Finite Range Couplings in a Tensor Renormalization Group Approach to 2D Classical Lattice Models

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Abstract

The Ising model is a remarkable model which originated in physics and chemistry but has a wide range of applications in other fields. However, it makes a crucial approximation: all far-range interactions are ignored in the Ising model for the sake of simplicity, even though far-range interactions are almost always present. It is unknown to what degree the inclusion of these interactions will affect the dynamics of the Ising model. We generalize the tensor renormalization group (TRG) method of analyzing 2D classical lattices to account for *next* nearest neighbor (NNN) interactions in a square lattice. We find that NNN interactions do *not* in fact have a significant impact on the behavior of the square Ising lattice. This adapted TRG method more rigorously justifies the nearest neighbor approximation, however, and could help resolve the long-standing problem of geometrical frustration in 2D lattices.

Summary

The Ising model is a remarkably elegant and powerful model in physics and chemistry, and is capable of explaining phenomena as varied as neuron interactions and de facto racial segregation in cities. However, the Ising model makes a crucial approximation: all far-range interactions are ignored in the Ising model for the sake of simplicity, even though far-range interactions are almost always present. It is unknown to what degree the inclusion of these interactions will affect the dynamics of the Ising model. We generalize an existing method for analyzing the Ising model to account for farther range interactions, and find that these interactions do *not* in fact have a significant impact on the behavior of the model. This generalized method more rigorously justifies the exclusion of far-range interactions in the Ising model, however, and could also help resolve some long-standing problems in statistical physics.

1 Introduction

In statistical mechanics, renormalization group methods are powerful tools for understanding the behavior of classical lattice structures, particularly at phase transitions. Perhaps the most famous is the square-lattice Ising Model, which is a simple model of ferromagnetism which displays a phase transition in two or more dimensions. The phase transition temperature, or critical point, corresponds to the Curie temperature of a material. The 2D Ising model is a particularly interesting physical system, in part because of its broad applications, which range from neural networks to lattice gases to de facto segregation in cities. The Ising model is also interesting because of its simplicity: it describes ferromagnets as a 2D lattice of magnetic spins of either $+1$ or -1, where each element only interacts with its nearest neighbors, as shown in Figure 1. The exact solution to the model was discovered by Lars Onsager in 1943 [1], making it an important benchmark in evaluating the accuracy of renormalization methods.

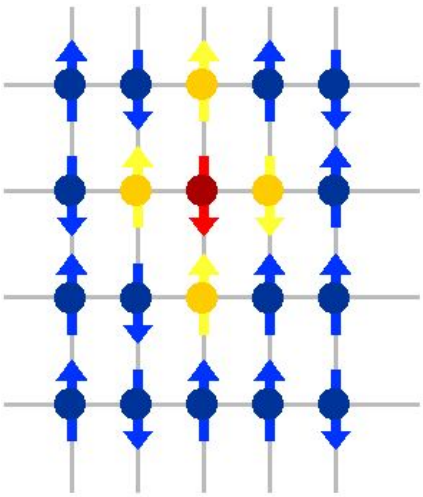


Figure 1: The Ising model with nearest neighbor interactions [2]

Renormalization group methods, in spirit, analyze a physical system at increasing length scales by coarse-graining over finer details to understand the macroscopic behavior of a

microscopic model. The quantities of particular interest in the analysis are critical exponents, which that quantitatively describe the behavior of a physical system near a phase transition.

Initial attempts to understand the Ising model lattice in 1895 [3] and 1907 [4] used mean field theory, which described the behavior of systems in terms of the effective magnetic spin of each element on the lattice. However, though mean field theory correctly predicts the existence of a phase transition in a ferromagnet in dimensions of two and greater (and fails in one dimension), the theory was a failure quantitatively [5]: for example, in two dimensions, it predicted a critical exponent of $\beta = 0.5$, whereas Onsager in 1944 proved that $\beta = 0.125$ [1]. Numerical Monte Carlo methods have also been used to understand the behavior of the 2D Ising model, but a more analytic, accurate approach would not come until the 1970s, when Kadanoff [6] used a block-spin renormalization method to analyze the properties of the Ising model.

