Kittel & Kroemer, Chapter 2, problem 1 [Entropy and temperature]: 3 points

Suppose $g(U) = CU^{3N/2}$, where C is a constant and N is the number of particles. (This form of g(U) actually applies to an ideal gas.)

(a)

Show that $U = \frac{3}{2}N\tau$.

The temperature τ is defined as

$$1/\tau \equiv (\partial \sigma/\partial U)_{N,V}$$
.

The entropy is given by

$$\begin{split} \sigma &\equiv \ln g \\ &= \ln(CU^{3N/2}) \\ &= \ln C + \frac{3N}{2} \ln U. \end{split}$$

Thus

$$\begin{split} 1/\tau &= \frac{\partial}{\partial U} [\ln C + \frac{3N}{2} \ln U] \\ &= \frac{3N}{2U}, \end{split}$$

which we can rearrange to find

$$U = \frac{3}{2}N\tau.$$

Note: This looks like the equipartition theorem! Each particle gets $\frac{1}{2}\tau$ energy for each of its degrees of freedom; each particle in a 3D ideal gas has 3 degrees of freedom.

(b)

Show that $(\partial^2 \sigma/\partial U^2)_N$ is negative.

From above,

$$\sigma = \ln C + \frac{3N}{2} \ln U.$$

So

$$(\partial^2 \sigma / \partial U^2)_N = \frac{\partial}{\partial U} \left(\frac{3N}{2U} \right)_N$$
$$= -\frac{3N}{2U^2}.$$

Since N > 0, this quantity is always negative.

(b)

(a)

Kittel & Kroemer, Chapter 2, problem 2 [paramagnetism]: 3 points

Find the equilibrium value at temperature τ of the fractional magnetization

$$M/Nm = 2\langle s \rangle/N$$

of the system of N spins each of magnetic moment m in a magnetic field B. The spin excess is 2s. Take the entropy as the logarithm of the multiplicity g(N, s) as given in (1.35):

$$\sigma(s) \simeq \ln g(N, 0) - 2s^2/N,$$

for $|s| \ll N$.

Hint 1: Show that in this approximation,

$$\sigma(U) = \sigma_0 - U^2 / 2m^2 B^2 N$$

with $\sigma_0 = \ln g(N,0)$. Further, show that $1/\tau = -U/m^2B^2N$, where U denotes $\langle U \rangle$, the thermal average energy.

Hint 2: In order to calculate the temperature, you need first to express the entropy in terms of the energy U, rather than the spin excess s. So write s in terms of U, and substitute into the formula for σ .

We showed in class (and it is given near the end of Chapter 1) that the energy of this system is given by

$$U = -2smB$$
,

which allows us to translate between the spin excess and the energy: s = -U/(2mB). Plugging this into the given entropy equation, we have

$$\sigma(U) = \sigma_0 - \frac{U^2}{2m^2B^2N}.$$

Now we can write down the temperature:

$$\begin{split} 1/\tau &\equiv (\partial \sigma/\partial U)_{N,V} \\ &= -\frac{U}{m^2 B^2 N}. \end{split}$$

Because we are now considering a system that is in contact with a reservoir at temperature τ , here U refers to its thermal average; we can connect this to the spin excess by taking the thermal average of the first equation we used above, $U = -2\langle s \rangle mB$. Translating back to the spin excess,

$$1/\tau = -\frac{-2\langle s \rangle mB}{m^2B^2N}$$
$$= -\frac{-2\langle s \rangle}{mBN},$$

or

$$\frac{2\langle s\rangle}{N} = -\frac{mB}{\tau}.$$

This result (specifically the $1/\tau$ dependence) is called Curie's law: it indicates that it gets more difficult to magnetize a material by applying a magnetic field as the temperature grows!

Page 3

Kittel & Kroemer, Chapter 2, problem 3 [quantum harmonic oscillator]: 4 points

(a)

Find the entropy of a set of N oscillators of frequency ω as a function of the total quantum number n. Use the multiplicity function (1.55) and make the Stirling approximation $\ln N! \simeq N \ln N - N$. Replace N-1 by N.

