PHYS 5130 Problem Set 4 Solution

1.

Solution: The number of microstates is $C_n^N C_n^{N'} = \frac{N!N'!}{(N-n)!(N'-n)!(n!)^2}$. Moreover, as creating a defect requires ϵ of energy, so number of defects $n = \frac{E}{\epsilon}$.
As $S = k\ln W$, entropy of the system could then be computed.

$$\begin{aligned} S &= k\ln W && (1)\\ &\approx k\left(N\ln N + N'\ln N' - (N-n)\ln(N-n) - (N'-n)\ln(N'-n) - 2n\ln(n)\right) && (2) \end{aligned}$$

One could then obtain $\frac{1}{T}$.

$$\begin{aligned} \frac{1}{T} &= \frac{\partial S}{\partial E} && (3)\\ &= \frac{\partial S}{\partial n}\frac{\partial n}{\partial E} && (4)\\ &= \frac{k}{\epsilon}\left(\ln(N-n) + 1 + \ln(N'-n) + 1 - 2 - 2\ln(n)\right) && (5)\\ &= \frac{k}{\epsilon}\ln\left(\left(\frac{N}{n}-1\right)\left(\frac{N'}{n}-1\right)\right) && (6) \end{aligned}$$

Rewriting this expression, one could then obtain $n(T)$.

$$\begin{aligned} \frac{1}{T} &= \frac{k}{\epsilon}\ln\left(\left(\frac{N}{n}-1\right)\left(\frac{N'}{n}-1\right)\right) && (7)\\ \frac{\epsilon}{kT} &= \ln\left(\left(\frac{N}{n}-1\right)\left(\frac{N'}{n}-1\right)\right) && (8)\\ e^{\left(\frac{\epsilon}{kT}\right)} &= \left(\frac{N}{n}-1\right)\left(\frac{N'}{n}-1\right) && (9)\\ e^{-\left(\frac{\epsilon}{kT}\right)} &= \left(\left(\frac{N}{n}-1\right)\left(\frac{N'}{n}-1\right)\right)^{-1} && (10)\\ e^{-\left(\frac{\epsilon}{kT}\right)} &= \frac{n^2}{(N-n)(N'-n)} && (11) \end{aligned}$$

As the number of defects n is typically much smaller than N or N', the above expression could be approximated as $e^{-\left(\frac{\epsilon}{kT}\right)} = \frac{n^2}{NN'}$, so $n = \sqrt{N'N}e^{-\frac{\epsilon}{2kT}}$.
The expression above could also be exactly solved by rewriting it into a quadratic equation of n.

$$n^2(1 - e^{-\left(\frac{\epsilon}{kT}\right)}) + n(N'+N)e^{-\left(\frac{\epsilon}{kT}\right)} - N'Ne^{-\left(\frac{\epsilon}{kT}\right)} = 0 \qquad (12)$$

Solving this quadratic equation and discarding the negative root, one obtains

$$n = \frac{\sqrt{(N-N')^2 + 4N'Ne^{\left(\frac{\epsilon}{kT}\right)}} - (N+N')}{2\left(e^{\left(\frac{\epsilon}{kT}\right)} - 1\right)} \qquad (13)$$

At low temperature, $\epsilon >> kT$, then the above expression is approximately,

$$\begin{aligned} n &\approx \frac{\sqrt{4N'Ne^{\left(\frac{\epsilon}{kT}\right)}}}{2e^{\left(\frac{\epsilon}{kT}\right)}} && (14)\\ &= \sqrt{N'N}e^{-\frac{\epsilon}{2kT}} && (15) \end{aligned}$$

2.