Recently, in 2008, Levin and Nave [7] developed a tensor renormalization approach to 2D classical lattice models, which is thought to be able to approximate the behavior of 2D lattices to a very high accuracy. This tensor approach is particularly interesting because it has the potential to resolve the long-standing problem of understanding geometrical frustration in antiferromagnetic triangular lattices [8].

Because it is energetically favorable for neighboring spins to have *opposite* directions in antiferromagnetic materials when only nearest neighbor (NN) interactions are taken into account, the behavior of antiferromagnetic triangular lattice structures is uncertain (as shown in Figure 2) and a large number of degenerate states[1] must be calculated.

To understand the true behavior of these geometrically frustrated structures, *next* nearest neighbor (NNN) couplings, or interactions, are analyzed in this paper, since they may play an important role in breaking the degeneracy of the model.

[1]Degenerate states are states that all have the same calculated energy, and thus no uniquely favorable state can be selected from among them.

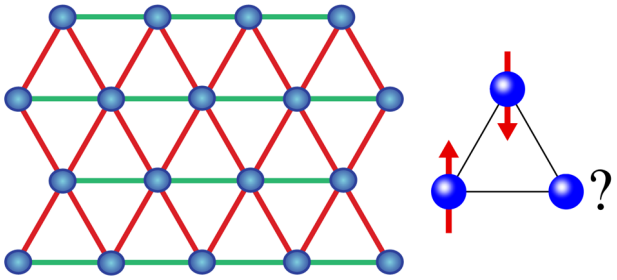


Figure 2: Geometrical frustration [9]

When two spins on a triangular lattice unit have defined spins, the third has no favorable energetic state, i.e. the state of the triangular unit is twofold degenerate. As the lattice is expanded, this degeneracy causes the analysis of the lattice to be extremely complex, as it is unclear what spin configuration is energetically favorable.

In addition, understanding the effects of NNN couplings on the behavior of an Ising lattice gives insight into the validity of the nearest-neighbor approximation and the effects of NNN couplings on Ising model dynamics. This paper analyzes the inclusion of NNN couplings in an Ising *square* lattice (as shown in Figure 3), keeping in mind the potential applications of the approach to a triangular lattice.

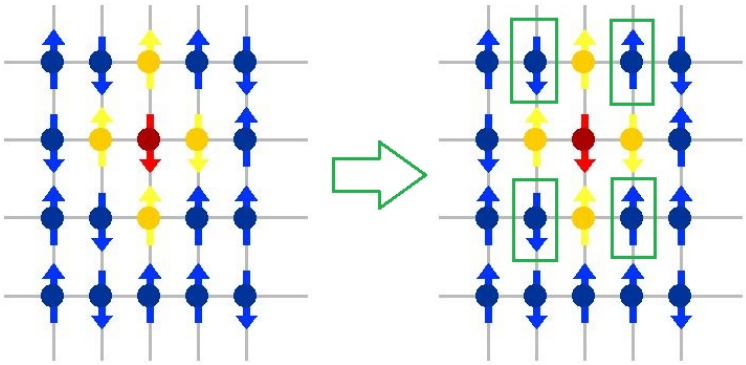


Figure 3: Next nearest neighbor couplings in the Ising model [2]

2 Generalized Tensor Renormalization Group Method

The higher order tensor renormalization group (HOTRG) method outlined in this paper closely follows that of Ueda et. al. [10]. We adapt the method to account for NNN interactions by redefining the hamiltonian in Equation (3), and analyze the consequences of including NNN interactions in the square lattice Ising model.

The quantity of interest for any model in statistical mechanics is the partition function Z. The partition function can be used to calculate many important quantities describing the system, such as the Helmholtz free energy $F = -T \log Z$, where T is the temperature.[2] The behavior of F around the critical point is what ultimately allows the calculation of the critical indices of the 2D Ising model.