The multiplicity for a system of oscillators is given as (1.55)

$$g(N,n) = \frac{(N+n-1)!}{n!(N-1)!}.$$

For large enough N, it won't make a difference to replace N-1 in the numerator and denominator by N. So, the entropy is

$$\begin{split} \sigma(N,n) &\equiv \ln g(N,n) = \ln \frac{(N+n)!}{n!N!} \\ &= \ln(N+n)! - \ln n! - \ln N! \\ &\simeq (N+n)\ln(N+n) - (N+n) - n\ln n + n - N\ln N + N \\ &= (N+n)\ln(N+n) - n\ln n - N\ln N \\ &= N\ln \frac{N+n}{N} + n\ln \frac{N+n}{n} \\ &= N\ln(1+n/N) + n\ln(1+N/n). \end{split}$$

[Grader: either of the last three lines is OK.]

(b)

Let U denote the total energy $n\hbar\omega$ of the oscillators. Express the entropy as $\sigma(U, N)$. Show that the total energy at temperature τ is

$$U = \frac{N\hbar\omega}{e^{\hbar\omega/\tau} - 1}.$$

This is the Planck result; it is derived again in Chapter 4 by a powerful method that does not require us to find the multiplicity function.

We can replace n in the expression for entropy above with $U/\hbar\omega$:

$$\sigma(U,N) = N \ln \left(1 + \frac{U}{N\hbar\omega} \right) + \frac{U}{\hbar\omega} \ln \left(1 + \frac{N\hbar\omega}{U} \right).$$

Then we can write down the temperature:

$$\begin{split} \frac{1}{\tau} &\equiv \left(\frac{\partial \sigma}{\partial U}\right)_N = N \frac{1}{1 + \frac{U}{N\hbar\omega}} \frac{1}{N\hbar\omega} + \frac{1}{\hbar\omega} \ln\left(1 + \frac{N\hbar\omega}{U}\right) + \frac{U}{\hbar\omega} \frac{1}{1 + \frac{N\hbar\omega}{U}} \left(-\frac{N\hbar\omega}{U^2}\right) \\ &= \frac{1}{\hbar\omega} \left[\frac{1}{1 + \frac{U}{N\hbar\omega}} + \ln\left(1 + \frac{N\hbar\omega}{U}\right) - \frac{N\hbar\omega}{1 + \frac{N\hbar\omega}{U}}\right]. \end{split}$$

(b)

(a)

The first and third terms above actually cancel each other out, and we are left with

$$\frac{1}{\tau} = \frac{1}{\hbar\omega} \ln\left(1 + \frac{N\hbar\omega}{U}\right).$$

We can now rearrange and solve for U:

$$\frac{\hbar\omega}{\tau} = \ln\left(1 + \frac{N\hbar\omega}{U}\right),\,$$

or

$$e^{\hbar\omega/\tau} = 1 + \frac{N\hbar\omega}{U},$$

or

$$U = \frac{N\hbar\omega}{e^{\hbar\omega/\tau} - 1}.$$

It's the Planck distribution!

(b)

Consider two systems of 10 spins each, i.e. $N_1 = N_2 = 10$. The systems are placed in a magnetic field, so configurations with different total spin have different energy. The systems are isolated from their surroundings, so their total energy (hence their total spin) is constant. Calculate all quantities in this problem exactly.

(a): 1 point

Initially, system 1 has all spins up, and system 2 has 2 up and 8 down. Using the notation of K&K, where 2s stands for the net excess of up spins, we have $s_1 = 5$, and $s_2 = -3$. What is the multiplicity of the combined system in its initial configuration?

The multiplicity of the individual two-state systems like this is given by the binomial coefficients:

$$g_1^0 = \frac{10!}{10!1!} = 1$$

 $g_2^0 = \frac{10!}{2!8!} = 45.$

Thus the initial multiplicity of the combined system is

$$(g_1g_2)^0 = g_1^0g_2^0 = 45.$$

(b): 2 points

Put the two systems in thermal contact with each other, so they can exchange energy with each other, but not with the outside world. So $s = s_1 + s_2 = 2$. Make a table showing all allowed combinations of s_1 and s_2 , the individual multiplicities g_1 and g_2 , and the combined multiplicity g_1g_2 . (Note: If you prefer, you can choose to label the configurations by the number of up spins, N_{\uparrow} , rather than by the spin excess s.) What is the total possible number of configurations available to the combined system? How much did the total entropy increase as a result of putting the two systems in thermal contact?