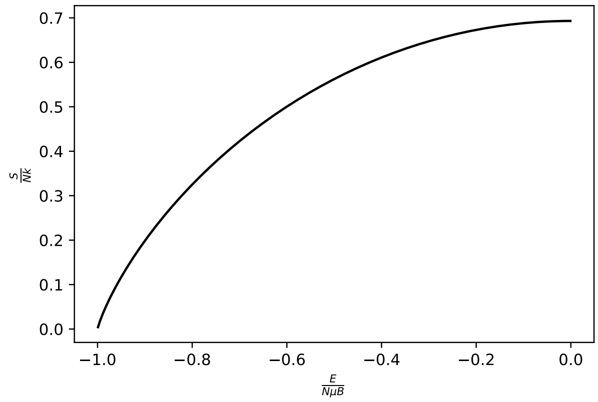
Solution:

(a) Given energy $E = -N\mu B + n(2\mu B)$, one could find the number of particles in the higher energy state. As each transition from lower energy state results in energy change of $\epsilon_{up} - \epsilon_{low} = 2\mu B$, one could identify n as the number of spins that are in the higher energy state.

Therefore, the number of microstates is given by C_n^N.

(b) As $S = k \ln W$, one obtains

$$S = k \ln \left(C_n^N\right) \tag{16}$$
$$= k \ln \left(\frac{N!}{(N-n)!n!}\right) \tag{17}$$
$$\approx k(N \ln N - (N-n)\ln(N-n) - n \ln n) \tag{18}$$



(c) As $n = n(E)$, one could write

$$\frac{1}{T} = \frac{\partial S}{\partial E} \tag{19}$$
$$= \frac{\partial S}{\partial E}\frac{\partial E}{\partial n} \tag{20}$$
$$= \frac{1}{2\mu B}\left(k \ln\left(\frac{N}{n} - 1\right)\right) \tag{21}$$
$$\frac{2\mu B}{kT} = \left(k \ln\left(\frac{N}{n} - 1\right)\right) \tag{22}$$
$$\frac{N}{n} - 1 = e^{\frac{2\mu B}{kT}} \tag{23}$$
$$n = \frac{N}{e^{\frac{2\mu B}{kT}} + 1} \tag{24}$$

Using $n = \frac{E + N\mu B}{2\mu B}$, one could then obtain

$$E = 2\mu B \frac{N}{e^{\frac{2\mu B}{kT}} + 1} - N\mu B = -N\mu B \tanh\left(\frac{\mu B}{kT}\right) \tag{25}$$

Then, heat capacity $C = \frac{\partial E}{\partial T}$ is given by

$$C = \frac{\partial E}{\partial T} \tag{26}$$
$$= -2\mu B \frac{N e^{\frac{2\mu B}{kT}}}{\left(e^{\frac{2\mu B}{kT}} + 1\right)^2}\left(\frac{-2\mu B}{kT^2}\right) \tag{27}$$
$$= Nk\left(\frac{2\mu B}{kT}\right)^2 \frac{e^{\frac{2\mu B}{kT}}}{\left(e^{\frac{2\mu B}{kT}} + 1\right)^2} \tag{28}$$
$$= Nk\left(\frac{\mu B}{kT}\right)^2 \operatorname{sech}^2\left(\frac{\mu B}{kT}\right) \tag{29}$$

In this problem, the temperature scale is set by the $2\mu B$ term, when $kT >> 2\mu B$, the temperature can be considered high. Conversely, the temperature is low when $kT << 2\mu B$.

At high temperature, with $kT >> 2\mu B$, $e^{\frac{2\mu B}{kT}} \to 1$. Therefore,

$$E \approx -N\frac{(\mu B)^2}{kT} \to 0 \tag{30}$$

and

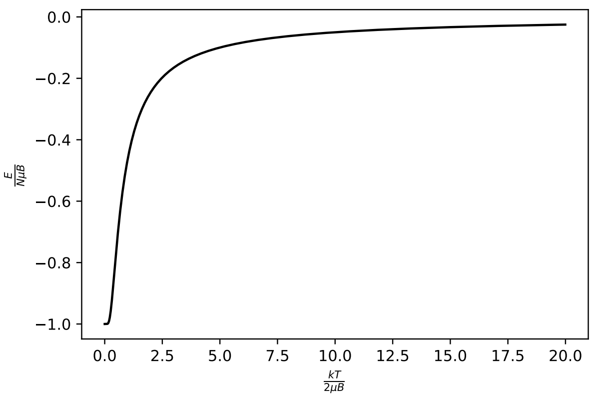
$$C \approx Nk\left(\frac{\mu B}{kT}\right)^2 \to 0. \tag{31}$$

