The Anatomy of a Spin: An Entropic Decomposition of the Antiferromagnetic Ising Model on a Triangular Lattice

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Using information-theoretic techniques developed by V.S. Vijayaraghavan, R.G. James and J.P. Crutchfield,[1] this work analyzes the collective behavior of the two-dimensional Antiferromagnetic Ising Model on a triangular lattice. The thermodynamic entropy of the system is decomposed into constituent pieces as a function of temperature both in the absence of an external field, in which case the lattice is frustrated, and in the presence of an external field.

I. INTRODUCTION

This articles considers the entropic properties of the Antiferromagentic Ising Model on a triangular lattice in two-dimensions (TAFIM). The TAFIM is an interesting system to study for several reasons. In the absence of an external field it is a frustrated spin system with finite non-zero entropy $H_0 = \frac{0.3231}{\ln(2)} = 0.4661$ bits at zero temperature, and no finite temperature phase transition. However, introducing an external field induces a second-order phase transition from a disordered paramagnetic phase, to an ordered phase at a critical temperature denoted as T_c.[2] Studying how different types entropic quantities vary as a function of temperature in these two regimes gives valuable insight into the role entropy plays in characterizing the behavior of classical spin systems and, more generally, the behavior of complex spatially extended systems with many coupled degrees of freedom. My results will show that if the *thermodynamic entropy density* h is decomposed into a *local entropy density* r and a *bound entropy density* b, as $T \to 0$ we see that $r > b$.

II. A FRUSTRATED ISING MODEL

The TAFIM is described by the Hamiltonian (energy function)

$$H = J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - B \sum_{i=1}^{N} \sigma_i \tag{1}$$

where $\sigma_i = \pm 1$ denotes a spin in the lattice. The first sum runs over all nearest-neighbors interactions characterized by an antiferromagnetic interaction constant $J > 0$, and the second sum runs over all N spins in the system, coupling them to an external field B. In the absence of an external field ($B = 0$) the system is frustrated, having an infinitely degenerate ground state in the thermodynamic limit, resulting in a non-zero entropy of $H_0 = \frac{0.3231}{\ln(2)} = 0.4661$ bits at zero temperature.[3] The frustration is a direct result of the antiferromagnetic nature of the nearest-neighbor interaction, and the underlying triangular lattice geometry. FIG. 1 displays a single triangle of interacting spins, showing that if one spin is spin-up (red) and the another spin is spin-down (blue), then the total energy of the triangle is $E = -J$, regardless of of whether the third spin is up or down. It is this type of degeneracy, present across the entire spatially extended lattice, that causes the frustration, resulting in a non-zero entropy at zero temperature.

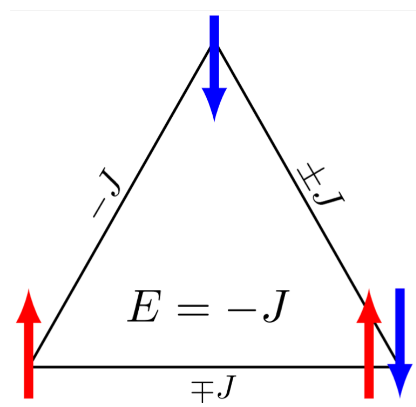

FIG. 1. Frustrated Triangle

Introducing a non-zero external field break the spin-symmetry of the system, lifting the degeneracy of the ground state. It also introduces a finite-temperature second-order phase transition from a paramagnetic phase above T_c, to an ordered phase below T_c, usually denoted ($\sqrt{3} \times \sqrt{3}$). To understand how this ordered phase is structured it is important to first realize that the triangular lattice is not a bipartite graph, but is rather a tripartite graph, meaning it can be split into three distinct sub-lattices (FIG. 2). In the ordered phase two of the three sub-lattices have the same spin, while the third sub-lattice has the opposite spin, giving the full lattice a net magnetization of $m = \frac{1}{3}$. FIG 3. shows the phase diagram for this system in the $B - T$ plane, displaying the phase boundary between the disordered paramagnetic phase and the ordered ($\sqrt{3} \times \sqrt{3}$) phase.[2]

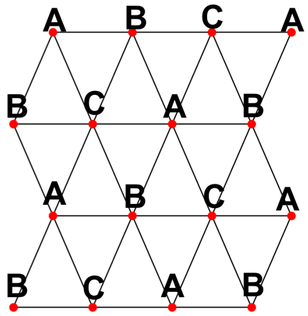

FIG. 2. Tripartite Triangular Lattice: each of the letters A, B and C denotes one of the three sub-lattices.

