Solution to Homework 2, 5163

Problem 1:

(a) Thermal equilibrium means

$$\boxed{T_L = T_R.} \tag{1}$$

We can use

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_{V,N}. \tag{2}$$

Using the entropy function from the assignment, we find

$$\left(\frac{\partial S}{\partial E}\right)_{V,N} = \frac{\lambda V^{1/2} N^{1/4}}{4E^{3/4}}. \tag{3}$$

Using Eq. (1), we have

$$\frac{\lambda V_L^{1/2} N_L^{1/4}}{4E_L^{3/4}} = \frac{\lambda V_R^{1/2} N_R^{1/4}}{4E_R^{3/4}} \tag{4}$$

or

$$\boxed{\frac{E_L^{3/4}}{E_R^{3/4}} = \frac{V_L^{1/2} N_L^{1/4}}{V_R^{1/2} N_R^{1/4}}.} \tag{5}$$

this eq. ensures equal temperatures on left and right (the wall conducts heat → thermal equilibrium)

Inserting $V_L = V_R$ and $N_L/N_R = 1/2$, we have

$$\frac{E_L^{3/4}}{E_R^{3/4}} = (1/2)^{1/4} \tag{6}$$

or

$$\frac{E_L}{E_R} = (1/2)^{1/3} \tag{7}$$

or

$$2^{1/3} E_L = E_R. \tag{8}$$

From $E_L + E_R = 600$ J, we find

$$E_R = 2^{1/3}(600 \text{ J} - E_R). \tag{9}$$

Finally

$$E_R = \frac{2^{1/3}}{1 + 2^{1/3}} 600 \text{ J} \approx 335 \text{ J}. \tag{10}$$

and

$$E_L = \frac{1}{1+2^{1/3}} 600 \text{ J} \approx 266 \text{ J}. \tag{11}$$

(b) The result does make sense. The energy flow from right to left allows for the two temperatures to be the same.
(c) From (a), we have

$$\boxed{\frac{V_L^{1/2} N_L^{1/4}}{E_L^{3/4}} = \frac{V_R^{1/2} N_R^{1/4}}{E_R^{3/4}}.} \tag{12}$$

from thermal equilibrium condition

Due to the fact that the partition is free to move, we have the additional mechanical equilibrium condition that

$$\boxed{P_L = P_R.} \tag{13}$$

mechanical equilibrium

Using the relation

$$P = T \left(\frac{\partial S}{\partial V} \right)_{E,N} \tag{14}$$

we find

$$\frac{\partial S_L}{\partial V_L} = \frac{\partial S_R}{\partial V_R}. \tag{15}$$

(for fixed E & N)

Using the entropy function from the assignment, we have

$$\left(\frac{\partial S}{\partial V} \right)_{E,N} = \frac{\lambda N^{1/4} E^{1/4}}{2V^{1/2}}. \tag{16}$$

Equation (15) thus yields

$$\boxed{\frac{N_L^{1/4} E_L^{1/4}}{V_L^{1/2}} = \frac{N_R^{1/4} E_R^{1/4}}{V_R^{1/2}}.} \tag{17}$$

from mechanical equilibrium condition

Combining Eqs. (12) and (17), we find

$$\frac{N_L^{1/2}}{E_L^{1/2}} = \frac{N_R^{1/2}}{E_R^{1/2}} \tag{18}$$

or

$$\frac{N_R}{N_L} = \frac{E_R}{E_L}. \tag{19}$$

Using that $N_R/N_L = 2$, we have

$$E_R = 2E_L, \tag{20}$$

implying $E_R = 400$ J and $E_L = 200$ J. From Eq. (17), we find

$$\frac{V_L}{V_R} = \frac{N_L^{1/2} E_L^{1/2}}{N_R^{1/2} E_R^{1/2}}. \tag{21}$$

Thus,

$$\frac{V_L}{V_R} = 1/2. \tag{22}$$

Using that $V_L + V_R = 2$ m^3, we find

$$V_R = \frac{4}{3} \text{ m}^3 \tag{23}$$

and

$$V_L = \frac{2}{3} \text{ m}^3. \tag{24}$$

(d) This is kind of an obvious result: We have twice as much of the right substance than of the left. Thus, the right takes up twice as much space as the left, and has twice the energy as the left. With the partition being movable and heat conducting, the cylinder in equilibrium contains one “homogeneous substance”.

