Physics 12c - Problem Set 2 - Solutions

April 22, 2016

[1] Energy Fluctuation (Problem 3.4 of Kittel/Kroemer)

Note first that:
\[ \langle (\epsilon - \langle \epsilon \rangle)^2 \rangle = \langle \epsilon^2 - 2\epsilon \langle \epsilon \rangle + \langle \epsilon \rangle^2 \rangle = \langle \epsilon^2 \rangle - \langle \epsilon \rangle^2. \]

Next we write the partition as a function of \( \beta = 1/\tau \) which would be a more natural definition of temperature.

\[ Z = \sum_i \exp(-\beta \epsilon_i) \]

Then

\[ U = \langle \epsilon \rangle = \frac{1}{Z} \sum_i \epsilon_i \exp(-\beta \epsilon_i) = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} \]

\[ \langle \epsilon^2 \rangle = \frac{1}{Z} \sum_i \exp(-\beta \epsilon_i) = \frac{1}{Z} \frac{\partial^2 Z}{\partial \beta^2}. \]

From these, with \( d\beta/d\tau = -1/\tau^2 \),

\[ \tau^2 \left( \frac{\partial U}{\partial \tau} \right)_V = \tau^2 \left( \frac{\partial U}{\partial \beta} \right)_V \frac{\partial \beta}{\partial \tau} = - \left( \frac{\partial U}{\partial \beta} \right)_V \]

\[ = \frac{\partial}{\partial \beta} \left( \frac{1}{Z} \frac{\partial Z}{\partial \beta} \right) = \frac{1}{Z} \frac{\partial^2 Z}{\partial \beta^2} - \frac{1}{Z^2} \left( \frac{\partial Z}{\partial \beta} \right)^2 \]

\[ = \langle \epsilon^2 \rangle - \langle \epsilon \rangle^2 \]


In one dimension, the orbital energies are, \( \epsilon_n = \epsilon_1 n^2 \), where \( \epsilon_1 = (\hbar^2/2M)(\pi/L)^2 \)

and \( n \) as a positive integer. The single-particle partition function is

\[ Z_1 = \sum_n \exp(-\epsilon_1 n^2/\tau) \approx \int_0^\infty \exp(-\epsilon_1 n^2/\tau) dn = (\pi \tau/4\epsilon_1)^{1/2} = \sqrt{\frac{L^2 M \tau}{2\pi \hbar^2}} \]

\( (\pi \tau/4\epsilon_1)^{1/2} = n_{Q_1} L, \)

where

\[ n_{Q_1} = \left( \frac{M \tau}{2\pi \hbar^2} \right)^{1/2} = (n_Q)^{1/3} \]
is the one-dimensional quantum concentration analogous to the three-dimensional quantum concentration \( n_Q \) defined in (62) and (63).

For \( N \) particles:

\[
Z_N = Z_N^1 / N!,
\]

\[
F = -\tau \log Z_N
= \tau \log N! - \tau N \log Z_1
= \tau (N \log N - N) - \tau N \log(n_Q, L)
= \tau N [\log(n/n_Q) - 1],
\]

where \( n = N/L \). With the help of \( \frac{\partial}{\partial \tau} \log n_Q^1 = 1/2 \tau \):

\[
\sigma = -\left( \frac{\partial F}{\partial \tau} \right)_n = N [\log(n_Q/n) + 3/2],
\]

which we should compare with (76).

[3] Model of Large Reservoir

(a). The total entropy of 2-subsystems is defined as,

\[
S_{total} = S_1(E_1) + S_2(E_2) \tag{S1}
\]

So that the change in total entropy, \( dS_{total} \), is

\[
dS_{total} = \frac{\partial S_1}{\partial E_1} dE_1 + \frac{\partial S_2}{\partial E_2} dE_2 = 0 \tag{S2}
\]

Because. total energy, \( E = E_1 + E_2 \), is constant, i.e., \( dE = dE_1 + dE_2 = 0 \), or

\[
dE_1 = -dE_2 \tag{S3}
\]

then (2) becomes,

\[
0 = \frac{\partial S_1}{\partial E_1} dE_1 - \frac{\partial S_2}{\partial E_2} dE_1
\]

or,

\[
\frac{\partial S_1}{\partial E_1} = \frac{\partial S_2}{\partial E_2}
\]

Recall that temperature, \( \tau \), is defined as \( \frac{1}{\tau} = \frac{\partial S}{\partial E} \). So that we have \( \tau_1 = \tau_2 \).

