PHYSICS 140A : STATISTICAL PHYSICS
HW ASSIGNMENT #3 SOLUTIONS

(1) Consider a generalization of the situation in §4.4 of the notes where now three reservoirs are in thermal contact, with any pair of systems able to exchange energy.

(a) Assuming interface energies are negligible, what is the total density of states $D(E)$? Your answer should be expressed in terms of the densities of states functions $D_{1,2,3}$ for the three individual systems.

(b) Find an expression for $P(E_1, E_2)$, which is the joint probability distribution for system 1 to have energy E_1 while system 2 has energy E_2 and the total energy of all three systems is $E_1 + E_2 + E_3 = E$.

(c) Extremize $P(E_1, E_2)$ with respect to $E_{1,2}$. Show that this requires the temperatures for all three systems must be equal: $T_1 = T_2 = T_3$. Writing $E_j = E_j^* + \delta E_j$, where E_j^* is the extremal solution ($j = 1, 2$), expand $\ln P(E_1^* + \delta E_1 \, , \, E_2^* + \delta E_2)$ to second order in the variations δE_j. Remember that

$$S = k_{\rm B} \ln D \quad , \quad \bigg(\frac{\partial S}{\partial E}\bigg)_{V,N} = \frac{1}{T} \quad , \quad \bigg(\frac{\partial^2 S}{\partial E^2}\bigg)_{V,N} = -\frac{1}{T^2 C_V} \; .$$

(d) Assuming a Gaussian form for $P(E_1, E_2)$ as derived in part (c), find the variance of the energy of system 1,

$$\mathsf{Var}(E_1) = \big\langle (E_1 - E_1^*)^2 \big\rangle \; .$$

Solution :

(a) The total density of states is a convolution:

$$D(E) = \int\limits_{-\infty}^{\infty} \! dE_1 \int\limits_{-\infty}^{\infty} \! dE_2 \int\limits_{-\infty}^{\infty} \! dE_3 \; D_1(E_1)\, D_2(E_2)\, D_3(E_3)\, \delta(E - E_1 - E_2 - E_3) \; .$$

(b) The joint probability density $P(E_1, E_2)$ is given by

$$P(E_1, E_2) = \frac{D_1(E_2)\, D_2(E_2)\, D_3(E - E_1 - E_2)}{D(E)} \; .$$

(c) We set the derivatives $\partial \ln P / \partial E_{1,2} = 0$, which gives

$$\frac{\partial \ln P}{\partial E_1} = \frac{\partial \ln D_1}{\partial E_1} - \frac{\partial D_3}{\partial E_3} = 0 \quad , \quad \frac{\partial \ln P}{\partial E_2} = \frac{\partial \ln D_3}{\partial E_2} - \frac{\partial D_3}{\partial E_3} = 0 \; ,$$

where $E_3 = E - E_1 - E_2$ in the argument of $D_3(E_3)$. Thus, we have

$$\frac{\partial \ln D_1}{\partial E_1} = \frac{\partial \ln D_2}{\partial E_2} = \frac{\partial \ln D_3}{\partial E_3} \equiv \frac{1}{T} \, .$$

Expanding $\ln P(E_1^* + \delta E_1 \, , \, E_2^* + \delta E_2)$ to second order in the variations δE_j, we find the first order terms cancel, leaving

$$\ln P(E_1^* + \delta E_1 \, , \, E_2^* + \delta E_2) = \ln P(E_1^* \, , \, E_2^*) - \frac{(\delta E_1)^2}{2k_{\rm B} T^2 C_1} - \frac{(\delta E_2)^2}{2k_{\rm B} T^2 C_2} - \frac{(\delta E_1 + \delta E_2)^2}{2k_{\rm B} T^2 C_3} + \ldots \, ,$$

where $\partial^2 \ln D_j / \partial E^2 = -1/2k_{\rm B} T^2 C_j$, with C_j the heat capacity at constant volume and particle number. Thus,

$$P(E_1, E_2) = \frac{\sqrt{\det(\mathcal{C}^{-1})}}{2\pi k_{\rm B} T^2} \exp\left(- \frac{1}{2k_{\rm B} T^2} \, \mathcal{C}^{-1}_{ij} \, \delta E_i \, \delta E_j \right) ,$$

where the matrix $\mathcal{C}^{-1}$ is defined as

$$\mathcal{C}^{-1} = \begin{pmatrix} C_1^{-1} + C_3^{-1} & C_3^{-1} \\ C_3^{-1} & C_2^{-1} + C_3^{-1} \end{pmatrix} .$$

One finds

$$\det(\mathcal{C}^{-1}) = C_1^{-1} \, C_2^{-1} + C_1^{-1} \, C_3^{-1} + C_2^{-1} \, C_3^{-1} \, .$$

The prefactor in the above expression for $P(E_1, E_2)$ has been fixed by the normalization condition $\int \! dE_1 \int \! dE_2 \, P(E_1, E_2) = 1$.