Problem 2:

We are given a "generic form" of the Hamiltonian:

$$\mathcal{H}(\vec{p}, \vec{q}) = \mathcal{H}_0(\vec{p}, \vec{q}) + \lambda \, \underbrace{h(\vec{p}, \vec{q})}_{\text{some function}}$$

parameter

We want to show:

$$\langle h \rangle = - T \frac{dS}{d\lambda} . \quad (*)$$

How to approach this? Let's try to look at the l.h.s. and r.h.s. of (*) and see if we can "connect" them.

Let's start w/ r.h.s.

$-T \frac{dS}{d\lambda}$ ⇝ we want to rewrite this

⇝ to do so, we need expressions for T and S

What is T?

$$T^{-1} \overset{\text{def.}}{=} \left(\frac{\partial S(E)}{\partial E} \right)_{V,N}$$

What is S?

$$S = k \log \big(\underbrace{\Sigma(E)}_{\frac{1}{N! \, h^{Nd}} \int \Theta(E - \mathcal{H}) \, d^{Nd}\vec{p} \, d^{Nd}\vec{q}} \big)$$

(we are assuming N particles in d dimensions) r.h.s.: $-T\ \dfrac{dS}{d\lambda} = -\left(\left(\dfrac{\partial S(E)}{\partial E}\right)_{V,N}\right)^{-1} \underbrace{\dfrac{d}{d\lambda}\left(k \log\left(\Sigma(E)\right)\right)}_{k \frac{d}{d\lambda}\left(\log(\Sigma(E))\right)}$

Before we manipulate this further, let's look at the l.h.s.:

What is $\langle h \rangle$?

$$\langle h \rangle \overset{\text{by definition}}{=} \frac{\int h\ \delta(E-\mathcal{H})\, d^{3N}\vec{p}\ d^{3N}\vec{q}}{\int \delta(E-\mathcal{H})\, d^{3N}\vec{p}\ d^{3N}\vec{q}}$$

Ok, we now have s.th. for the l.h.s. – let's go back to r.h.s.:

$$-T\frac{dS}{d\lambda} = -\left(\left(\frac{\partial S(E)}{\partial E}\right)_{V,N}\right)^{-1} k\frac{d}{d\lambda}\underbrace{\left(\log\left(\frac{1}{N!\,h^{Nd}}\int \theta(E-\mathcal{H})\ d^{Nd}\vec{p}\, d^{Nd}\vec{q}\right)\right)}_{\log\int\theta(E-\mathcal{H})d^{Nd}\vec{p}\,d^{Nd}\vec{q}\ -\ \log \cancel{N!\,h^{Nd}}}$$

goes away when taking $\dfrac{d}{d\lambda}$

$$= -\left(\left(\frac{\partial S(E)}{\partial E}\right)_{V,N}\right)^{-1} k\ \frac{d}{d\lambda}\left(\log\left(\int\theta(E-\mathcal{H})\, d^{Nd}\vec{p}\ d^{Nd}\vec{q}\right)\right)$$

What is $\left(\frac{\partial S(E)}{\partial E}\right)_{V,N}$?

$$\left(\frac{\partial}{\partial E}\left(k \log\left(\frac{1}{N!\,h^{Nd}}\int \theta(E-\mathcal{H})\, d^{Nd}\vec{p}\, d^{Nd}\vec{q}\right)\right)\right)_{V,N}$$

$$= k\left(\frac{\partial}{\partial E}\left(\log\left(\int \theta(E-\mathcal{H})\, d^{Nd}\vec{p}\, d^{Nd}\vec{q}\right)\right)\right)_{V,N}$$

Now we use a "trick": $\frac{d}{dE}\log f = \frac{\frac{df}{dE}}{f}$ (trick 1)

$$= k\,\frac{\left(\frac{\partial}{\partial E}\int \theta(E-\mathcal{H})\, d^{Nd}\vec{p}\, d^{Nd}\vec{q}\right)_{V,N}}{\int \theta(E-\mathcal{H})\, d^{Nd}\vec{p}\, d^{Nd}\vec{q}}$$

Use this in $-T\frac{dS}{d\lambda}$:

$$-T\frac{dS}{d\lambda} = -\frac{\int \theta(E-\mathcal{H})\, d^{Nd}\vec{p}\, d^{Nd}\vec{q}}{k\left(\frac{\partial}{\partial E}\int \theta(E-\mathcal{H})\, d^{Nd}\vec{p}\, d^{Nd}\vec{q}\right)_{V,N}}$$

this is T (inverse of the equation above)

$$\times\, k\,\frac{\frac{d}{d\lambda}\int \theta(E-\mathcal{H})\, d^{Nd}\vec{p}\, d^{Nd}\vec{q}}{\int \theta(E-\mathcal{H})\, d^{Nd}\vec{p}\, d^{Nd}\vec{q}}$$

the red pieces cancel

I am applying trick 1 again

$$= -\frac{\frac{d}{d\lambda}\int \theta(E-\mathcal{H})\, d^{Nd}\vec{p}\, d^{Nd}\vec{q}}{\left(\frac{\partial}{\partial E}\int \theta(E-\mathcal{H})\, d^{Nd}\vec{p}\, d^{Nd}\vec{q}\right)_{V,N}}$$

Okay: We have s.th. for the r.h.s. in terms of a step function.

