

# **A Simple Model for Teaching Upper Division Statistical Physics**

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## **ABSTRACT**

Teaching upper division statistical physics can often be clouded by the theory and complex examples used. To better help students appreciate the fundamental statistical concepts and how they are connected to thermodynamic principles this paper suggests using a simple abstract model. Using Atkins' Model students can see these ideas clearly connected and have a straightforward reference to help understand the behavior of more complicated cases.

**Keywords:** Statistical physics, thermodynamics, Atkins' Model, Upper division.

## INTRODUCTION

In my upper division Statistical Physics course, I find that the students often focus too much of the mathematics and neglect to see the fundamental statistical relationships. Considering the complexity of the some of the systems we look at, this is not surprising. However, I consider it very important that the students appreciate how the fundamental idea of accessible states leads to the well-known thermodynamic relationships, like the 2<sup>nd</sup> Law.

Furthermore, the statistical methods used in physics could be applied to any system, while I think many students believe that they are somehow just of use in the study of gases and other special physical systems. This demonstrates my primary concern that they do not appreciate the fundamental statistics and why it is related to thermodynamic laws.

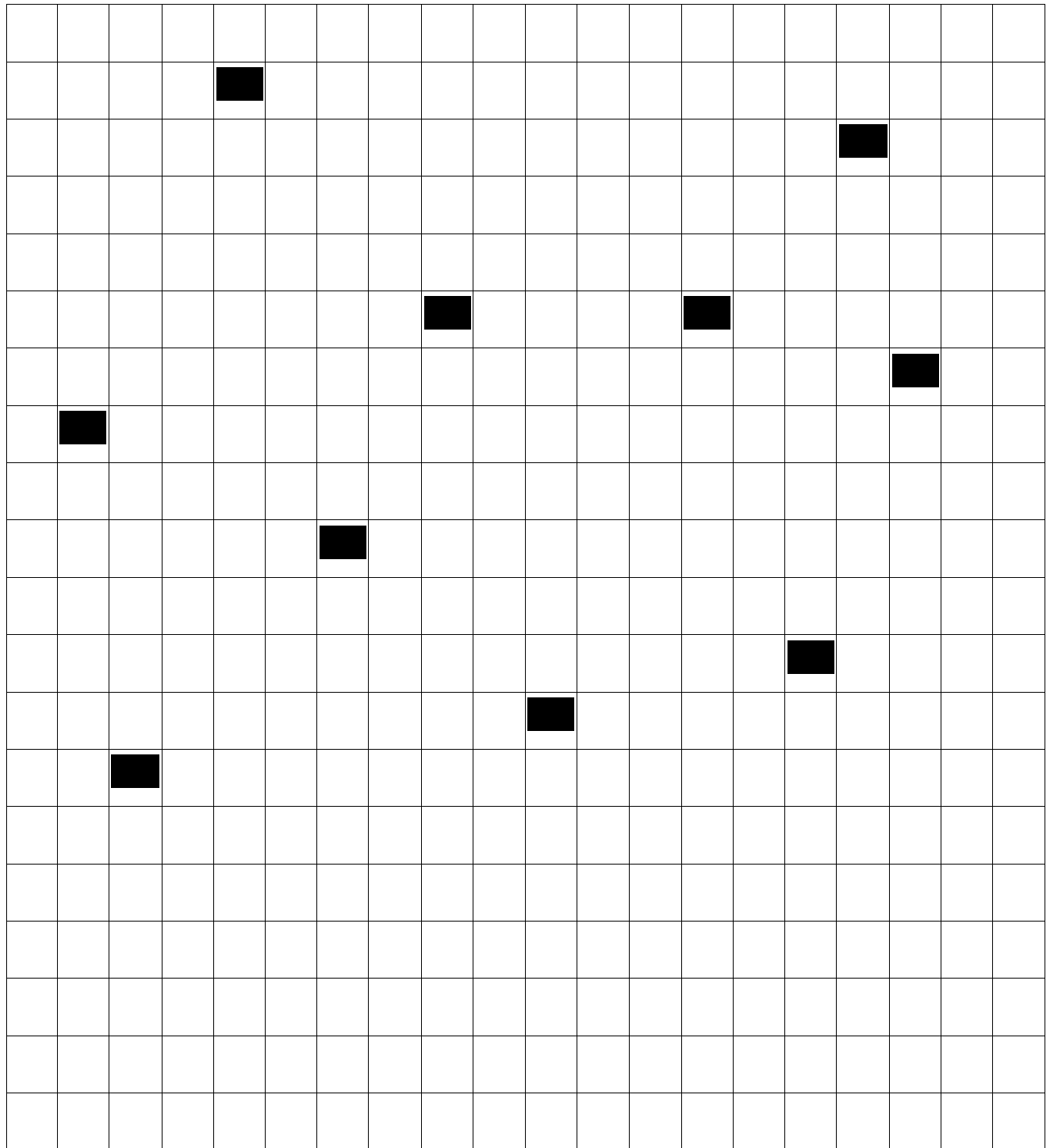
To address this I have begun looking at a simple system that has been well developed by Atkins (1984). Using this straightforward statistical model, I think that students gain a better understanding of how and why the thermodynamic laws have their particular form. They also gain a simple conceptual model to help understand more complex systems.

