Utilizing exact and Monte Carlo methods to investigate properties of the Blume Capel Model applied to a nine site lattice

Nick Franciose

Writing various exact and Monte Carlo computer algorithms in C language, I used the Blume Capel Model to evaluate some thermodynamic properties of a nine site lattice. I first investigated the lattice using exact methods, and then moved on to Monte Carlo methods, and then compared the two sets of results for consistency. The results from the Monte Carlo method proved to be comparable to those of the exact method to a high degree of accuracy.

Introduction. The Blume Capel Model is used to evaluate properties of a lattice in one, two, three or higher dimensions. For this project I chose to observe nine site lattices. Each site in the lattice can assume a spin of -1, +1, or 0. The energy is evaluated according to the Hamiltonian:

$$E = - J \Sigma \ S_i S_j + \Delta \Sigma \ S_i^2$$

The expression consists of two sums. The S represents a site's spin, but in a very general way. In fact it is used merely to designate a microstate, and doesn't necessarily imply spin as we normally think about it. A spin equal to 1 could represent an atom of iron, a spin of -1 could represent an atom of copper, and a spin of zero could represent a vacancy. If depends entirely on how you define your system.

The first term constitutes the Ising Model, and evaluates the interactions between neighboring sites. Sites vertically and horizontally adjacent contribute to the term but diagonal neighbors are neglected. The J is a variable interaction parameter.

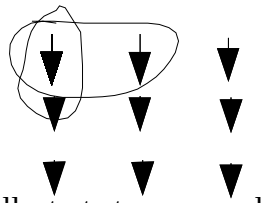

Figure 1: The drawn loops illustrate two examples of neighboring sites in a nine site lattice.

The second term incorporates energy contributions of vacancies in the lattice, and is a summation of the square of each site's spin and is acted upon by a Δ term. The delta term is a variable parameter called the “vacancy concentration.”

The following example configurations will illustrate better how the expression serves to evaluate different configurations.

$$E = - J \Sigma \ S_i S_j \ + \Sigma \ \Delta_i \ S_i^2$$

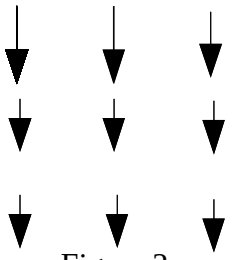

Figure 2.

For all sites S = -1
If J = 1 and Δ=1
E= -1*(1+1+1+1+1+1+1+1+1+1+1+1) + 1*(1+1+1+1+1+1+1+1+1)
E = -12 + 9
E = -3 (lowest energy)

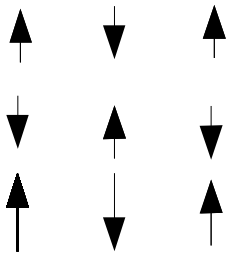

Figure 3.
Sites equal 1 and -1 alternately
If J = 1 and Δ=1
E= -1*(-1+ -1+ -1+ -1+ -1+ -1+ -1+ -1+ -1+ -1+ -1+ -1) + 1*(1+1+1+1+1+1+1+1+1)
E = 12 + 9
E = 21 (highest energy)

If J is *negative*, the left term will have lower energy when S_i and S_j are antiparallel (+1 and -1). If J is *positive*, the left term will have lower energy when S_i & S_j are parallel (+1 and +1, or -1 and -1). If Δ is negative, the right term will have the lowest energy when sites have spin. If Δ is positive, the right term will have the lowest energy when sites have a spin of zero. For this reason, Delta is called the "vacancy concentration." There is a competition between the two terms and the thermodynamics of the system will be determined by the ratio of J and Δ.

Monte Carlo methods are a class of computational algorithms for simulating the

behavior of various physical and mathematical systems. They are distinguished from other simulation methods by being stochastic, that is nondeterministic in some manner - usually by using random numbers (or more often pseudo-random numbers) - as opposed to deterministic algorithms, which were used for the exact approach.

Results and Discussion. I wrote a program to evaluate exactly the energy all 19,683 different configurations.