The partition function is defined as

$$Z = \sum_{\{s\}} e^{-\beta H} = \sum_{\{s\}} e^{-\frac{H}{T}}, \tag{1}$$

where $\beta = \frac{1}{k_B T} \equiv \frac{1}{T}$, H is the hamiltonian of the system, and the sum is taken over all possible microstates of the system.

In the classical Ising model,

$$H = -K \sum_{\langle i,j \rangle} S_i S_j, \tag{2}$$

where K is a positive constant, $\langle i, j \rangle$ denotes each pair of nearest neighbors, and $S_i \in \{-1, 1\}$ [11]. Thus, the energy is minimized when the spins are parallel, and maximized when the spins are antiparallel.

In this paper, the effects of next nearest neighbor couplings, as shown in Figure 4, are analyzed, so that

[2] Temperature is measured in units of energy, such that the Boltzmann constant $k_B = 1$.

$$H = -K \sum_{\langle i,j \rangle} S_i S_j - K' \sum_{\langle i,k \rangle} S_i S_k, \tag{3}$$

where $\langle i, k \rangle$ denotes each pair of *next* nearest neighbors and K' is the coupling constant for NNN interactions. It is assumed that $K' < K$ in all real-world situations.

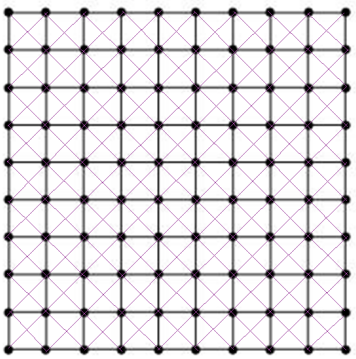


Figure 4: Square lattice with next nearest neighbor interactions

In order to account for all NN interactions, we define tensors on a dual lattice, where each tensor represents the magnetic spin interactions of one unit square. The indices of the tensor are *not* the vertex spins S. Instead, the indices are the link variables σ, as shown in Figure 5. Each σ is a scalar equal to either $+1$ or -1, and is the product of adjacent spins on the lattice. Thus, $\sigma_{x_i} \equiv S_1 S_2$.

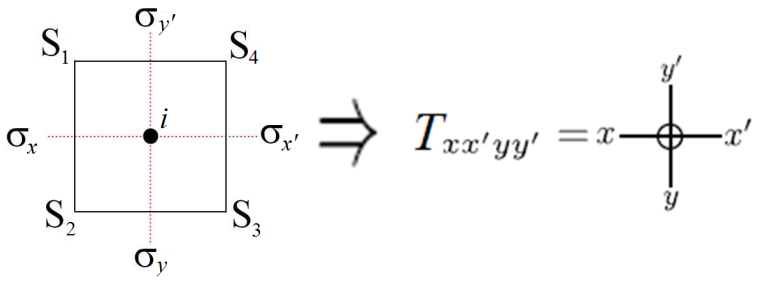


Figure 5: Definition of tensors on the square lattice [10, 11]

Because we define a tensor at the center of *every* unit square of the lattice in Figure 4 (in

constrast with the more common checkerboard lattice approach[3] [12]), we can account for all NNN interactions by defining the diagonal spin variables σ_{D_1} and σ_{D_2} on every tensor, where $\sigma_{D_1} \equiv S_1 S_3$ and $\sigma_{D_2} \equiv S_2 S_4$. Because the indices of the tensor are $\sigma_{x_i}, \sigma_{x_i'}, \sigma_{y_i}$, and $\sigma_{y_i'}$, *not* σ_{D_1} and σ_{D_2}, we evaluate $\sigma_{D_1}$and σ_{D_2} by defining $S_1 \equiv 1$ [4] and recursively calculating $S_1\sigma_x = S_2$, $S_2\sigma_y = S_3$, and $S_3\sigma_{x'} = S_4$. For any real (i.e. possible) configuration of link variables $(\sigma_{x_i}, \sigma_{x_i'}, \sigma_{y_i}, \sigma_{y_i'}), S_4\sigma_{y'} = S_1 = 1$, or, equivalently, $S_1 S_4 = \sigma_{y'}$. [5]

