Solution for week 2

PDF version of solutions

1. Entropy and Temperature (K&K 2.1)
   a) We begin by finding the entropy given the provided multiplicity.

   \[ S(U, N) = k_B \log g(U, N) \quad (1) \]
   \[ = k_B \log \left( C U^{3N/2} \right) \quad (2) \]
   \[ = k_B \left( \log C + \log \left( U^{3N/2} \right) \right) \quad (3) \]
   \[ = k_B \log C + \frac{3}{2} N k_B \log U \quad (4) \]

   In the last two steps there, we made use of properties of \( \log \). If these are not obvious to you, you absolutely must take the time to review the properties of logarithms. They are absolutely critical to this course!

   \[ T = \left( \frac{\partial S}{\partial U} \right)_{V, N} \quad (6) \]
   \[ = \frac{3}{2} N k_B \frac{1}{U} \quad (7) \]
   \[ U = \frac{3}{2} N k_B T \quad (8) \]

   Yay.

   b) We just need to take one more derivative, since we already found \( \left( \frac{\partial S}{\partial U} \right)_{V, N} \) in part (a).

   \[ \left( \frac{\partial^2 S}{\partial U^2} \right)_{V, N} = -\frac{3}{2} N k_B \frac{1}{U^2} \quad (9) \]
   \[ < 0, \quad (10) \]

   where in the last step we only needed to assume that \( N > 0 \) (natural for the number of particles) and that the energy \( U \) is real (which it always must be). Thus ends the solution.

   Because the second derivative of the entropy is always negative, the first derivative is monotonic, which means that the temperature (which is positive) will always increase if you increase the energy of the system and vice versa.

2. Paramagnetism (K&K 2.2)

   Okay, here we can understand the fractional magnetization if we think \( N m \) as being the maximum possible magnetization (all spins are pointing the same way). The quantity \( s \) is defined as the total value of the spin. Because each spin has a value of \( \pm \frac{1}{2} \), twice \( s \) per particle also tells us the fractional magnetization.

   To convert from \( S(s) \) to \( S(U) \) we need to relate the energy to the excess spin \( s \). This relies on the energy expression

   \[ U = -B2sm \quad (11) \]

   which uses the equations given. At this point, it is a simple substitution of \( s = -\frac{U}{2mB} \): \n
   \[ S(U) = S_0 - k_B \frac{2 \left( \frac{U}{2mB} \right)^2}{N} \quad (12) \]
   \[ = S_0 - k_B \frac{U^2}{2m^2B^2N} \quad (13) \]

   To determine \( 1/kT \), we just need to take a derivative:

   \[ \frac{1}{T} = \left( \frac{\partial S}{\partial U} \right)_V \quad (14) \]
   \[ = -k_B \frac{U}{m^2B^2N} \quad (15) \]
   \[ \frac{1}{k_BT} = \frac{U}{m^2B^2N} \quad (16) \]

   At this point we have finished the problem, with just a bit of algebra. It is helpful at this stage to do a bit of checking. The left hand side here is an inverse energy. On the right hand side, \( mB \) is an energy, so we have an energy over an
energy squared, so all is good. $N$, of course, is dimensionless. However, it is also extensive, as is $U$. This is good, because the left hand side is intensive, so the right hand side should be also.

The equilibrium fractional magnetization is thus given by

$$\frac{\mu_{\text{tot}}}{Nm} = -\frac{U}{NmB}$$  \hspace{1cm} (17)

$$= -\frac{1}{NmB} \left( -\frac{m^2 B^2 N}{kT} \right)$$  \hspace{1cm} (18)

$$= \frac{mB}{kT}$$  \hspace{1cm} (19)

Thus the fractional magnetization is just equal to the ratio between $mB$ (which is the energy of one spin in the magnetic field) to $kT$ (which is a measure of the available energy).

**Of interest** This relationship is very different than the one we saw in the previous problem! Previously, we saw the temperature being proportional to the internal energy, and here we see it as inversely proportional, meaning that as the energy approaches zero the temperature becomes infinite.

We also previously had an energy that was positive. Here we have a negative sign, which suggests that the energy should be negative in order to maintain a positive temperature. This relates to the energy of a single spin always being either positive or negative, with equal and opposite options.

