Problem 1

Kittel & Kroemer, Chapter 3, problem 9 [Partition function for two systems]: 2 points

Show that the partition function $Z(1+2)$ of two independent systems **1** and **2** in thermal contact at a common temperature τ is equal to the product of the partition functions of the separate systems:

$$Z(1+2) = Z(1)Z(2)$$

Partition function formula:

$$Z = \sum_s e^{-\epsilon_s/\tau}$$

Let's multiply two of these together

$$Z_1 = \sum_{s_1} e^{-\epsilon_{s_1}/\tau}$$

$$Z_2 = \sum_{s_2} e^{-\epsilon_{s_2}/\tau}$$

$$Z_1 Z_2 = \sum_{s_1} \sum_{s_2} e^{-\epsilon_{s_1}/\tau} e^{-\epsilon_{s_2}/\tau}$$

$$= \sum_{s_1} \sum_{s_2} e^{(-\epsilon_{s_1}-\epsilon_{s_2})/\tau}$$

Somehow we have to deal with these summations.

The states availiable to system 1 and 2 combined are $g_{1,2} = g_1 g_2$, so they make sense logically.

States in the combined system $\bold1 + \bold2$ can be represented as (s_1, s_2). The energy ϵ depends on $U(s)$, and $\epsilon_{s_1,s_2} = U_{tot}(s_1, s_2) = U_1(s_1) + U_2(s_2) = \epsilon_{s_1} + \epsilon_{s_2}$.

As such, $Z(\bold1 + \bold2) = \sum_{(s_1,s_2)} e^{-\epsilon_{(s_1,s_2)}/\tau}$. All states possible can be indexed by two summations, so

$$\sum_{(s_1,s_2)} e^{-\epsilon_{(s_1,s_2)}/\tau} = \sum_{s_1} \sum_{s_2} e^{(-\epsilon_{s_1}-\epsilon_{s_2})/\tau}$$

$$Z_{1,2} = Z_1 Z_2$$

Problem 2

Adapted from: Kittel & Kroemer, Chapter 3, problem 2 [Magnetic susceptibility]: 6 points

(a): 2 points

Find the partition function first for a single spin, then for N independent spins, using the result from the first problem on this homework set.

(b): 2 points

Find the magnetization M directly from the partition function using the Boltzmann factor. (You don't eed to find F as the book suggests). You can work either with the energy U or the spin excess s, which are related as $U = -2mb\langle s \rangle$. M is then a function of U or s.

(c): 1 point

Show that the magnetic susceptibility is $\chi = nm^2/\tau$ in the high-temperature limit.

(d): 1 point

Compare your answer with the one you obtained on Problem 2 of the previous homework assignment. There you calculated the dimensionless magnetization per atom, M/Nm, for a spin system. (That answer was only valid at high temperatures where $s \ll N$.) Calculate the magnetic susceptibility from that problem, and compare it with your answer to part (c) above. The inverse temperature dependence you found for the magnetic susceptibility is called the "Curie Law", and is very famous.

(a)

For one particle:

$$s = \{\uparrow, \downarrow\}$$
$$Z(s) = e^{-\epsilon_\uparrow/\tau} + e^{-\epsilon_\downarrow/\tau}$$
$$\epsilon_s = U(s) = \pm mb$$
$$Z(s) = e^{-mb/\tau} + e^{mb/\tau} = 2\cosh(mb/\tau)$$

N particles:

$$Z(s^N) = Z^N(s) = \left(e^{-mb/\tau} + e^{mb/\tau}\right)^N$$
$$= 2^N \cosh^N(mb/\tau)$$

(b)

If all spins are aligned we have $M = Nm/V$, but unalignd they are

$$M = \langle 2s \rangle m/V = 2\langle s \rangle m/V$$

Let's find $\langle s \rangle$ using Z

$$\mathcal{U} = \tau^2 \frac{\partial \ln Z}{\partial \tau} = -Nmb \tanh(mb/\tau)$$
$$\mathcal{U} = -2mb\langle s \rangle$$
$$\langle s \rangle = \frac{-Nmb \tanh(mb/\tau)}{-2mb} = \frac{N \tanh(mb/\tau)}{2}$$
$$M = 2\langle s \rangle m/V = (Nm/V)\tanh(mb/\tau) = nm \tanh(mb/\tau)$$

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In [25]:  import sympy as sym
          from sympy import cosh, ln, tanh

          n, N, m, b, tau = sym.symbols('n N m b tau')

          Z = 2**N * (cosh(m*b/tau))**N
          sym.diff(ln(Z), tau) * tau**2
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Out[25]:
$$-\frac{Nbm \sinh\left(\frac{bm}{\tau}\right)}{\cosh\left(\frac{bm}{\tau}\right)}$$

Yippie!