The highest possible s_1 is 5 (this means all of the spins are up); we will count down from there. For each g we will use the multiplicity $g(10, s) = \frac{10!}{(5+s)!(5-s)!}$. Also recall that 0! = 1.

s_1	s_2	g_1	g_2	$g_{1}g_{2}$
5	-3	1	45	45
4	-2	10	120	1200
3	-1	45	210	9450
2	0	120	252	30240
1	1	210	210	44100
0	2	252	120	30240
-1	3	210	45	9450
-2	4	120	10	1200
-3	5	45	1	45
			Sum:	125970

(b): 2 points

(a): 1 point

There are 125970 possibilities available to the combined system. The initial entropy before contact was $\sigma^0 = \ln[(g_1g_2)^0] = \ln(45)$. The final entropy after thermal contact is $\sigma = \ln(125970)$. The change in entropy is thus $\sigma - \sigma^0 = 7.94$.

(c): 1 points

What is the total probability that the combined system will be found in the most probable state $(s_1 = \hat{s}_1)$, or in one of the nearby states with $s_1 = \hat{s}_1 \pm 1$? What is the probability that the system will be found in its initial state?

The probability of being found in the most probable state $(s_1 = \hat{s}_1 = 1)$ is 44100/125970 = .350. The probability of being found in one of the nearby states with $s_1 = \hat{s}_1 \pm 1 = 0, 2$ is (30240 + 30240)/125970 = .480, so the combined probability of being found in any of these three states is .350 + .480 = .83. Quite likely!

(c): 1 points

The probability of being found in the starting state $s_1 = 5$ is 45/125970 = .000357. Very unlikely.

Now let's combine what you learned in problems 2 and 4 above. Consider two systems of spins in a uniform magnetic field. The energy of a state with spin excess s is U = -2smB, where m is the magnetic moment of a spin and B is the magnetic field. System 1 has $N_1 = 10^4$ spins, while system 2 has $N_2 = 2 \times 10^4$ spins. Initially, system 1 has half its spins up and half down, so its spin excess is $s_1 = 0$. Initially, system 2 has a spin excess $s_2 = 1500$. Use the Gaussian approximation to the multiplicity that we derived in class for all parts of this problem, and ignore the first term $\sqrt{\frac{2}{\pi N}}$.

(a): 1 point

What is the initial energy and entropy of each system?

The multiplicity we will work with is

$$g(N,s) \sim 2^N e^{-2s^2/N}$$

ignoring the $\sqrt{2/\pi N}$ prefactor. Thus the initial multiplicities of the systems are

$$g_1^0(10^4, 0) = 2^{10^4}$$

 $g_2(2 \times 10^4, 1500) = 2^{2 \times 10^4} e^{-(1500)^2/10^4}.$

The entropies are thus

$$\sigma_1^0 = \ln(g_1^0) = 6931$$

 $\sigma_2^0 = \ln(g_2^0) = 13640.$

The energies are

$$U_1^0 = 0$$

$$U_2^0 = -3000mB$$

(b): 2 points

What is the initial temperature of each system? (Your answer for system 1 may be counter-intuitive.) Notice that the temperature τ in our textbook has units of energy.

To find temperature, we must write the entropy in terms of the energy. The entropy is

$$\sigma \equiv \ln g = \ln 2^N + \ln(e^{-2s^2/N})$$

= $N \ln 2 - 2s^2/N$.

Since s = -U/(2mB), we can write the entropy as

$$\sigma = N \ln 2 - \frac{2U^2}{4m^2B^2N}.$$

Then

$$1/\tau \equiv \left(\frac{\partial \sigma}{\partial U}\right)_N = -\frac{U}{m^2 B^2 N},$$

(a): 1 point

(b): 2 points

or

$$\tau = -\frac{m^2 B^2 N}{U}.$$

Using the initial energies for part (a), we can find that the initial temperatures for the two spin systems are

$$\begin{split} \tau_1^0 &= -\frac{m^2 B^2 N_1}{U_1^0} = \infty \\ \tau_2^0 &= -\frac{m^2 B^2 N_2}{U_2^0} = \frac{2mB \times 10^4}{3000} = 6.67mB. \end{split}$$

(b): 2 points

(c): 1 point

Infinite temperature! It won't burn you; it simply means that adding a little bit of energy to System 1 won't increase the number of available states at all (it's already at the maximum possible), so when it comes into thermal contact with another system, energy is guaranteed to flow out of system 1 and into the other system (as long as the other system isn't also at $\tau = \infty$).