This paper first details the Atkins' model and then looks at several derivations that are commonly carried out in an upper division statistical physics course.

## ATKIN'S MODEL

P.W. Atkins introduces the model used in this paper in his book "The Second Law" (Atkins, 1984) which was part of the Scientific American Library Series. Impressively, Atkins doesn't just look at the 2<sup>nd</sup> Law of Thermodynamics, as discussed in this paper, but includes a broad range of phenomena. Included are discussions of Boltzmann's Demon, simple engines, and chemical transformations (including burning). All explained through this simple model.

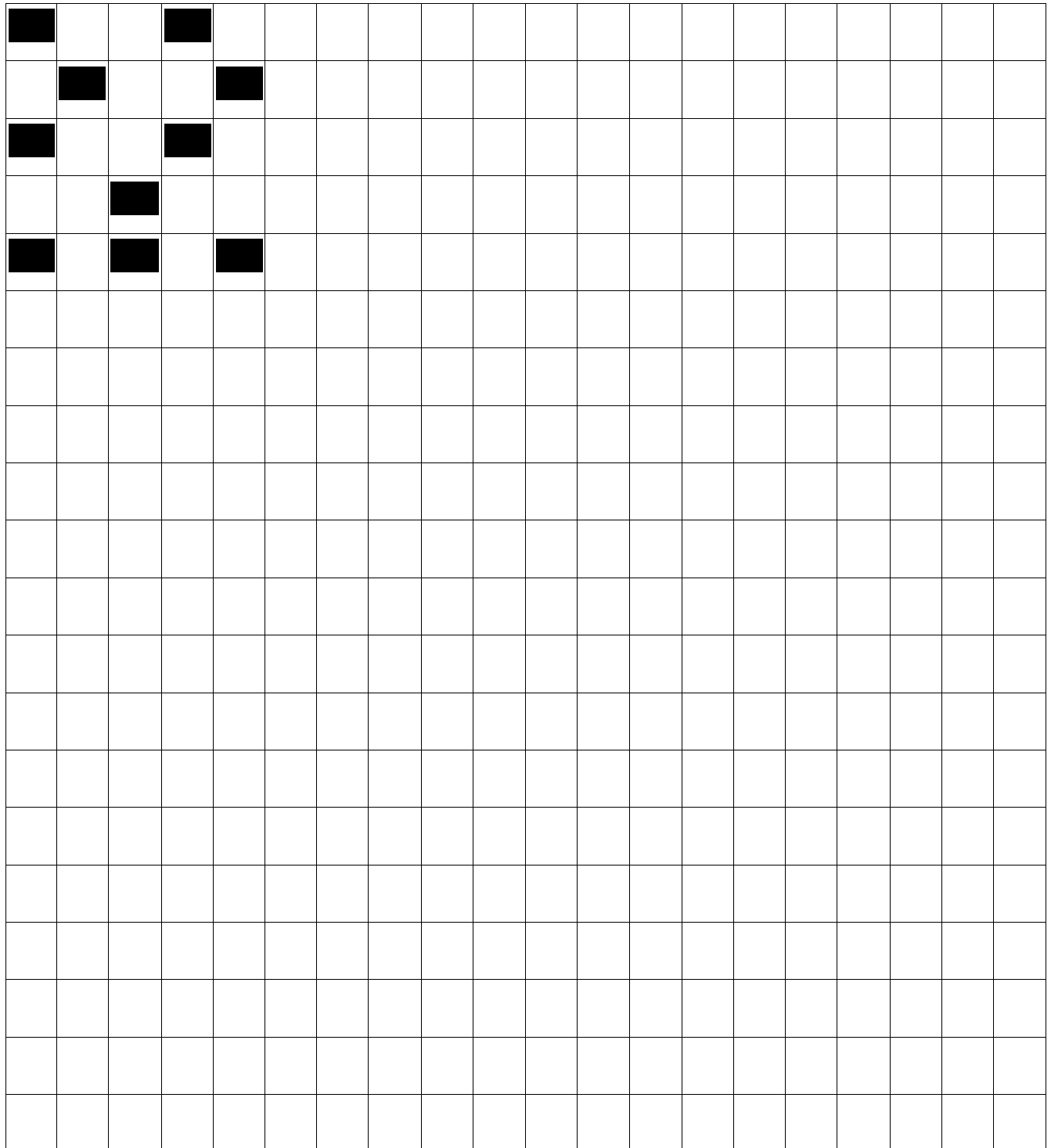
Atkins' Model is discussed in detail by the previous research (Atkins, 1984; Kincanon, 2013; Mattis, 2003, Nuffield, 1972; Styer, 2000). Here is presented a summary of that work that follows that primarily using the discussions of Kincanon. This model uses a grid of cells as shown in Figure 1. This is a 20 x 20 grid of cells, but any number of cells is fine. Each cell has the characteristic of either being ON or OFF. In the grid, several cells are shown as ON by being filled in:



**Figure 1.** Atkins model for heat flow with 10 cells ON

A cell being ON is a model of it having energy that is not possessed by the OFF cells. The transfer of energy or heat flow is modeled by the ONs not being static in their positions. During each time step they migrate to one of the eight surrounding cells with the caveat that no cells can leave the grid and no cell can possess two ONs. So, the number of ONs is conserved, representing conservation of energy. (Though it is not necessary to require only one ON per cell, I think that it makes for a simpler visual representation that is still consistent with qualitative predictions.) Temperature is modeled in this grid by dividing the number of ONs by the total number of cells in the grid; or in other words, by the density of the ONs.

To clarify how this model's heat flow, consider what one would expect to happen if the ONs started all near one corner as in Figure 2.



**Figure 2.** Atkins model for heat flow with 10 cells ON, but concentrated in one region

As the ONs migrate randomly one would expect, given enough time, that each ON would have equal probability of occupying any cell and also, as students easily predict, one does not expect to see all of the ONs back up in the corner. This is a model of heat flow.

If we took the ONs all in the corner as my hot cup of coffee at the beginning of my lecture and the rest of the cells, the ones outside of the 5 x 5 corner, as the lecture room, we could understand why the temperature of the coffee eventually matches the temperature of the room. As we allow the ONs in Figure 2 to migrate around we expect, after a lot of time steps, to see a situation with the ONs spread throughout the grid. Though we would not predict a particular configuration of the ONs, we do expect to see a uniform density. The students can see why the initial high ON density coffee and low-density room lead to an equal ON density of the coffee cup and room. (Students usually agree with this quickly.) And since temperature is defined as the density of ONs, they can see how this models the progression to thermal equilibrium. There is however a problem.

If the ONs are moving around randomly then it is possible that an initial configuration of the room and coffee at the same temperature could be followed by the coffee heating up and the room cooling. Since the ONs are moving around randomly there is a chance that they will occupy the corner 5 x 5 section and so it does seem possible that the coffee will heat up. This also makes "sense" to the students but hopefully they also realize that they have never observed that occurring. Why not?

The key concept here is the distinction between a particular arrangement of ONs and what we measure, the temperature. Since temperature is a measure of the density of ONs, there are many possible arrangements of ONs for a given temperature. Now I introduce the concepts of microstates and macrostates. A microstate is a particular arrangement of ONs while a macrostate is a particular temperature. So, a given macrostate corresponds to many different microstates. And, critical to the student understanding, is that different macrostates are associated with different probabilities of occurrence.

This can be seen by considering the microstates first. Since the ONs move randomly each microstate has the same probability. Since each macrostate corresponds to a different number of microstates, each macrostate has a different probability. So, the macrostate that corresponds to the largest number of microstates is the most probable. This explains why the room temperature coffee is not observed to heat up. The number of microstates associated with the coffee being hot is very small compared the number of microstates with the room and coffee being near the same temperature. It is important it note that though the probability of my coffee heating up as the lecture goes on is small it is not zero.