(c)

$$\chi = \frac{\partial M}{\partial b} = \frac{\partial}{\partial b} nm \tanh(mb/\tau)$$
$$= nm^2/\tau \left(1 - \tanh^2(mb/\tau)\right)$$

Since $\lim_{x \to 0} \tanh = 0$, this gives us

$$\lim_{\tau \to \infty} \chi = nm^2/\tau \left(1 - 0^2\right) = nm^2/\tau$$

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In [28]:  M = n*m*tanh(m*b/tau)
          sym.diff(M, b)
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Out[28]:
$$\frac{m^2 n \left(1 - \tanh^2\left(\frac{bm}{\tau}\right)\right)}{\tau}$$

(d) The end result didn't have a volume/density dependency

$$\tau = \frac{-m^2 b^2 N}{-Mb}$$
$$M = \frac{bNm^2}{\tau}$$
$$\chi = \frac{Nm^2}{\tau}$$

Problem 3

Kittel & Kroemer, Chapter 3, problem 4 [Energy fluctuations]: 3 points

Consider a system of fixed volume in thermal contact with a reservoir. Show that the mean square fluctuation in the energy of the system is

$$\langle (\epsilon - \langle \epsilon \rangle)^2 \rangle = \tau^2 (\partial U / \partial \tau)_V.$$

Here U is the conventional symbol for $\langle \epsilon \rangle$.

Hint: Use the partition function Z to relate $\partial U / \partial \tau$ to the mean square fluctuation. Also, multiply out the term $(\cdots)^2$.

Note: The temperature τ of a system is a quantity that by definition does not fluctuate in value when the system is in thermal contact with a reservoir. Any other attitude would be inconsistent with our definition of the temperature of a system. The energy of such a system may fluctuate, but the temperature does not. Some workers to not adhere to a rigorous definition of temperature. Thus Landau and Lifshitz give the result

$$\langle (\Delta \tau)^2 \rangle = \tau^2 / C_V,$$

but this should be viewed as just another form of the result of this problem with $\Delta \tau$ set ot $\Delta U / C_V$. We know that $\Delta U = C_V \Delta \tau$, whence $\langle (\Delta U)^2 \rangle = \tau^2 C_V$, which is our result.

Fortunately we worked through the LHS in class

First off we'll expand the variance.

$$\langle (\epsilon - \langle \epsilon \rangle)^2 \rangle = \langle \epsilon^2 \rangle - \langle \epsilon \rangle^2$$
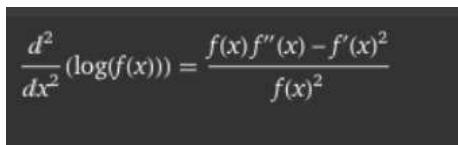
We have formulas for each of these

$$\langle \epsilon \rangle = \mathcal{U} = -\frac{\partial \ln Z}{\partial \beta}$$

$$\langle \epsilon^2 \rangle = \frac{1}{Z} \frac{\partial^2 Z}{\partial \beta^2}$$

(I use $\mathcal{U}$ since we're in canonical ensemble)
This gives us the left side in terms of Z

$$\langle \epsilon^2 \rangle - \langle \epsilon \rangle^2 = \frac{1}{Z} \frac{\partial^2 Z}{\partial \beta^2} - \left(\frac{\partial \ln Z}{\partial \beta} \right)^2 = \frac{\partial^2 \ln Z}{\partial \beta^2}$$

That last step comes down to chain rule I believe.

$$\frac{d^2}{dx^2} (\log(f(x))) = \frac{f(x) f''(x) - f'(x)^2}{f(x)^2}$$

Let's convert from $\mathcal{U}$ to Z on the right side. We'll need to go from τ to β

$$\frac{\partial}{\partial \tau} = \frac{\partial \beta}{\partial \tau} \frac{\partial}{\partial \beta} = -\frac{1}{\tau^2} \frac{\partial}{\partial \beta}$$

This gives us

$$\tau^2 \frac{\partial U}{\partial \tau} = \tau^2 \frac{\partial}{\partial \tau} \left(-\frac{\partial}{\partial \beta} \ln Z \right)$$

$$= \frac{\partial^2 \ln Z}{\partial \beta^2}$$