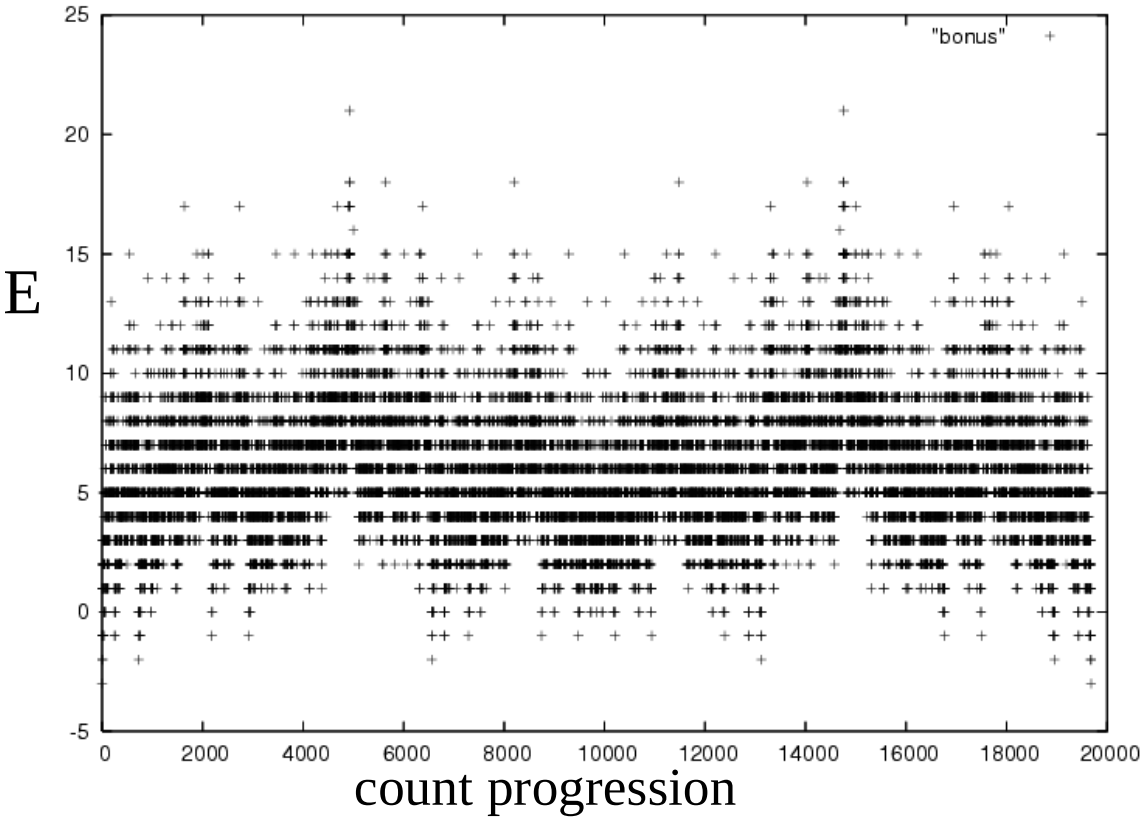

Figure 4: Energy histogram for J =1, Δ =1.

In figure 4, the histogram represents the energies of each of the configurations, ranging from E= -3 to E= 21 and having integer values between the extremes. The histogram appears in bands each each energy because it is restricted to integer values due to the selection of J and Δ. The configurations assume some energies more often than others. Energies of 5, 6, and 7 are very dense, but energies of -3 or 21 only occur twice each. This is so because only two possible configurations will produce an energy of -3 (all spins equaling -1, or all spins equalling +1), and only two will produce an energy of 21 (alternating spin sites, one beginning with -1 in the top left site, and one beginning with +1 in the top left site). The density of the line at E= 5 reflects that many different configurations will produce that energy. The following figure illustrates how many configurations assume each energy value.