(c): 1 point

Bring the two systems into thermal contact with each other. In thermal equilibrium, what is the average spin excess for each system, \hat{s}_1 and \hat{s}_2 ? What is the final (common) temperature of the two systems?

From the previous part of the problem, we see that the temperature of these spin systems is

$$\tau = -\frac{m^2 B^2 N}{U},$$

or written in terms of the spin excess,

$$\tau = \frac{mBN}{2s}.$$

In thermal equilibrium, we know the temperatures τ_1 and τ_2 of the two systems should be equal to each other, and also equal to the temperature of the *combined* system:

$$\frac{mBN_1}{2\hat{s}_1} = \frac{mBN_2}{2\hat{s}_2} = \frac{mBN}{2s}$$

or

$$\frac{N_1}{\hat{s}_1} = \frac{N_2}{\hat{s}_2} = \frac{N}{s}.$$

From the problem statement, $N = 3 \times 10^4$ and s = 1500. Thus

$$\hat{s}_1 = \frac{N_1}{N} s = 500$$

$$\hat{s}_2 = \frac{N_2}{N} s = 1000.$$

The final common temperature is

$$\tau = \frac{mBN}{2s} = 10mB.$$

Problem 5 continued on next page...

(d): 2 points

By how much did the total entropy increase during the process of thermal equilibration? (Hint: Ignore the constant terms $N \ln 2$ and just look at the part of the entropy that changed. You may approximate the entropy by $\ln(g_1g_2)_{\text{max}}$, so don't do any sums or integrals!) By what factor did the total multiplicity of the combined system increase?

The change in total entropy of the system can be found from the initial and final multiplicities, using $g(N,s) \sim 2^N e^{-2s^2/N}$ as above:

$$\sigma^{f} - \sigma^{0} = \ln(g_{1}g_{2})_{\text{max}} - \ln(g_{1}g_{2})_{0} = \ln\left(\frac{(g_{1}g_{2})_{\text{max}}}{(g_{1}g_{2})_{0}}\right)$$

$$= \ln\left(\frac{2^{N_{1}}2^{N_{2}}e^{-2\hat{s}_{1}^{2}/N_{1}-2\hat{s}_{2}^{2}/N_{2}}}{2^{N_{1}}2^{N_{2}}e^{-2\hat{s}_{1}^{2}/N_{1}-2\hat{s}_{2}^{2}/N_{2}}}\right)$$

$$= \ln\left(e^{-2(\hat{s}_{1}^{2}-s_{1}^{2})/N_{1}-2(\hat{s}_{2}^{2}-s_{2}^{2})/N_{2}}\right)$$

$$= -2(\hat{s}_{1}^{2}-s_{1}^{2})/N_{1}-2(\hat{s}_{2}^{2}-s_{2}^{2})/N_{2}.$$

(d): 2 points

Here $s_1 = 0$, $\hat{s}_1 = 500$, $s_2 = 1500$, and $\hat{s}_2 = 1000$. Plugging everything in, we find

$$\sigma^f - \sigma^0 = 75.$$

For the multiplicity, this means that it increased by a factor of $e^{75} = 3.7 \times 10^{32}$. It is this much more likely to be found in the equilibrium state than the initial state. It is not *impossible* for heat to flow from low-to high-temperature, but we can see that it is vanishingly unlikely.

After you do part (d), think about what it means. Does energy (heat) always have to flow from the hotter system to the colder system? It wouldn't violate energy conservation to have energy flow the other way, but the probability for that to happen in a macroscopic system is incredibly small!

You should also have noticed in doing this problem that spin temperatures can be infinite or even negative! What does that mean? When there are more spins in the high-energy state than the low-energy state, we call that an "inverted" spin population, and it has a negative temperature. But you can never use such a system to cool another system, because a system with an inverted spin population has higher energy than a system with a normal (noninverted) spin population. The moral of the story is, be careful about using equilibrium concepts such as temperature to describe nonequilibrium situations! By the way, inverted populations are the basis for lasers.