

1. K&K, chapter 10, problem 4. The one dimensional case is discussed in the example on pages 285-286 of K&K. (We skipped it in lecture.)
2. K&K, chapter 10, problem 5.
3. K&K, chapter 10, problem 6. You may want to review pages 252-256 in chapter 8 of K&K. This gives a quick overview of magnetic energy in superconductors.
4. K&K, chapter 10, problem 8. Here you need to review Debye theory covered in K&K, chapter 4 or lecture 10.
5. This is to test your strength in calculating when you have to solve for things numerically. Consider a van der Waals gas isotherm with $\hat{\tau} = 0.90$. What is the pressure range over which the volume is a triple valued function of the pressure? What are the two volumes on the gas branch and the two volumes on the liquid branch at these two extremes of pressure? Finally, what is the pressure for which a mixture of liquid and gas is the equilibrium state? Hint: you want $\int \hat{V} d\hat{p} = 0$ when this is evaluated along the isotherm from the point where the mixture is all gas to the point where the mixture is all liquid. You can write this as a function only of \hat{V} with $\int \hat{V} (d\hat{p}/d\hat{V}) d\hat{V}$. This can be evaluated analytically to give an expression involving the volume where the mixture is all gas and the volume where the mixture is all liquid. The problem is that the volumes must be at the intersection of a constant pressure line with the gas and liquid branches. So, can you pick a pressure, evaluate the volumes, evaluate the integral, make a correction based on the error, and repeat?
6. In lecture 24 and in K&K, chapter 10, a simple model of ferromagnetism is developed. Show that the energy per unit volume in this model is $U/V = -\lambda M^2/2 = -n\tau_c m^2/2$. The variables are defined in the notes or the text; briefly, $m = M/n\mu$ is the magnetization in units of the maximum possible magnetization, μ is the magnetic dipole moment, n is the concentration of magnetic moments, and $\tau_c = n\mu^2\lambda$ is the Curie temperature. Determine the heat capacity per unit volume for temperatures below the Curie temperature. Make a sketch (heat capacity versus temperature) of your results. Note that we found a relation between the dimensionless magnetization and the temperature in units of the Curie temperature ($t = \tau/\tau_c$), namely $m = \tanh(m/t)$. This can be solved for t in terms of m , so you should be able to obtain a system of parametric equations.

7. This problem looks long, but it's not really. Our goal is to investigate the algorithm for placing a two state system in contact with a heat bath in a Monte Carlo simulation. To start with, get on the web and learn about Monte Carlo simulations of the Ising model. You will find that many of these simulations use something called the "Metropolis algorithm" for deciding whether to flip a spin.

(a) What is the Metropolis algorithm?

Most computer software libraries come with a "random number generator" capable of generating pseudo-random numbers uniformly distributed between 0 and 1. Suppose we are simulating a two state system with energies 0 and E in contact with a heat bath at temperature τ .

(b) How would you use a random number x , uniformly distributed between 0 and 1 to put the system in one of the two states with canonical probabilities (i.e. $p(E)/p(0) = \exp(-E/\tau)$)?

Suppose we want to implement a Monte Carlo algorithm to simulate the Ising model. We visit a spin and must decide whether it should flip. Again, we take the low energy state to have energy $E_0 = 0$, the high energy state to have energy $E_1 = E$ and the temperature to be τ . When we visit the spin, let the probabilities that it's in state 0 or 1 be $p_0(0)$ and $p_1(0)$. Note that depending on how the system was prepared, these probabilities can be anything between 0 and 1 and, of course, they must sum to 1. After we visit once, the probabilities can be written as $p_0(1)$ and $p_1(1)$. After n visits, $p_0(n)$ and $p_1(n)$.

Aside: we are simplifying the problem by imagining that only the spin we are visiting is changing, that all other spins remain the same. In a real simulation we would visit many other spins before returning to the original spin, so the energies of the two states might have changed. We are trying to figure out how to decide on a spin flip, which will be based on the energies and temperature at the time we visit, so this shouldn't matter.

We might think of transition probabilities. For example, t_{01} is the probability that the spin goes to state 0 from state 1. Then we can write

$$\begin{pmatrix} p_0(n) \\ p_1(n) \end{pmatrix} = \begin{pmatrix} t_{00} & t_{01} \\ t_{10} & t_{11} \end{pmatrix} \begin{pmatrix} p_0(n-1) \\ p_1(n-1) \end{pmatrix}.$$

Since the t_{ij} are transition probabilities, it must be true that $0 \leq t_{ij} \leq 1$. Also it must be true that $t_{00} + t_{10} = 1$ and $t_{01} + t_{11} = 1$.

(c) Why?

We are trying to find conditions on t_{ij} because these are the probabilities you must choose in deciding whether to flip a spin. The previous two conditions reduce the number of

variables to be chosen “arbitrarily” to 2. However we want the output probabilities to be canonical or to become canonical after the spin has been in contact with the heat bath for a long time (which means we’ve made many decisions on whether to flip it). We might impose the condition that if the input probabilities ($p_{0 \text{ or } 1}(n-1)$) are canonical then the output probabilities ($p_{0 \text{ or } 1}(n)$) are also canonical.

(d) Show that this leads to the additional condition that

$$t_{00} = 1 - e^{-E/\tau} (1 - t_{11})$$

So, if one chooses t_{11} arbitrarily in the range $0 \leq t_{11} \leq 1$, the other transition probabilities can be chosen consistently. One choice is $t_{11} = 1$. This makes the transition probability matrix the identity matrix which is not very exciting and would not drive a system towards thermal equilibrium if it were out of equilibrium. Another choice is the value required for the Metropolis algorithm.

(e) What is the transition probability matrix in this case?

Aside: note that the Metropolis algorithm does not necessarily produce canonical probabilities if the input probabilities are not canonical. To see this, suppose one or the other of the input probabilities is 1 (and the other is 0). A question that you might want to think about (not to be handed in) is whether repeated application of the Metropolis algorithm produces thermal equilibrium (canonical probabilities) starting from an arbitrary, non-equilibrium input.

A third choice for t_{11} and the transition matrix might be that value that produces canonical outputs no matter what the input.

(f) What is the transition probability matrix in this case?

Comment: I find the Metropolis algorithm to be unphysical with its requirement that any spin found in the high energy state be immediately flipped to the low energy state. The problem can most easily be seen at the limit of infinite temperature. In this limit, half the spins are in the high energy state and half are in the low energy state, but there are fluctuations. Your answer to (e) should become $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and your answer to (f) becomes $\begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$. If you think about it, you will see that in this limit, the Metropolis algorithm just causes every spin to flip at every visit. The probabilities from (f) cause a random half (on the average) of the spins to flip. The probability that a spin stays in one state after n visits is 2^{-n} . In other words the spin exponentially decays to the other state. This is a much more physical situation!