frac{e^{-2\epsilon/kT}}{\sum_{j=1}^3 e^{-\epsilon_j/kT}} = \frac{e^{-\epsilon_3/kT}}{\sum_{j=1}^3 e^{-\epsilon_j/kT}} \quad \checkmark$$

Comments:

notice that as u increases from 0 to 1, entropy increases and Temperature increases. But as u increases from 1 to 2, the entropy decreases, since there are no higher energy levels. So the material gets more ordered. As a result, the Temperature is negative.