Thus, we define the tensor T, which represents the magnetic spin interactions of one unit square in the lattice, as

$$T_{x_i x_i' y_i y_i'} = \frac{1 + \sigma_{x_i}\sigma_{x_i'}\sigma_{y_i}\sigma_{y_i'}}{2} \exp\left[\frac{K}{2T}(\sigma_{x_i} + \sigma_{x_i'} + \sigma_{y_i} + \sigma_{y_i'}) + \frac{K'}{T}(\sigma_{D_1} + \sigma_{D_2})\right]. \qquad (4)$$

Because some spin configurations $(\sigma_{x_i}, \sigma_{x_i'}, \sigma_{y_i}, \sigma_{y_i'})$ are impossible, e.g. $(+1, +1, +1, -1)$, we include the term $\frac{1+\sigma_{x_i}\sigma_{x_i'}\sigma_{y_i}\sigma_{y_i'}}{2}$ in Equation (4) to restrict $T_{x_i x_i' y_i y_i'}$ to allowed dual lattice microstates. For any real configuration of spins, $\sigma_{x_i}\sigma_{x_i'}\sigma_{y_i}\sigma_{y_i'} = (S_1S_2)(S_2S_3)(S_3S_4)(S_4S_1) = (S_1)^2(S_2)^2(S_3)^2(S_4)^2 = 1$. For every impossible spin configuration, where $\sigma_{y'} \neq S_4S_1$ (as shown in the recursive process previously described), $\sigma_{x_i}\sigma_{x_i'}\sigma_{y_i}\sigma_{y_i'} = -1$ [11].

In 2010, Xiang et. al. demonstrated that the partition function in Equation (1) can be reformulated in terms of tensors such as that in Equation (4) [11]. This reformulated partition function is shown in Equation (5).

[3] In the checkerboard lattice approach, only every *other* square on the lattice has a tensor defined on it. Naturally, this makes accounting for all NNN couplings difficult, so we employ a dual-lattice approach which allows us to define a tensor on every square of the lattice.

[4] This is necessary because a set of link variables $(\sigma_{x_i}, \sigma_{x_i'}, \sigma_{y_i}, \sigma_{y_i'})$ defines *two* sets of vertex spin variables (S_1, S_2, S_3, S_4). This is because both (S_1, S_2, S_3, S_4) and $(-S_1, -S_2, -S_3, -S_4)$ are represented by the same set of link variables $(\sigma_{x_i}, \sigma_{x_i'}, \sigma_{y_i}, \sigma_{y_i'})$. In the calculation of σ_{D_1} and σ_{D_2}, it does not matter whether S_1 is defined as $+1$ or -1, only that an explicit set of vertex spins (S_1, S_2, S_3, S_4) is calculated.

[5] This is valid because $S^2 = 1$. Thus, $S_4\sigma_{y'} = S_1$ can be rewritten as $S_4(S_4\sigma_{y'}) = S_4(S_1) = \sigma_{y'}$.

$$Z = \mathrm{Tr} \prod_i T_{x_i x'_i y_i y'_i} \tag{5}$$

The trace is defined on all bond indices, and is the equivalent of the sum over all possible states in Equation (1). The product $\prod_i T_i$ is over all tensors in the lattice. Note that the $\frac{K}{T}$ term in Equation (4) is halved because each nearest neighbor coupling is summed twice in the product $\prod_i T$. Thus, Equations (4) and (5) account for every NN and NNN interaction once, and together are equivalent to Equation (1).

To actually evaluate the partition function, we begin with one tensor $W^{(0)}_{xx'yy'} = T_{x_i x'_i y_i y'_i}$, where W is the vertex weight of the current lattice, and 2^0 is the linear dimension L of the current lattice structure. Thus, a weight $W^{(n)}_{x_a x'_a y_a y'_a}$ describes a lattice with dimensions $L \times L$, where $L = 2^n$. The subscripts x_a, x'_a, y_a, and y'_a are defined as $\{x_1, x_2 ... x_L\}, \{x'_1, x'_2 ... x'_L\}$, etc., as shown in Figure 6.