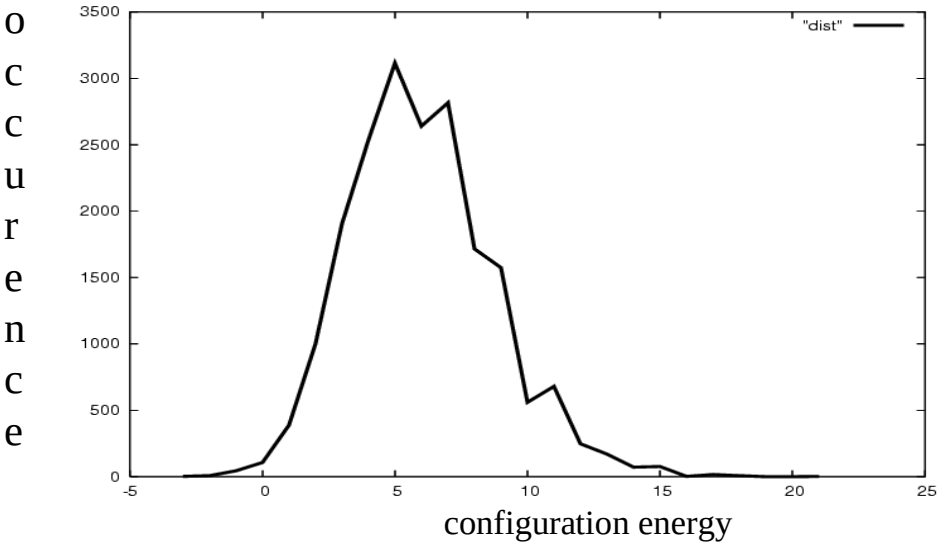

Figure 5. Number of configurations that assume each energy value.

Including temperature, the average energy can be evaluated using the partition function.

$$\langle E \rangle = \Sigma E_j e^{-Ej/T} / \Sigma e^{-Ej/T}$$

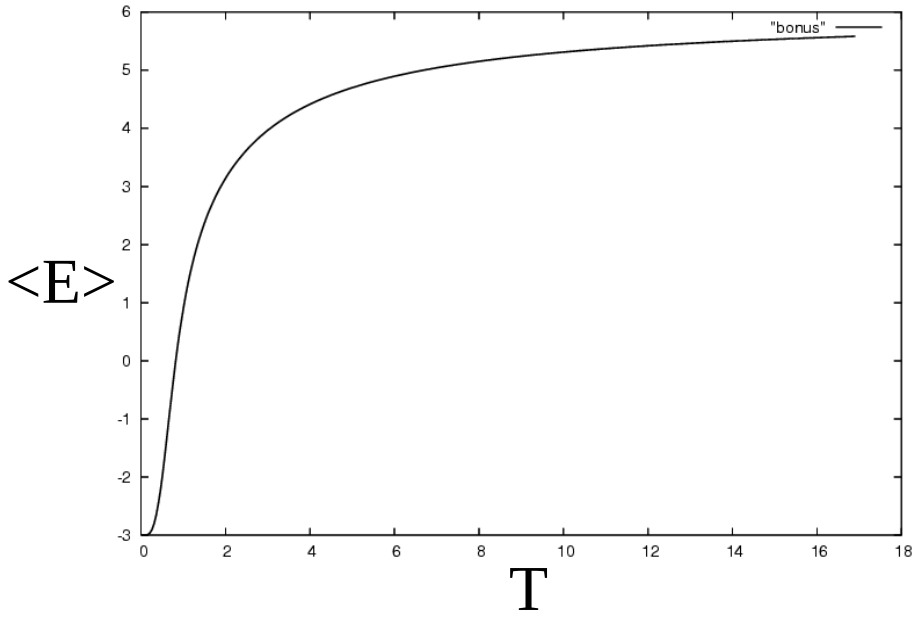

Figure 6. Average energy vs T

So far, we have only seen results from the exact enumeration, which is fine for a nine site lattice, as it only has 3^9 possible configurations. But exploring larger lattices becomes impractical very quickly. For example, evaluating a 6x6 lattice, which has 3^{36} possible

configurations, would take a 3.2 GHz processor about a year and a half. Evaluating a 7x7 lattice, having 3^{49} possible configurations, would take about ten million years. It is apparent that a new method is needed. The method that I used was Monte Carlo.

I used a random number generator to produce a number (r) between zero and one to dictate a random state change. Moving from site 1 to site 9 sequentially, a state change was made randomly at each location, using the following conditions:

if $r < 1/3$, spin at site changed to -1
if $1/3<r<2/3$, spin at site changed to 0
if $r>2/3$, spin at site changed to 1

After a state change was made, the energy of the new configuration was evaluated. Figure 7 shows the number of times an energy was assumed in creating new configurations randomly.

