Physics 112, Fall 2017: Holzapfel
Problem Set 2 (6 problems). Due Friday, September 15, 5 PM

Problem 1: **Paramagnetism**
(a) Kittel, Problem 2.2

(b) Roughly plot the entropy and the temperature as a function of energy. Notice that the temperature is negative for some values of U. If a system a with negative temperature is brought into contact with a system at positive temperature, which way will the energy flow? You may wish to consult "Thermodynamics and statistical mechanics at negative absolute temperatures", Phys. Rev. **103**, 20 (1956).

Problem 2: **Crystal Disorientations**
N atoms are arranged to lie on a simple cubic lattice. Then M of these atoms are moved from their lattice sites to lie at the interstices of the lattice, that is points which lie centrally between the lattice sites. Assume that the atoms are placed in the interstices in a way which is completely independent of the positions of the vacancies.

a) Show that the number of ways of taking M atoms from the N lattice sites and placing them on the N interstices is:

$$g(N,M) = \left(\frac{N!}{M!(N-M)!}\right)^2. \tag{1}$$

(b) Suppose that the energy required to move an atom from its lattice site into any interstitial site is ε. The energy of the system is then $U = M\varepsilon$ if there are M displaced atoms. Use our definition of entropy and temperature in terms of the entropy to show that:

$$\frac{M}{N} = \frac{1}{\exp(\varepsilon/2k_bT)+1}. \tag{2}$$

Problem 3: **More Crystal Disorientations**
Consider a cubic crystal like that in the previous problem. However, in this case when an atom is displaced it moves to one of β sites immediately surrounding its original position. Assume that the atoms act independently and the energy associated with a displaced atom is ε for all β states.

(a) Show that the number of displaced atoms is:

$$\frac{M}{N} = \frac{\beta}{\exp(\varepsilon/k_bT)+\beta}. \tag{3}$$

(b) Consider the limiting cases for this experiment. For each case, find a value for M/N and provide an explanation for your result.
i) $\beta \to \infty$
ii) $T \to \infty$
iii) $T \to 0$

Problem 4: **Paramagnet Entropy**.

(a) Show that the entropy of a two-state paramagnet, expressed as a function of temperature, is

$$S = Nk_b[\ln(2\cosh x) - x\tanh x], \tag{4}$$

where $x = (mB/k_bT)$ and B is an external magnetic field.

(b) Sketch the result of part (a) as a function of (k_bT/mB) for both positive and negative temperatures. Demonstrate that this formula has the expected behavior for both $T \to 0$ and $T \to \infty$. From the form of the result for part (a), you might have already guessed that this function only depends on $|x|$ and not on the sign. Explain the significance of the results for negative temperatures.

Problem 5: **Quantum Harmonic Oscillator**.
In discussion section, we talked about a system of N harmonic oscillators with a total of q quanta of energy. As you'll see later in the course, this result describes the physics of black body radiation and lattice vibrations in solids. We found the multiplicity for this system to be:

$$g(N,q) = \frac{(q+N-1)!}{q!(N-1)!}. \tag{5}$$

(this result is derived in a different way on page 24-25 of Kittel)

(a) Show that in the limit of large N and q that:

$$g(N,q) \approx \left(\frac{q+N}{q}\right)^q \left(\frac{q+N}{N}\right)^N. \tag{6}$$

(b) Find an expression for the entropy of this system as a function of N and q. You should verify for yourself that the factors of $\sqrt{N}$ and $\sqrt{q}$ left out in the derivation of part (a), are not important.

(c) Use the result of part (a) to calculate the temperature of the system as a function of its energy. (The energy is $U = q\varepsilon$, where ε is a constant.)

(d) Use the results of part (c) to find the energy as a function of temperature.

(e) Differentiate the result of part (d) to find an expression of the heat capacity. Show that in the limit as $T \to \infty$, the heat capacity $C \to Nk_b$. Is this the result you expect?

(f) Sketch the heat capacity as a function of k_bT/ε. Pay particular attention to the low and high temperature limits. How do you expect the heat capacities for materials such as lead and diamond to differ? Without worrying about the exact values of ε, sketch your estimates for the relative heat capacities of lead and diamond on the same plot.

(g) Find an expression for the heat capacity of this system at high temperature. Keeping terms up to $(\varepsilon/k_bT)^2$ in the final result, show that

$$C \approx Nk_b\left[1 - \frac{1}{12}\left(\frac{\varepsilon}{k_bT}\right)^2\right]. \tag{7}$$

Problem 6: **Entropy and Reversibility**.

A kilogram of water has a nearly constant heat capacity of 4.2 kJ/K over the temperature range of 0° C to 100° C. The water starts at 0° C and is brought into contact with a thermal reservoir at 100° C.

(a) After the water comes into equilibrium with the thermal reservoir, what is the entropy change of the water and of the Universe.

(b) What is the ratio of the final to the original multiplicity of the water.

(c) This process is now divided into two stages: first the water is placed in contact with a heat bath at 50° C and comes into thermal equilibrium; then it is placed in contact with the heat bath at 100° C and again comes to thermal equillibrium. What is the entropy change of the Universe for this two step process.

(d) If we were to continue this subdivision into an infinite number of steps with thermal reservoirs at intermediate temperatures, what would the entropy change of the Universe be? What does this say about the reversibility of the process in this limit?