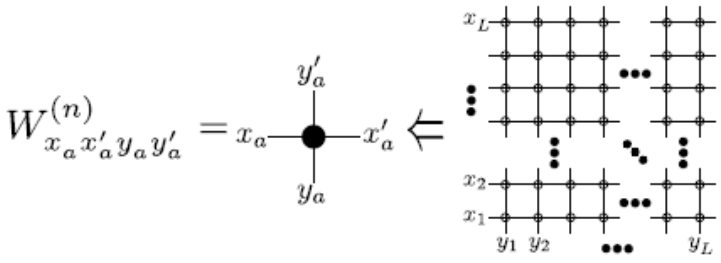


Figure 6: Definition of spins on the square lattice [10]

We begin with $W^{(0)}_{xx'yy'}$ and continually expand the lattice through the renormalization group process $W^{(0)} \to M^{(0,1)} \to W^{(1)} \to M^{(1,2)} \to W^{(2)} \ldots$ We expand the lattice by linking two tensor weights $W^{(n)}_{x_a x'_a y_a y'_a}$ and $W^{(n)}_{x_b x'_b y_b y'_b}$ vertically by summing over a common indice y (shown graphically in Figure 7), obtaining a composite tensor

$$M^{(n,n+1)}_{x_a x_b x'_a x'_b y_a y'_b} = \sum_y W^{(n)}_{x_a x'_a y_a y} W^{(n)}_{x_b x'_b y y'_b}, \tag{6}$$

where $W^{(n)}_{x_b x'_b y_b y'_b}$ is above $W^{(n)}_{x_a x'_a y_a y'_a}$. $M^{(n,n+1)}_{x_a x_b x'_a x'_b y_a y'_b}$ represents a lattice with dimensions $L \times 2L$. We rewrite the index pairs $\{x_a x_b\}$ and $\{x'_a x'_b\}$ as X_{ab} and X'_{ab}, respectively, so that $M^{(n,n+1)}$ is once again a rank four tensor, with bond dimensions[6] (D^2, D^2, D, D). The result is shown in Figure 7.

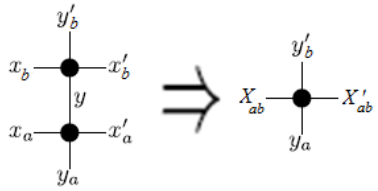


Figure 7: Vertical tensor contraction and index redefinition [10]

Now, we perform a higher-order singular value decomposition (HOSVD) to truncate the bond dimension of X_{ab} and X'_{ab} down to D. We do this by performing an orthogonal transformation on $M_{XX'yy'}$, where the orthogonal matrix O is chosen according to the theory of HOSVD [13], so that

$$\sum_{X'yy'} M_{X_1 X' yy'} M_{X_2 X' yy'} = M'_{X_1 X_2} = O_{X_1 I} \Lambda_{IJ} O^T_{J X_2}, \tag{7}$$

where O is a $D^2 \times D^2$ matrix of of eigenvectors, and Λ is a diagonal matrix of eigenvalues, such that the eigenvalues are in decreasing order. Using a largest eigenvalue approximation, justified in the thermodynamic limit of the system, we then truncate the second dimension of O_{XI} from D^2 to D, calling this new truncated matrix $O_{X\mu}$. [7]

We now update the expanded vertex weight $M^{(n,n+1)}$ such that

$$M^{(n,n+1)}_{\mu\mu' yy'} = \sum_{X,X'} O_{X\mu} O_{X'\mu} M^{(n,n+1)}_{XX'yy'} \tag{8}$$

[6]The bond dimension of a tensor index is the number of degrees of freedom of the index.

[7]Throughout this paper, following the convention of Ueda et. al. [10], we use Greek letters such as μ and ν to denote renormalized variables which have at most D degrees of freedom.