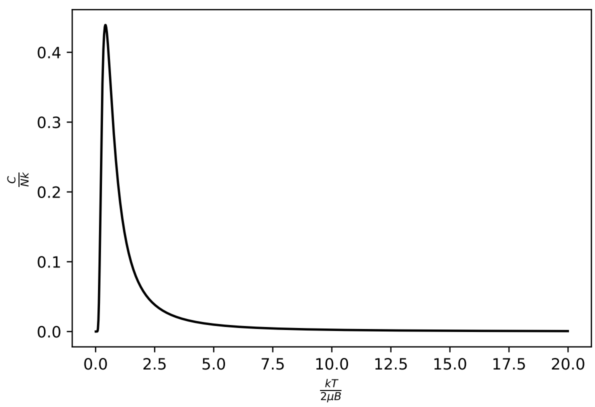
At low temperature,

$$E \approx 2\mu B e^{-\frac{2\mu B}{kT}} - N\mu B \to -N\mu B \tag{32}$$

and

$$C \approx Nk\left(\frac{2\mu B}{kT}\right)^2 e^{-\frac{2\mu B}{kT}} \to 0. \tag{33}$$





(d) From the expression for E obtained in part c, one could see that $E < 0$, for $E > 0$, one needs $T < 0$.

(e) Depending on the energy state, each particle contributes either μ or $-\mu$ to the total dipole moment, the net dipole moment is therefore given by $M = \mu((N-n)-n) = \mu(N-2n)$. Using the result from part c, one obtains

$$M = N\mu\left(1 - \frac{2}{e^{\frac{2\mu B}{kT}}+1}\right) = N\mu\tanh\left(\frac{\mu B}{kT}\right) \tag{34}$$

(f) When $T \to \infty$, $e^{\frac{2\mu B}{kT}} \to 1$, so $M \to 0$.

(g)

$$\begin{aligned}
\chi &\propto \frac{\partial M}{\partial B} && (35)\\
&= 2N\mu\frac{e^{\frac{2\mu B}{kT}}}{\left(e^{\frac{2\mu B}{kT}}+1\right)^2}\frac{2\mu}{kT} && (36)\\
&= \frac{4N\mu^2}{kT}\frac{e^{\frac{2\mu B}{kT}}}{\left(e^{\frac{2\mu B}{kT}}+1\right)^2} && (37)\\
&= \frac{N\mu^2}{kT}\operatorname{sech}^2\left(\frac{\mu B}{kT}\right) && (38)
\end{aligned}$$

At high temperature, $e^{\frac{2\mu B}{kT}} \to 1$, therefore

$$\chi \propto \frac{N\mu^2}{kT}, \tag{39}$$

So, $\chi \propto \frac{1}{T}$, which is the Curie's Law.

3.

Solution: First, one might define the following quantities, $\tilde{p} = \frac{p}{\sqrt{2m}}$ and $\tilde{x} = \sqrt{\frac{m\omega^2}{2}}x$. Then the Hamiltonian of each oscillator could be expressed as $h = \tilde{p}^2 + \tilde{q}^2$.