To prove that it’s a maximum, we first note that

\[
dS_{total}(E_1, E - E_1) = \frac{\partial S_{total}}{\partial E_1} dE_1 \quad \Rightarrow \quad \frac{\partial S}{\partial E_1} = \frac{1}{\tau_1} - \frac{1}{\tau_2}
\]

Taking the second derivative, using the chain rule and eq.(S3), we find:

\[
\frac{\partial^2 S}{\partial E_1^2} \bigg|_{\tau_2 = \tau_1} = \left( -\frac{1}{\tau_1^2} \frac{\partial \tau_1}{\partial E_1} + \frac{1}{\tau_2} \frac{\partial \tau_2}{\partial E_1} \right) \bigg|_{\tau_2 = \tau_1} = \left( -\frac{1}{\tau_1^2} \frac{\partial \tau_1}{\partial E_1} - \frac{1}{\tau_2^2} \frac{\partial \tau_2}{\partial E_2} \right) \bigg|_{\tau_2 = \tau_1}.
\]

Since the specific heat \( C_V = \frac{\partial E_i}{\partial \tau_i} \) is positive, we find a local maximum for \( S_{total} \).
(b). We want to generalize the above to the N-subsystem case. Let’s start with $N = 2$. It has been shown in part (a) that at thermal equilibrium (total entropy is maximized), $\tau_1 = \tau_2$.

Suppose that a system consisting of $k$ subsystems reaches thermal equilibrium when $\tau_1 = \tau_2 \cdots = \tau_k = \tau$. After a system consisting of $k$ subsystems reaches thermal equilibrium, it can be regarded as a system with temperature $\tau$ and energy $E = \sum_{i=1}^{k} E_i$ and entropy $S_{(k)}$.

Now, we put it together with the $(k+1)^{th}$ system. It’s total entropy is

$$S_{tot} = S_{(k)}(E) + S_{k+1}(E_{k+1}).$$

Via the argument of part (a), the two reach thermal equilibrium when $\tau = \tau_{k+1}$.

Through mathematical induction, we generalized the result in (a) to any number of subsystem.

(c) For an N-indetical subsystem each with entropy $S(E/N)$, where $\xi = E/N$ is the energy of each subsystem. Then the total entropy is,

$$S_{total}(E) = NS\left(\frac{E}{N}\right) = NS(\xi)$$  \hspace{1cm} (S4)

Taylor expanding the total entropy,

$$S_{tot}(E + \Delta E) = S_{tot}(E) + \frac{\partial S}{\partial E}S_{tot}(E)\Delta E + \frac{1}{2} \frac{\partial^2 S}{\partial E^2}S_{tot}(E)(\Delta E)^2 + O(\Delta E)^3$$

$$= NS(\xi) + N \frac{\partial S(\xi)}{\partial E} \Delta E + \frac{1}{2} N \frac{\partial^2 S(\xi)}{\partial E^2} (\Delta E)^2 + O(\Delta E)^3$$

$$= NS(\xi) + N \frac{\partial S(\xi)}{\partial \xi} \frac{\partial \xi}{\partial E} \Delta E + \frac{1}{2} N \frac{\partial^2 S(\xi)}{\partial \xi^2} \left( \frac{\partial \xi}{\partial E} \right)^2 (\Delta E)^2 + O(\Delta E)^3$$

$$= NS + N \frac{\partial S}{\partial \xi} \left( \frac{\Delta E}{N} \right) + \frac{1}{2} N \frac{\partial^2 S}{\partial \xi^2} \left( \frac{\Delta E}{N} \right)^2 + O(\Delta E)^3$$