Using this process, we can then join two tensors $M^{(n,n+1)}$ horizontally, to obtain an expanded tensor $W^{(n+1)}_{\mu\mu'\nu\nu'}$ representing a lattice with dimensions $2L \times 2L$. We iterate through this process while imposing the normalization

$$\gamma_n \sum_{\mu\nu} M^{(n,n+1)}_{\mu\mu\nu\nu} = \gamma'_n \sum_{\mu\nu} W^{(n+1)}_{\mu\mu\nu\nu} = 1, \tag{9}$$

We retain the normalization constants γ_n and γ'_n, and use them to obtain the ultimate value of the partition function per site,[8]

$$\log z = \sum_{i=0}^{n} \frac{1}{2^{2i}} (\log \gamma_i + \frac{1}{2} \log \gamma'_i) \tag{10}$$

By calculating the free energy of the lattice via $F = -T \log Z$, we analyze the effect of different coupling constant ratios ${}^{K'}/_{K}$ on the phase transition behavior of the square-lattice Ising model.

We then use the TRG process to compute the spontaneous magnetization M of the lattice via Equation (11) below,

$$M = -\left(\frac{\partial F}{\partial B}\right)_T, \tag{11}$$

where the temperature T is constant. In order to calculate M, we must evaluate F as a function of an external magnetic field B. We do this by generalizing the hamiltonian in Equation (3) to include interactions with B, as shown in Equation (12).

$$H = -K \sum_{\langle i,j \rangle} S_i S_j - K' \sum_{\langle i,k \rangle} S_i S_k - B \sum_i S_i \tag{12}$$

[8]The $\frac{1}{2^{2i}}$ term divides each γ_i by the total size of the lattice (L^2) when γ_i was computed. Since each horizontal expansion doubles the size of the lattice, $\log \gamma'_i$ requires another $\frac{1}{2}$ term for normalization. Thus, (9) takes the sum of each $\log \gamma$ per site, ultimately calculating the value of the partition function for every site.

Including external field interactions in a tensor defined on a dual lattice is non-trivial because a set of spins $(\sigma_{x_i}, \sigma_{x_i'}, \sigma_{y_i}, \sigma_{y_i'})$ defines *two* sets of vertex spin variables (S_1, S_2, S_3, S_4). Unlike the case of NNN interactions, $\sum_i S_i$ is not invariant under the transformation $(S_1, S_2, S_3, S_4) \rightarrow (-S_1, -S_2, -S_3, -S_4)$. Thus, to account for both sets of vertex spins, the number degrees of freedom of the tensor $T_{x_i x_i' y_i y_i'}$ must be increased from two to four. The full process of generalizing the tensor to account for an external magnetic field is not outlined here.

After $F = -T \log Z$ is evaluated as a function of B, the quantity $-\frac{\partial F}{\partial B}|_{B=0}$ is computed. This is a one sided derivative, because, when the temperature is below the critical point T_c, M is an even function which is not differentiable at $B = 0$. However, due to spontaneous symmetry breaking, when $T < T_c$, the right and left derivatives $-\frac{\partial F}{\partial B}|_{B=0}$ are opposite each other, finite, and nonzero. From the relationship between the magnetization $|M|$ and the temperature T, we hope to calculate the critical exponent β, where $M \propto \left|\frac{T-T_c}{Tc}\right|^{\beta}$, and compare it to the exact value calculated by Onsager [1], $\beta = 0.125$. Further work is still to come.

3 Results and Conclusion

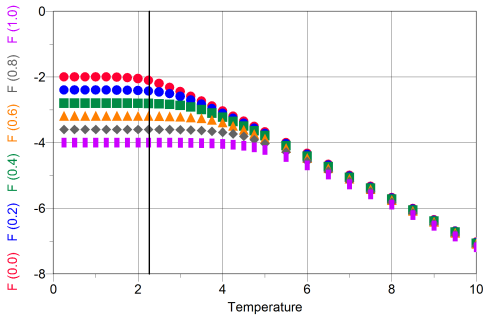
We analyze the effect of differing coupling constant ratios $^{K'}/_{K}$ on the relationship between free energy and temperature[9], as shown in Figure 8.