(d) Integrating over E_2, we obtain $P(E_1)$:

$$P(E_1) = \int\limits_{-\infty}^{\infty} \! dE_2 \, P(E_1, E_2) = \frac{1}{\sqrt{2\pi k_{\rm B} \widetilde{C}_1 T^2}} \, e^{-(\delta E_1)^2 / 2k_{\rm B} \widetilde{C}_1 T^2} \, ,$$

where

$$\widetilde{C}_1 = \frac{C_2^{-1} + C_3^{-1}}{C_1^{-1} \, C_2^{-1} + C_1^{-1} \, C_3^{-1} + C_2^{-1} \, C_3^{-1}} \, .$$

Thus,

$$\langle (\delta E_1)^2 \rangle = \int\limits_{-\infty}^{\infty} \! dE_1 \, (\delta E_1)^2 = k_{\rm B} \widetilde{C}_1 T^2 \, .$$

(2) Consider a two-dimensional gas of identical classical, noninteracting, massive relativistic particles with dispersion $\varepsilon(\boldsymbol{p}) = \sqrt{\boldsymbol{p}^2 c^2 + m^2 c^4}$.

(a) Compute the free energy $F(T, V, N)$.

(b) Find the entropy $S(T,V,N)$.

(c) Find an equation of state relating the fugacity $z = e^{\mu/k_B T}$ to the temperature T and the pressure p.

Solution :

(a) We have $Z = (\zeta A)^N/N!$ where A is the area and

$$\zeta(T) = \int \frac{d^2p}{h^2}\, e^{-\beta\sqrt{p^2c^2+m^2c^4}} = \frac{2\pi}{(\beta hc)^2}\left(1+\beta mc^2\right) e^{-\beta mc^2} \,.$$

To obtain this result it is convenient to change variables to $u = \beta\sqrt{p^2c^2+m^2c^4}$, in which case $p\,dp = u\,du/\beta^2c^2$, and the lower limit on u is mc^2. The free energy is then

$$F = -k_B T\,\ln Z = Nk_B T\ln\!\left(\frac{2\pi\hbar^2c^2N}{(k_B T)^2 A}\right) - Nk_B T\ln\!\left(1+\frac{mc^2}{k_B T}\right) + Nmc^2 \,.$$

where we are taking the thermodynamic limit with $N\to\infty$.

(b) We have

$$S = -\frac{\partial F}{\partial T} = -Nk_B\ln\!\left(\frac{2\pi\hbar^2c^2N}{(k_B T)^2 A}\right) + Nk_B\ln\!\left(1+\frac{mc^2}{k_B T}\right) + Nk_B\left(\frac{mc^2+2k_B T}{mc^2+k_B T}\right) .$$

(c) The grand partition function is

$$\Xi(T,V,\mu) = e^{-\beta\Omega} = e^{\beta pV} = \sum_{N=0}^{\infty} Z_N(T,V,N)\, e^{\beta\mu N} \,.$$

We then find $\Xi = \exp\left(\zeta A\, e^{\beta\mu}\right)$, and

$$p = \frac{(k_B T)^3}{2\pi(\hbar c)^2}\left(1+\frac{mc^2}{k_B T}\right) e^{(\mu-mc^2)/k_B T} \,.$$

Note that

$$n = \frac{\partial(\beta p)}{\partial\mu} = \frac{p}{k_B T} \quad\Longrightarrow\quad p = nk_B T \,.$$

(3) A three-level system has energy levels $\varepsilon_0 = 0$, $\varepsilon_1 = \Delta$, and $\varepsilon_2 = 4\Delta$. Find the free energy $F(T)$, the entropy $S(T)$ and the heat capacity $C(T)$.