So,

$$\Delta S_{total} = \frac{\partial S}{\partial \xi} \Delta E + \frac{1}{2N} \frac{\partial^2 S}{\partial \xi^2} \Delta E^2 = \frac{\Delta E}{\tau} - \frac{(\Delta E)^2}{2NC_v\tau^2}$$

For large $N$ the second term can be ignored. Notice that we can express $\partial^2 S/\partial \xi^2 = \frac{\partial}{\partial \xi} \frac{\partial S}{\partial E} = \frac{\partial}{\partial \xi} (1/\tau) = \frac{\partial \tau}{\partial \xi} \frac{\partial}{\partial \tau} (1/\tau) = -1/(C_v \tau^2)$, where $C_v = \partial \xi/\partial \tau$. 

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(a). The rate of going from stat $g$ to $e$ is
\[ N(g)\Gamma(g \rightarrow e). \]
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\[ N(e)\Gamma(e \rightarrow g). \]
Therefore, at equilibrium
\[ \frac{dN(e)}{dt} = N(g)\Gamma(g \rightarrow e) - N(e)\Gamma(e \rightarrow g) = 0. \]
And
\[ N(g)\Gamma(g \rightarrow e) = N(e)\Gamma(e \rightarrow g). \]

(b). From (a)
\[ \exp\left(-\frac{E_g}{\tau}\right) \exp\left(-\frac{E_e}{\tau}\right) = N(g)N(e) = \Gamma(e \rightarrow g)\Gamma(g \rightarrow e) = 2 \]
So
\[ \frac{E_e - E_g}{\tau} = \frac{\hbar \omega}{\tau} = \log(2) \]
\[ \tau = \frac{\hbar \omega}{\log 2} \]

[5] Anisotropic Well

(a).
\[ Z_1 = \sum_{n_1} \sum_{n_2} \sum_{n_3} \exp\left(-\frac{\hbar}{\tau}(\omega_1 n_1 + \omega_2 n_2 + \omega_3 n_3)\right) \]
\[ = \sum_{n_1} \exp\left(-\frac{\hbar \omega_1 n_1}{\tau}\right) \sum_{n_2} \exp\left(-\frac{\hbar \omega_2 n_2}{\tau}\right) \sum_{n_3} \exp\left(-\frac{\hbar \omega_3 n_3}{\tau}\right) \]
\[ = \frac{1}{(1 - \exp(-\frac{\hbar \omega_1}{\tau}))(1 - \exp(-\frac{\hbar \omega_2}{\tau}))(1 - \exp(-\frac{\hbar \omega_3}{\tau}))} \]

(b). Since it’s distinguishable
\[ Z_N = \sum_{n_{11}} \sum_{n_{12}} \sum_{n_{13}} \sum_{n_{21}} \sum_{n_{22}} \sum_{n_{23}} \cdots \sum_{n_{N1}} \sum_{n_{N2}} \sum_{n_{N3}} \cdots \sum_{k=1}^{N} \exp\left(-\frac{\hbar}{\tau}(\omega_1 n_{k1} + \omega_2 n_{k2} + \omega_3 n_{k3})\right) = Z_1^N. \]

(c).
\[ U = \tau^2 \frac{\partial \log(Z)}{\partial \tau} = N \sum_{n=1}^{3} \frac{\hbar \omega_n}{\exp(\frac{\hbar \omega_n}{\tau}) - 1} \]

(d). As $\tau \rightarrow \infty$, we Taylor expand the exponential $e^x \approx 1 + x$ to find
\[ U \rightarrow N \sum_{n=1}^{3} \frac{\hbar \omega_n}{1 + \frac{\hbar \omega_n}{\tau} - 1} = 3N\tau \]
\[ \frac{\partial U}{\partial \tau} = 3N \]