The graphs in Figure 8 suggest that taking into account NNN interactions increases the critical temperature T_c of the lattice, which was expected. At low temperatures, the magnetic spins are well-ordered due to the interactions among nearby lattice elements. As the temperature increases, this order is broken as the increasing thermal energy scrambles the magnetic interactions among the spins.

When NNN interactions are taken into account, higher temperatures are required to

[9]Again, temperature is measured in units of energy.

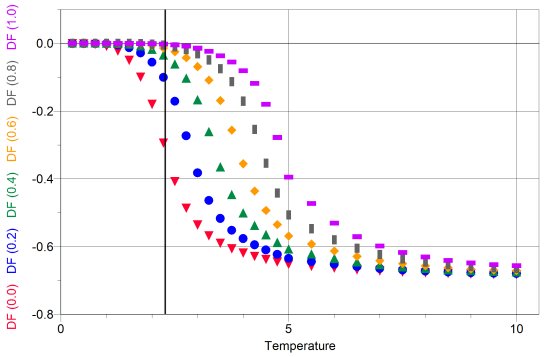
Figure 8: Effect of NNN couplings on the behavior of free energy



The black line at Temperature = 2.26918531 is the phase transition temperature T_c which was exactly determined by Onsager [1]. It corresponds to the critical point of $F(0)$, where ${}^{K'}/_{K} = 0$. These values were each calculated at $K = 1$ after $n = 12$ iterations, with an approximation degree of $D = 12$.

break the magnetic ordering of the lattice, and thus the critical temperature T_c is greater. This is more clearly shown in Figure 9.

Figure 9: Derivative of free energy with respect to temperature

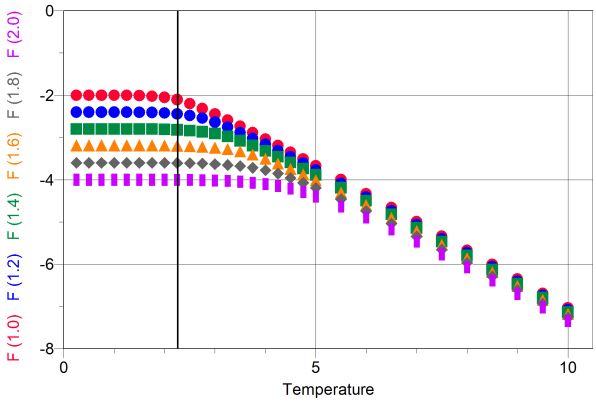


These graphs are the numerical derivatives of the free energy curves in Figure 8.

However, though the inclusion of NNN interactions increases the critical temperature T_c, so does merely increasing the coupling constant K. In Figure 10 below, we adapt Figure 8 so that $K_{new} = K + K'$ and $K'_{new} = 0$.

Thus, an increase in K has the same effect as including NNN interactions. This is demonstrated in Figure 11. In Figure 11, it can be seen that when the strength of the NN interaction is replaced by an equally great NNN interaction (i.e. $K + K'$ is conserved), the relationship

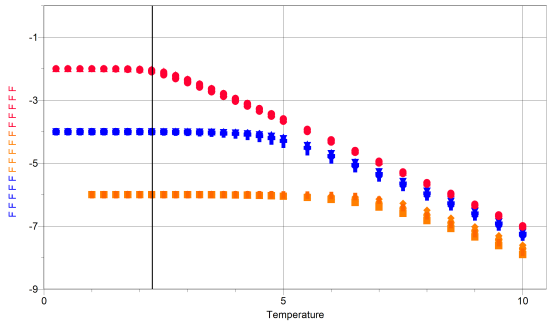
Figure 10: Effect of stronger NN interactions on the behavior of free energy



Graphs are of the form $F(K)$, where $K' = 0$. Values were calculated with $n = 12$ iterations, with an approximation degree of $D = 12$.

between free energy and temperature is nearly unchanged.