Solution :

We have

$$Z = \mathrm{Tr}\; e^{-\beta H} = 1 + e^{-\beta\Delta} + e^{-4\beta\Delta} \,.$$

The free energy is

$$F = -k_B T \ln Z = -k_B T \ln\big(1 + e^{-\Delta/k_B T} + e^{-4\Delta/k_B T}\big) \, .$$

To find the entropy S, we differentiate with respect to temperature:

$$S = -\frac{\partial F}{\partial T}\bigg|_{V,N} = k_B \ln\big(1 + e^{-\Delta/k_B T} + e^{-4\Delta/k_B T}\big) + \frac{\Delta}{T} \cdot \frac{e^{-\Delta/k_B T} + 4e^{-4\Delta/k_B T}}{1 + e^{-\Delta/k_B T} + e^{-4\Delta/k_B T}} \, .$$

Now differentiate with respect to T one last time to find

$$C_{V,N} = k_B \left(\frac{\Delta}{k_B T}\right)^2 \cdot \frac{e^{-\Delta/k_B T} + 16\, e^{-4\Delta/k_B T} + 9\, e^{-5\Delta/k_B T}}{\big(1 + e^{-\Delta/k_B T} + e^{-4\Delta/k_B T}\big)^2} \, .$$

(4) Consider a many-body system with Hamiltonian $\hat{H} = \frac{1}{2}\hat{N}(\hat{N}-1)\,U$, where $\hat{N}$ is the particle number and $U > 0$ is an interaction energy. Assume the particles are identical and can be described using Maxwell-Boltzmann statistics, as we have discussed. Assuming $\mu = 0$, plot the entropy S and the average particle number N as functions of the scaled temperature $k_B T/U$. (You will need to think about how to impose a numerical cutoff in your calculations.)

Solution :

The grand partition function is

$$\Xi(T,\mu) = e^{-\beta\Omega} = e^{\beta p V} = \sum_{N=0}^{\infty} e^{-N(N-1)\beta U/2} \, ,$$

where we have taken $\mu = 0$ and we have assumed that each state of definite particle number ,$|\, N \,\rangle$, is nondegenerate. We then have the grand potential

$$\Omega(T,\mu) = -k_B T \ln \Xi = -k_B T \ln\left(\sum_{N=0}^{\infty} e^{-N(N-1)\,U/2k_B T}\right)$$

The entropy is

$$S = -\frac{\partial\Omega}{\partial T} = k_B \ln\left(\sum_{N=0}^{\infty} e^{-N(N-1)\,U/2k_B T}\right) + \frac{U}{2T} \cdot \frac{\sum_{N=0}^{\infty} N(N-1)\, e^{-N(N-1)U/2k_B T}}{\sum_{N=0}^{\infty} e^{-N(N-1)\,U/2k_B T}} \, .$$

This must be evaluated numerically. The results are shown in Fig. 1. Note that $\lim_{T\to 0} S(T) = k_B \ln 2$, which indicates a doubly degenerate ground state. This is because both $|\, N = 0 \,\rangle$ and $|\, N = 1 \,\rangle$ have energy $E_0 = E_1 = 0$.

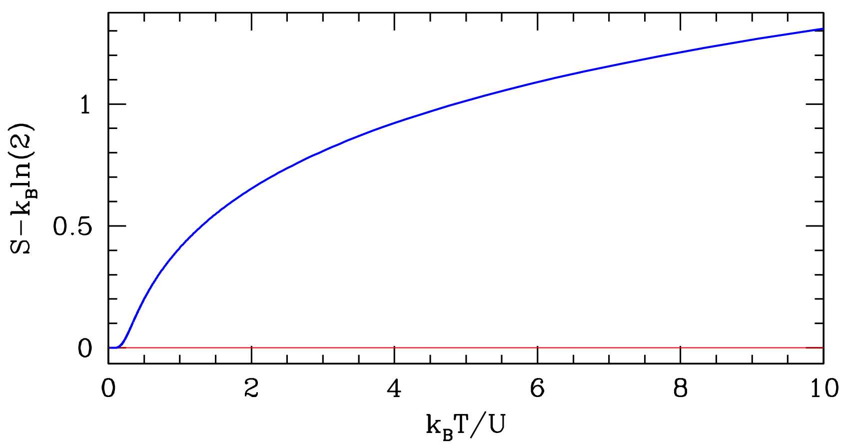

Figure 1: Entropy as a function of dimensionless temperature for problem #4. Note that $S(T=0) = \ln 2$ because the states $|\, N=0 \,\rangle$ and $|\, N=1 \,\rangle$ are degenerate.