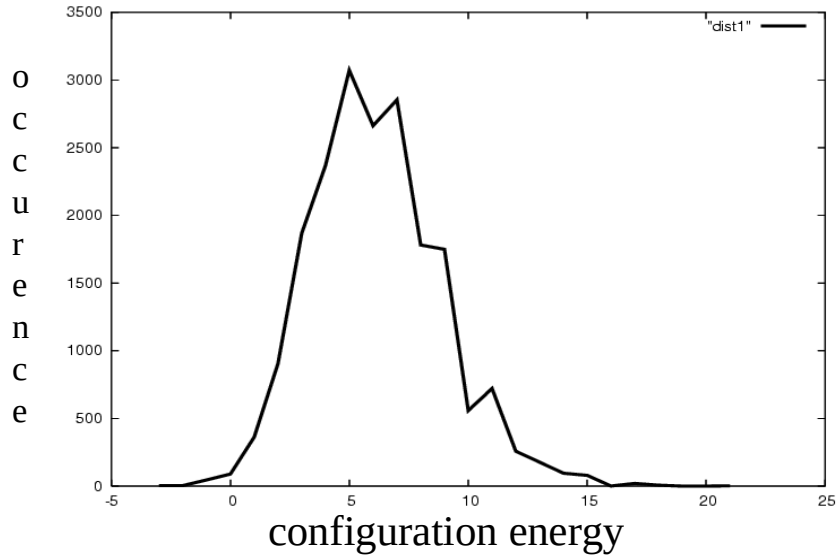

Figure 7. Number of configurations that assume each energy value using Monte Carlo method.

It is evident how similar this distribution is to the exact method.

To evaluate the average energy of the system, is is necessary to include an energy condition for each state change: if $r > e^{-\Delta E/T}$ then state change is rejected. This energy condition is used to restrict the system to configurations of realistic energy, that is, configurations of high energy are only made available when high enough temperatures have been reached. This energy condition, which applies to every microscopic state change results in reproducing the thermodynamics found using the exact method.

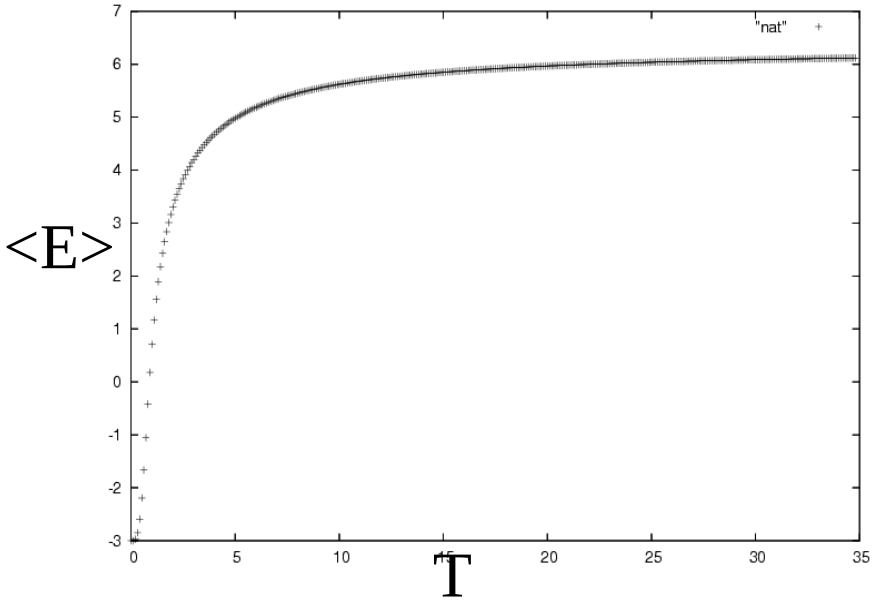

Figure 8. Average energy found using Monte Carlo method.

Conclusion. The Monte Carlo method is a powerful tool for describing a system's properties, and it can be used to explore simple lattices as well as systems with a high degree of complexity. It is more flexible than exact approaches because, by virtue of its randomness, as it doesn't require every possible configuration to be explored, so long as an adequate sampling is made to represent the range of a system's possible configurations. The Blume Capel Model is an elegant and compact expression which offers a surprising amount of complexity. Further projects could explore various other properties of the model. Possible research could be conducted to describe larger lattices, or lattices in three dimensions. Also the consequences of changing delta at each spin site could be explored. This might simulate interesting materials with non uniform vacancy concentrations.

References.

D. Stauffer, D.M. Saul, and M. Wortis, Phys. Rev. B9, 4964 (1972).