Figure 11: Effect of preserving total coupling strength $K + K'$ on the behavior of free energy

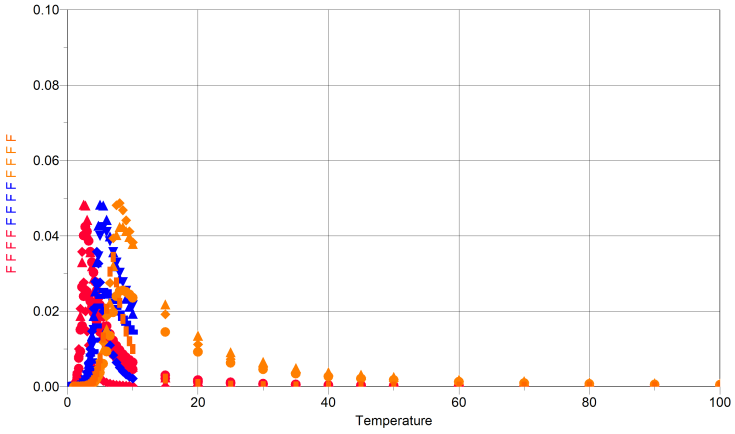


There are fifteen different graphs shown in this figure. If each graph is of the form $F(K, K')$, the red plot $(K + K' = 1)$ is of $F(1, 0), F(0.75, 0.25)$, $F(0.5, 0.5)$, and $F(0.25, 0.75), F(0, 1)$. The blue plot $(K + K' = 2)$ is of $F(2, 0), F(1.5, 0.5)$, $F(1, 1)$, $F(0.5, 1.5)$, and $F(0, 2)$. The yellow plot $(K + K' = 3)$ is of $F(3, 0), F(2.25, 0.75), F(1.5, 1.5), F(0.75, 2.25), F(0, 3)$.

To decide whether the relative error between the graphs of each color is acceptable, we plot the errors in Figure 12, where the error is relative to $F(1, 0), F(2, 0)$, or $F(3, 0)$. We define the error as $\left|\frac{F(a,b)-F(K+K',0)}{F(K+K',0)}\right|$, where a and b are the coupling constants for each graph, excluding $F(1, 0), F(2, 0)$, and $F(3, 0)$. Thus, $a + b = K + K'$.

As all of the relative errors are below .05, and go to zero as the temperature increases,

Figure 12: Relative Error



Graphs of the form $F(K)$, where $K' = 0$. Values were calculated with $n = 12$ iterations, with an approximation degree of $D = 12$.

we conclude that the behavior of $F(a, b)$ closely follows that of $F(K + K', 0)$, and that the presence of K' does not substantially affect the qualitative behavior of the lattice; the inclusion of NNN interactions do not seem to affect the fundamental structure of the free energy curve. In addition, because of the apparent interchangeability of K and K' in the free energy graphs (as shown in Figure 11), we predict that the exclusion of NNN interactions does not quantitatively affect fundamental properties of the phase transition (which are independent of the value of the coupling constant), such as the critical exponents.

4 Further Study

Although the procedure for calculating the spontaneous magnetization and critical exponent β of the Ising square lattice with NNN interactions has been fully worked out and shown to be correct, there has not been an opportunity to carry out the procedure. Further work on explicitly evaluating β is soon to come.

Though we demonstrate in this paper how to account for NNN couplings with relative ease in square lattices, accounting for NNN couplings in other lattice structures, such as

triangular, hexagonal, and kagome, is still an open problem. Although the specific dual-lattice approach to accounting for NNN interactions taken in this paper is not clearly applicable to other lattices, the general strategy of redefining the tensor to encompass all NNN interactions is powerful. Generalizing the TRG method to triangular lattices in particular would be interesting, as it could give insight into how to solve the problem of geometrical frustration in antiferromagnetic triangular lattices.

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