This problem illustrates a weird phenomenon: if the energy is positive, then we must conclude that the temperature is negative. Furthermore, the temperature discontinuously passes from $\infty$ to $-\infty$ as the energy passes through zero. There are different interpretations of these “negative temperature” states. You cannot reach them by heating a system (adding energy via heating), and they cannot be exist in equilibrium if the system has contact with any quantity of material that can have kinetic energy. So I consider these to be unphysical (or non-equilibrium) states. Since temperature is an equilibrium property, I would not say that a negative temperature is physically meaningful. That said, there is an analogy that can be made to population inversion in a laser, which is a highly non-equilibrium system that is pretty interesting.

3. **Quantum harmonic oscillator** (K&K 2.3)

a) Given the multiplicity, we just need to take a logarithm, and simplify.

$$S(N, n) = k \log g(N, n) \quad \text{(20)}$$

$$= k \log \left( \frac{(N + n - 1)!}{n!(N - 1)!} \right) \quad \text{(21)}$$

$$\approx k \left( \log(N + n + 1) - \log n! - \log(N - 1)! \right) \quad \text{(22)}$$

$$\approx k \left( (N + n) \log(N + n) - n \log n - N \log N \right) \quad \text{(23)}$$

$$= k \left( N \log \left( \frac{N + n}{N} \right) + n \log \left( \frac{N + n}{n} \right) \right) \quad \text{(24)}$$

$$= k \left( N \log (1 + n/N) + n \log (1 + N/n) \right) \quad \text{(25)}$$

You need not simplify your answer this far, but it is good to get practice simplifying answers, particularly involving logarithms. In particular, it is usually helpful at this point in a computation to verify that the entropy is indeed extensive. Both $N$ (the number of oscillators) and $n$ (the sum of all the quantum numbers of all the oscillators) are extensive quantities. Thus $n/N$ and $N/n$ are intensive, which is good because otherwise we could not add them to 1. Each term is now clearly extensive, and the entropy behaves as we expect.
b) Now we want to find $U(T)$, which will require us to find $S(U)$ (via simple substitution of $n = U/\hbar\omega$) and $T$ from a derivative of that.

$$S(U) = Nk \log \left( 1 + \frac{U}{Nh\omega} \right) + Nk \frac{U}{Nh\omega} \log \left( 1 + \frac{Nh\omega}{U} \right)$$

(27)

Now we just have a derivative to take, and then a mess of algebra to simplify.

$$\frac{1}{T} = \left( \frac{\partial S}{\partial U} \right)_{N,V}$$

$$= \frac{Nk}{1 + \frac{U}{Nh\omega}}$$

$$+ Nk \frac{1}{Nh\omega} \log \left( 1 + \frac{Nh\omega}{U} \right)$$

$$- Nk \frac{U}{Nh\omega} \frac{1}{1 + \frac{Nh\omega}{U^2}}$$

(28)

(29)

(30)

(31)

And now to simplify...

$$\frac{\hbar\omega}{kT} = \frac{1}{1 + \frac{U}{Nh\omega}} + \log \left( 1 + \frac{Nh\omega}{U} \right) - \frac{Nh\omega}{1 + \frac{Nh\omega}{U}}$$

$$= \frac{Nh\omega}{1 + \frac{Nh\omega}{U}} + \log \left( 1 + \frac{Nh\omega}{U} \right) - \frac{Nh\omega}{1 + \frac{Nh\omega}{U}}$$

$$= \log \left( 1 + \frac{Nh\omega}{U} \right)$$

(32)

(33)

(34)

Well, didn’t that simplify down nicely? The key was to multiply the first term by $Nh\omega/U$ so that it shared a denominator with the last term (and ended up being equal and opposite).

Solving for $U$ is not bad at all, now, we’ll just take an exponential of both sides:

$$e^{\frac{Nh\omega}{U}} = 1 + \frac{Nh\omega}{U}$$

(35)

$$\frac{Nh\omega}{U} = e^{\frac{Nh\omega}{U}} - 1$$

(36)

$$U = \frac{Nh\omega}{e^{\frac{Nh\omega}{U}} - 1}$$

(37)

Note As I mentioned in the homework, this is the hard way to solve this problem. That said, it wasn’t actually particularly hard, you just need to be comfortable doing algebra with logarithms, and simplifying annoying ratios.