And we have s.th. for the l.h.s. in terms of a δ-function.

Natural question? Can we "turn" the step function into a δ-fct.?

Yes!

$$\frac{d}{d\lambda}\,\theta(E-\mathcal{H}_0-\lambda h) = -h\,\delta(\underbrace{E-\mathcal{H}_0-\lambda h}_{E-\mathcal{H}})$$

$$\frac{\partial}{\partial E}\,\theta(E-\mathcal{H}) = \delta(E-\mathcal{H})$$

The r.h.s. thus becomes:

$$-T\,\frac{dS}{d\lambda} = \underbrace{\frac{\int h\,\delta(E-\mathcal{H})\,d^{Nd}\vec{p}\,d^{Nd}\vec{q}}{\int \delta(E-\mathcal{H})\,d^{Nd}\vec{p}\,d^{Nd}\vec{q}}}_{\text{but this is } \langle h\rangle}$$

Assignment 2, Problem 3:

(a) We want to calculate the entropy $S(N, E, A)$

The Hamiltonian has similarities with the ideal gas Hamiltonian ⇝ this suggests that we want to follow a similar approach to tackling the problem.

Recall: $S = k \log(\Sigma(E))$

So: if we know $\Sigma(E)$, we can calculate S.

$$\Sigma(E) = \frac{1}{N!\, h^{3N}} \int_{\mathcal{H}<E} d^{3N}p \; d^{3N}q$$

our variables are $x_1, y_1, \theta_1, x_2, y_2, \theta_2, \ldots, x_N, y_N, \theta_N$

$p_{x_1}, p_{y_1}, p_{\theta_1}, p_{x_2}, p_{y_2}, p_{\theta_2}, \ldots, p_{x_N}, p_{y_N}, p_{\theta_N}$

⇝ so, we need a factor of h^{3N}

$$= \frac{1}{N!\, h^{3N}} \int \theta(E - \mathcal{H}) \, d^{3N}p \, d^{3N}q$$

$$\mathcal{H} = \sum_{i=1}^{N} \frac{p_{x_i}^2 + p_{y_i}^2}{2m} + \sum_{i=1}^{N} \frac{p_{\theta_i}^2}{2J}$$

Let us first integrate over the $\vec{q}$ coordinates.

Look at first molecule:

$$\underbrace{dx_1\, dy_1}\, d\theta_1$$

integrating over x_1 and y_1 gives the area $\mathcal{A}$

integrating over θ_1 gives a factor of 2π

$\Rightarrow$ the integration over $\vec{q}$ gives a factor of

$\mathcal{A}^N (2\pi)^N$

$$\Rightarrow \Sigma(E) = \frac{\mathcal{A}^N (2\pi)^N}{N!\, h^{3N}} \int \theta\left(E - \sum_{i=1}^{N}\left(\frac{p_{xi}^2 + p_{yi}^2}{2m} + \frac{p_{\theta i}^2}{2J}\right)\right) d^{3N}p$$

define $u_{xi} = \frac{p_{xi}}{\sqrt{2m}}$

$u_{yi} = \frac{p_{yi}}{\sqrt{2m}}$

$\omega_i = \frac{p_{\theta i}}{\sqrt{2J}}$

$\Rightarrow dp_{xi} = \sqrt{2m}\; du_{xi}$

$dp_{yi} = \sqrt{2m}\; du_{yi}$

$dp_{\theta i} = \sqrt{2J}\; d\omega_i$

Thus:

$$\Sigma'(E) = \frac{\mathcal{A}^N (2\pi)^N (8m^2 J)^{N/2}}{N!\ h^{3N}} \underline{\int \theta\left(E - \sum_{i=1}^{N} (u_{xi}^2 + u_{yi}^2 + w_i^2)\right) d^{3N}p}$$

this integral is of the exact same form as the integral we encountered in the ideal gas problem

$$= E^{3N/2} \underbrace{\frac{\pi^{3N/2}}{\Gamma\left(\frac{3N}{2}+1\right)}}_{C_{3N}}$$

in the large N limit:

$$C_{3N} \to \frac{3N}{2} \log \pi - \frac{3N}{2} \log \frac{3N}{2} + \frac{3N}{2}$$