### ADVANCED CALCULATION EXAMPLES

There are, of course, a lot of calculations and derivations that are done in a typical statistical physics course. Here, two examples are given that illustrate how the Atkins' Model can be used. These are finding the total energy as a function of temperature and looking at the conditions under which equilibrium occurs.

For both of these examples one needs to use the relationship between the temperature parameter,  $b$ , and the number of accessible states,  $\Omega$ . Assuming that there are  $m$  ON's in a grid of  $N$  cells, the number of accessible states is given by:

$$\Omega = \frac{N!}{(N-m)!} \tag{1}$$

$b$  and  $\Omega$  are related by: (Reif, 1965)

$$b = \partial \ln \Omega / \partial E \tag{2}$$

It is reasonable to assume that the energy,  $E$ , is proportional to the number of ON's,  $m$ . For simplicity a proportionality constant of 1 is used. So, since  $E = m$ , the above equation becomes:

$$b = \partial \ln \Omega / \partial m \tag{3}$$

Combining this with the original expression for  $\Omega$  gives:

$$\beta = \frac{\partial}{\partial m} [\ln N! - \ln(N - m)!] \tag{4}$$

Eliminating the parenthesis and using the approximation for large  $n$  that:

$$\frac{d \ln n!}{dn} = \ln n \tag{5}$$

Gives:

$$\beta = \ln(N - m) \tag{6}$$

Since  $b = 1/kT$ , where  $k$  is Boltzmann's Constant and  $T$  is the temperature, one has:

$$1/kT = \ln(N - m) \tag{7}$$

Equation (7) can be used to easily find the relationship between the energy,  $E$ , and the temperature. Since  $E = m$ , equation (7) yields:

$$E = N - e^{1/kT} \tag{8}$$

How this matches intuition, can be seen by looking at a limiting case. As  $T$  approaches  $\infty$ , it is seen that  $E$  approaches  $N-1$ . One would expect that in this limit one would see that  $E$  approaches  $N$ . But, and this comes up often in statistical physics, the derivations are assuming that  $N$  is very large. (It is the underlying assumption that gives equation 1.) So,  $N-1$  is  $N$  for very large  $N$  and the expected result matches.

As another example consider the thermal interaction between two systems  $A$  and  $A'$ . Equilibrium is obtained when the Entropy is a maximum. The Entropy,  $S$ , is given by

$$S = k \ln \Omega$$

One has for the combined systems that the total Entropy is given by:

$$S = k \ln \Omega + k \ln \Omega'$$

Saying that  $S$  is a maximum at equilibrium is requiring that:

$$0 = \frac{\partial}{\partial m} k \ln \Omega + \frac{\partial}{\partial m'} k \ln \Omega'$$

Now, using the original equation for  $\Omega$  and the fact that  $\frac{\partial}{\partial m} = -\frac{\partial}{\partial m'}$ , one gets that:

$$\beta = \beta'$$

which is of course equivalent to  $T = T'$ . So, it has been demonstrated that maximum Entropy corresponds to thermal equilibrium (Details of this calculation can be found in Reif (1965))



So, these two examples show that the methods of statistical physics give expected thermodynamic results even for an abstract system. Using the fundamental equation for  $\Omega$  all of the relationships of thermodynamics for the Atkins' Model could also be found.

## SUMMARY

Using Atkins' Model and applying the techniques of statistical physics gives the expected results for thermodynamic behavior. Though this should not be surprising, by using such a simple model, students can better appreciate how the statistical physics functions and what the thermodynamic relationships mean fundamentally.

Given here were just two examples of using Atkins' Model. In fact, *any* relationship in statistical physics that includes reference to the number of accessible states can be applied to this model. The examples presented here were chosen to emphasize fundamental relationships between  $\Omega$  and particular thermodynamic quantities. Since Statistical Physics reduces all of Thermodynamics to characteristics of  $\Omega$  there are no limits to this application. One can look at engine efficiencies, Maxwell's Demon or any other topic covered in Statistical Physics. The challenge is to choose cases in which this model gives students a better insight into the statistical relationships and is not just a mathematical exercise.

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