Physics 12c - Problem Set 2 - Solutions

April 22, 2016

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

Note first that:

$$\langle(\epsilon - \langle\epsilon\rangle)^2\rangle = \left\langle \epsilon^2 - 2\epsilon\langle\epsilon\rangle + \langle\epsilon\rangle^2 \right\rangle = \langle\epsilon^2\rangle - \langle\epsilon\rangle^2.$$

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

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

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

¿From these, with $d\beta/d\tau = -1/\tau^2$,

$$\begin{aligned}\tau^2\left(\frac{\partial U}{\partial\tau}\right)_V &= \tau^2\left(\frac{\partial U}{\partial\beta}\right)_V\frac{\partial\beta}{\partial\tau} = -\left(\frac{\partial U}{\partial\beta}\right)_V \\ &= \frac{\partial}{\partial\beta}\left(\frac{1}{Z}\frac{\partial Z}{\partial\beta}\right) = \frac{1}{Z}\frac{\partial^2 Z}{\partial\beta^2} - \frac{1}{Z^2}\left(\frac{\partial Z}{\partial\beta}\right)^2 \\ &= \langle\epsilon^2\rangle - \langle\epsilon\rangle^2\end{aligned}$$

[2] Energy Fluctuation (Problem 3.11 of Kittel/Kroemer)

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: $Z_N = Z_1^N/N!$,

$$\begin{aligned} F &= -\tau \log Z_N \\ &= \tau \log N! - \tau N \log Z_1 \\ &= \tau(N \log N - N) - \tau N \log(n_{Q_1} L) \\ &= \tau N[\log(n/n_{Q_1}) - 1], \end{aligned}$$

where $n = N/L$. With the help of $\frac{\partial}{\partial \tau} \log n_{Q_1} = 1/2\tau$:

$$\sigma = -(\partial F/\partial \tau)_n = N[\log(n_{Q_1}/n) + 3/2],$$

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, τ, 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

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

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

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

Since the specific heat $C_V = \partial E_i/\partial \tau_i$ 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 $\tau_1 = \tau_2 \cdot \cdot = \tau_k = \tau$. After a system consisting of k subsystems reaches thermal equilibrium, it can be regarded as a system with temperature τ 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,

$$S_{total}(E) = NS(\frac{E}{N}) = NS(\xi) \tag{S4}$$

Taylor expanding the total entropy,

$$\begin{aligned}
S_{tot}(E+\Delta E) =& S_{tot}(E) + \frac{\partial}{\partial E} S_{tot}(E)\Delta E + \frac{1}{2}\frac{\partial^2}{\partial E^2} S_{tot}(E)(\Delta E)^2 + \mathcal{O}(\Delta E)^3 \\
=& NS(\xi) + N\frac{\partial S(\xi)}{\partial E}\Delta E + \frac{1}{2}N\frac{\partial^2 S(\xi)}{\partial E^2}(\Delta E)^2 + \mathcal{O}(\Delta E)^3 \\
=& NS(\xi) + N\frac{\partial S(\xi)}{\partial \xi}\frac{\partial \xi}{\partial E}\Delta E + \frac{1}{2}N\frac{\partial^2 S(\xi)}{\partial \xi^2}\left(\frac{\partial \xi}{\partial E}\right)^2 (\Delta E)^2 + \mathcal{O}(\Delta E)^3 \\
=& NS + N\frac{\partial S}{\partial \xi}\left(\frac{\Delta E}{N}\right) + \frac{1}{2}N\frac{\partial^2 S}{\partial \xi^2}\left(\frac{\Delta E}{N}\right)^2 + \mathcal{O}(\Delta E)^3
\end{aligned}$$

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 $\partial^2 S/\partial \xi^2 = \frac{\partial}{\partial \xi}\frac{\partial S}{\partial \xi} = \frac{\partial}{\partial \xi}(1/\tau) = \frac{\partial \tau}{\partial \xi}\frac{\partial}{\partial \tau}(1/\tau) = -1/(C_v\tau^2)$, where $C_v = \partial \xi/\partial \tau$

[4] Atoms and Photons

(a).The rate of going from stat g to e is

$$N(g)\Gamma(g \to e).$$

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$$N(e)\Gamma(e \to g).$$

Therefore, at equilibrium

$$\frac{dN(e)}{dt} = N(g)\Gamma(g \to e) - N(e)\Gamma(e \to g) = 0.$$

And

$$N(g)\Gamma(g \to e) = N(e)\Gamma(e \to g).$$

(b). From (a)

$$\frac{\exp(-E_g/\tau)}{\exp(-E_e/\tau)} = \frac{N(g)}{N(e)} = \frac{\Gamma(e \to g)}{\Gamma(g \to e)} = 2$$

So

$$\frac{E_e - E_g}{\tau} = \frac{\hbar\omega}{\tau} = \log(2)$$
$$\tau = \frac{\hbar\omega}{\log 2}$$

[5] Anisotropic Well

(a).

$$\begin{aligned} Z_1 &= \sum_{n_1}\sum_{n_2}\sum_{n_3} \exp(-\frac{\hbar}{\tau}(\omega_1 n_1 + \omega_2 n_2 + \omega_3 n_3)) \\ &= \sum_{n_1} \exp(-\frac{\hbar\omega_1 n_1}{\tau}) \sum_{n_2} \exp(-\frac{\hbar\omega_2 n_2}{\tau}) \sum_{n_3} \exp(-\frac{\hbar\omega_3 n_3}{\tau}) \\ &= \frac{1}{(1-\exp(-\frac{\hbar\omega_1}{\tau})(1-\exp(-\frac{\hbar\omega_2}{\tau})(1-\exp(-\frac{\hbar\omega_3}{\tau})} \end{aligned}$$

(b).Since it's distinguishable

$$Z_N = \sum_{n_{11}}\sum_{n_{12}}\sum_{n_{13}}\sum_{n_{21}}\sum_{n_{22}}\sum_{n_{23}} \cdots \sum_{n_{N1}}\sum_{n_{N2}}\sum_{n_{N3}} \prod_{k=1}^{N} \exp(-\frac{\hbar}{\tau}(\omega_1 n_{k1} + \omega_2 n_{k2} + \omega_3 n_{k3})) = Z_1^N.$$

(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 $\tau \to \infty$, we Taylor expand the exponential $e^x \approx 1 + x$ to find

$$U \to N \sum_{n=1}^{3} \frac{\hbar\omega_n}{1 + \frac{\hbar\omega_n}{\tau} - 1} = 3N\tau$$

$$\frac{\partial U}{\partial \tau} = 3N$$