So: $\Sigma'(E) = \dfrac{\left(2\pi \mathcal{A} \sqrt{8m^2 J}\right)^N}{N!\ h^{3N}} E^{3N/2}\ C_{3N}$

We want to calculate $S = k \log(\Sigma(E))$

$$\Rightarrow \boxed{S = k \log\left(\frac{\left(2\pi \mathcal{A} \sqrt{8m^2 J}\right)^N}{N!\ h^{3N}} E^{3N/2} C_{3N} \right)} \quad (*)$$

(b) We want to find the energy and the pressure $P = T\left(\frac{\partial S}{\partial A}\right)_{E,N}$

First, we need to find the energy. From (*):

$$e^{S/k} = \frac{\left(2\pi A\sqrt{8m^2 J}\right)^N}{N!\, h^{3N}}\, C_{3N}\, E^{3N/2}$$

$$\Rightarrow E = \left(\frac{N!\, h^{3N}}{\left(2\pi A\sqrt{8m^2 J}\right)^N C_{3N}}\right)^{2/3N} e^{2S/(3Nk)}$$

From this, we can calculate $T = \frac{\partial E}{\partial S}$ for fixed V and N

$$T = \frac{2}{3Nk} E \Rightarrow \frac{3Nk}{2} T = E \Rightarrow \boxed{\frac{E}{N} = \frac{3}{2} kT}$$

We also need $\left(\partial S/\partial A\right)_{E,N}$:

$$\left(\frac{\partial S}{\partial A}\right)_{E,N} = \frac{kN}{A}$$

$$\Rightarrow \boxed{P =} T\frac{kN}{A} = \boxed{Tkn}$$

where the density $n = \frac{N}{A}$

(c)

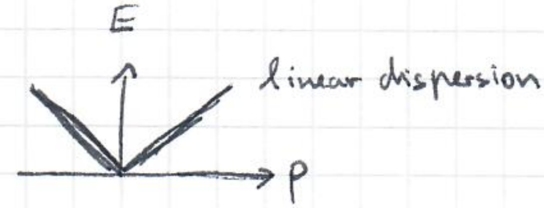
We want to find $C_V = N^{-1}\left(\frac{\partial E}{\partial T}\right)_V$ (here, $V = A$)

Using $E = \frac{3NkT}{2}$, we find $\frac{\partial E}{\partial T} = \frac{3Nk}{2}$

$$\Rightarrow \boxed{C_V = \frac{3k}{2}}$$

Assignment 2, Problem 4:

For a single massless particle in 1D, the energy is $c\,|p|$



$$\Rightarrow \quad \mathcal{H} = \sum_{i=1}^{N} c\,|p_i|$$

We can calculate the entropy from the expression

$$S = k \log\left(\Sigma(E)\right),$$

where $\Sigma(E) = \dfrac{1}{N!\,h^N} \displaystyle\iint \theta(E - \mathcal{H})\, d^N q\, d^N p.$

The integration over $\vec{q}$ gives a factor of L^N:

$$\Rightarrow \Sigma(E) = \frac{L^N}{N!\,h^N} \int \theta\left(E - \sum_{i=1}^{N} c\,|p_i|\right) d^N p$$

$$\text{let } \varepsilon_1 = c\,p_1$$
$$\varepsilon_2 = c\,p_2$$
$$\vdots$$
$$\Rightarrow \quad d\varepsilon_i = c\,dp_i$$

With this change of variables, we have

$$\Sigma(E) = \frac{L^N}{(ch)^N N!} \int \theta\left(E - \sum_{i=1}^{N} |\varepsilon_i|\right) d^N \varepsilon$$

the integral goes over all space:

using that the θ fct depends on the absolute values $|\varepsilon_i|$, we can restrict the integral to $\int_0^\infty$, provided we add a factor of 2 for each of the coordinates

$$\Rightarrow \Sigma(E) = \left(\frac{2L}{ch}\right)^N \frac{1}{N!} \int_0^\infty \dots \int_0^\infty \theta\left(E - \sum_{i=1}^N |\varepsilon_i|\right) d\varepsilon_1\, d\varepsilon_2 \dots d\varepsilon_N$$

I will solve the integral by looking at $N=1$, $N=2$, and $N=3$, and deducing a general formula from that (for a more rigorous treatment, see below).