One could then compute the total number of states with energy less than E, given by

$$W^< = h^{-3N} \underbrace{\int dp_1 \int dp_2 \ldots \int dx_1 \int dx_2 \ldots \int dx_{3N}}_{\sum_i h_i \leq E} \tag{40}$$

By change of variables, $dp = \sqrt{2m}d\tilde{p}$ and $dx = \sqrt{\frac{2}{m\omega^2}}d\tilde{x}$. The expression can be rewritten into

$$\begin{aligned} W^< &= h^{-3N}(2m)^{\frac{3}{2}N}\left(\frac{2}{m\omega^2}\right)^{\frac{3}{2}N} \underbrace{\int d\tilde{p}_1 \ldots \int d\tilde{x}_{3N}}_{\sum_i h_i \leq E} && (41) \\ &= \frac{2^{3N}}{\omega^{3N}h^{3N}} \underbrace{\int d\tilde{p}_1 \ldots \int d\tilde{x}_{3N}}_{\sum_i h_i \leq E} && (42) \end{aligned}$$

As $E = \sum_i^{3N} h = \sum_i^{3N} \tilde{p}^2 + \tilde{x}^2$, one could identify the integration above as finding the volume of a 6N dimensional hypersphere with radius $\sqrt{E}$. Therefore, using the expression for volume of a N dimensional hypersphere provided in the lecture notes, one could obtain

$$W^< = \frac{2^{3N}\pi^{3N}}{\omega^{3N}h^{3N}3N!}E^{3N} \tag{43}$$

Then, the density of state could be obtained from

$$\begin{aligned} W &= \frac{\partial W^<}{\partial E} && (44) \\ &= \frac{2^{3N}\pi^{3N}}{\omega^{3N}h^{3N}(3N-1)!}E^{3N-1} && (45) \end{aligned}$$

Then, one could obtain entropy of the system

$$\begin{aligned} S &= k\ln(W\Delta E) && (46) \\ &\approx 3Nk\ln E - 3Nk\ln\left(\frac{h\omega}{2\pi}\right) - 3Nk\ln(3N) + 3Nk && (47) \end{aligned}$$

Using $T^{-1} = \frac{\partial S}{\partial E}$, one could obtain

$$E = 3NkT \tag{48}$$

Therefore, one obtains $C = 3Nk$, which is the same result as that obtained for quantum oscillator at high temperature.

4.

Solution: Before the two subsystems are placed in thermal contact, the number of accessible microstates is given by $C_2^{(3-1+2)} \times C_{14}^{(5-1+14)} = 18360$, therefore the total entropy of the system is $9.818k$.

After the two system are brought into thermal contact, energy exchange is allowed between the two subsystem, therefore the 16ϵ of energy could be shared among the two subsystems.

Distribution (E_1, E_2)	W_1	W_2	Total number of microstates ($W_1 \times W_2$)
(0, 16)	1	4845	4845
(1,15)	3	3876	11628
(2,14)	6	3060	18360
(3,13)	10	2380	23800
(4,12)	15	1820	27300
(5,11)	21	1365	28665
(6,10)	28	1001	28028
(7,9)	36	715	25740
(8,8)	45	495	22275
(9,7)	55	330	18150
(10,6)	66	210	13860
(11,5)	78	126	9828
(12,4)	91	70	6370
(13,3)	105	35	3675
(14,2)	120	15	1800
(15,1)	136	5	680
(16,0)	153	1	153

So the total number of accessible microstates is 245157, and entropy of the system is $12.41k$, which is higher than initial state. Therefore, the process is irreversible.

The dominating distribution is $E_1 = 5$, $E_2 = 11$, which gives $\frac{E_1}{N_1-1} \approx \frac{E_2}{N_2-1}$. Initially, the two subsystems are out of equilibrium, with the second system "having higher temperature", after the two systems are allowed to equilibrate, the two subsystems have "roughly the same temperature".

It can be seen that states like (4, 12), (5, 11), (6, 10) contributes similar number of mircostates, the relatively large spread of distribution is due to the small size of the system. As the system size increases, the relatively spread of distribution decreases.

One could see that with total energy being constant, the W_1 increases with E_1, whereas W_2 decreases with E_1. So under equilibrium condition, with $S = k\ln(W_1W_2)$ being maximum, the most probable distribution is determined by $\frac{\partial \ln W_1}{\partial E_1} = \frac{\partial \ln W_2}{\partial E_2}$.