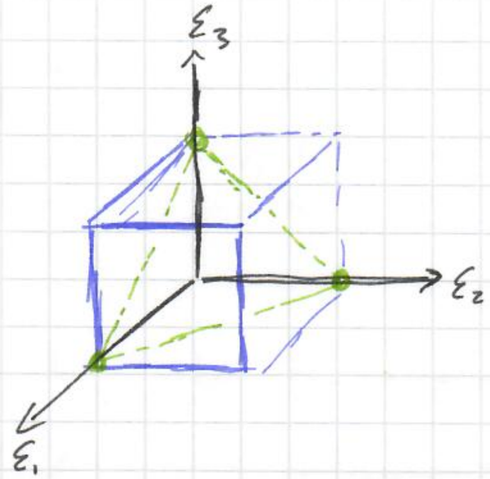
$$\int_0^\infty \theta(E - \varepsilon_1)\, d\varepsilon_1 = E \quad \text{(by inspection)}$$

$$\int_0^\infty \int_0^\infty \theta(E - \varepsilon_1 - \varepsilon_2)\, d\varepsilon_1\, d\varepsilon_2 = \underbrace{\frac{1}{2}}_{\frac{1}{2!}} E^2 \quad \text{(by inspection, see sketch)}$$

$$\int_0^\infty \int_0^\infty \int_0^\infty \theta(E - \varepsilon_1 - \varepsilon_2 - \varepsilon_3)\, d\varepsilon_1\, d\varepsilon_2\, d\varepsilon_3 = \frac{1}{6} E^3$$

$$= \underbrace{\frac{1}{1\cdot 2\cdot 3}}_{\frac{1}{3!}} E^3$$

again by inspection



So, we deduce: $\int_0^\infty \cdots \int_0^\infty \theta(E - \varepsilon_1 - \varepsilon_2 - \ldots - \varepsilon_N)\, d\varepsilon_1 \cdots d\varepsilon_N = \frac{E^N}{N!}$

$$\Rightarrow \Sigma(E) = \left(\frac{2EL}{ch}\right)^N \frac{1}{(N!)^2}$$

It follows: $S = k \log \Sigma(E)$

$$\Rightarrow \boxed{S = k \log\left(\left(\frac{2EL}{ch}\right)^N \frac{1}{(N!)^2}\right)}$$

Let's evaluate the integral in a mathematically rigorous manner:

$$J_N(E) = \underbrace{\int \cdots \int}_{\substack{N \text{ integrals,} \\ 0 \text{ to } \infty \text{ each}}} \theta(E - \varepsilon_1 - \varepsilon_2 - \ldots - \varepsilon_N)\, d\varepsilon_N\, d\varepsilon_{N-1} \cdots d\varepsilon_1$$

We can change the integration limits to: $0 \ldots E$ since the argument of the θ fct. takes negative values when one of the $\varepsilon_i > E$.

$$J_N(E) = \underbrace{\int_0^E \cdots \int_0^E}_{N \text{ integrals}} \theta(E - \varepsilon_1 - \varepsilon_2 - \ldots - \varepsilon_N)\, d\varepsilon_N\, d\varepsilon_{N-1} \cdots d\varepsilon_1$$

We can also write:

$$J_{N-1}(E) = \underbrace{\int_0^E \cdots \int_0^E}_{N-1 \text{ integrals}} \theta(E - \varepsilon_1 - \ldots - \varepsilon_{N-1})\, d\varepsilon_{N-1} \ldots d\varepsilon_1$$

But this also means that we can express $J_N(E)$ in terms of $J_{N-1}(E)$:

$$J_N(E) = \int_0^E J_{N-1}(E - \varepsilon_N)\, d\varepsilon_N$$

now, let's do a variable transformation:

let $y = E - \varepsilon_N$

$$\Rightarrow dy = -d\varepsilon_N$$

the limits change to $\int_{E-0}^{E-E} \rightarrow \int_{E}^{0} \rightarrow -\int_{0}^{E}$

$$\Rightarrow J_N(E) = \int_0^E \underbrace{J_{N-1}(y)}\, dy$$

we have $N-1$ "hidden" integrals

$\rightsquigarrow$ we want to go to the case where we have only one integral to do

$$J_1(E) = \int_0^E \theta(E - \varepsilon_1)\, d\varepsilon_1$$

$$= \int_0^E \theta(y)\, dy = E$$

$$\Rightarrow J_2(E) = \int_0^E J_1(y)\, dy$$

$$= \int_0^E E\, dE = \frac{1}{2} E^2$$

$$\Rightarrow J_3(E) = \frac{1}{2 \cdot 3} E^3 \quad \& \quad J_N(E) = \frac{E^N}{N!}$$