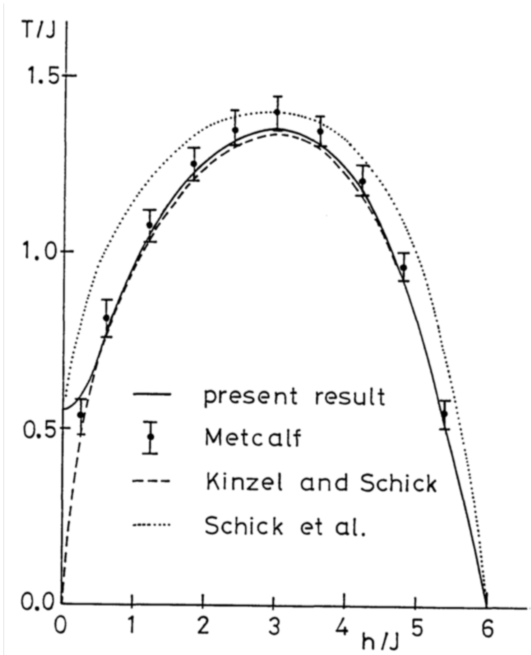

FIG. 3. Phase diagram of antiferromagnetic Ising Model on a triangular lattice.[2]

III. AN ENTROPIC DECOMPOSITION OF CLASSICAL SPIN SYSTEMS

Before I review the different entropic quantities that will be studied in this paper, it is worth spending a moment specifying notation. In this article σ will denote a specific lattice spin configuration, and $\boldsymbol{\sigma}$ will specify the set of all possible configurations such that $\sigma \in \boldsymbol{\sigma}$. A specific spin in the lattice is given by σ_i where $i \in \mathbb{Z} \cap [1, N]$ and N is the size of the lattice. Finally, we will denote the lattice with a single spin σ_i removed as $\sigma_{\setminus i}$. All entropies are computed assuming that the TAFIM is in the canonical ensemble (fixed temperature and lattice size). Therefore the Boltzmann distribution $p(\sigma) = \frac{1}{Z} e^{-H(\sigma)/T}$ gives the probability of a lattice configuration σ occurring, where Z is the partition function that normalizes this distribution. Finally, we define the magnetization of the lattice as $m = \frac{1}{N} \sum_{i=0}^{N} \sigma_i$.

With these definitions in hand we first define the thermodynamic *entropy density* that is traditionally used in thermodynamics and statistical mechanics,

$$h = -\frac{1}{N} \sum_{\sigma \in \boldsymbol{\sigma}} p(\sigma) \log_2 p(\sigma). \tag{2}$$

Next, we specify an *isolated spin entropy*[1] given by

$$H[\boldsymbol{\sigma}_0] = -p(\uparrow) \log_2 p(\uparrow) - p(\downarrow) \log_2 p(\downarrow), \tag{3}$$

where the probability of an up-spin is give by $p(\uparrow) = \frac{1+m}{2}$. Therefore, $H[\boldsymbol{\sigma}_0]$ is the entropy associated with treating each spin as an entirely independent spin that behaves like a biased coin.

Next we define the *localized entropy density*[1] as

$$\begin{aligned} r &= -\frac{1}{N} \sum_{i=1}^{N} H[\sigma_i | \sigma_{\setminus i}] \\ r &= -\frac{1}{N} \sum_{i=1}^{N} H[\sigma_i | \sigma_{nn}]. \end{aligned} \tag{4}$$

This expression is simplified using that fact that the entropy of a given spin conditioned on the rest of the lattice $H[\sigma_i|\sigma_{\setminus i}]$ is equal to entropy of that same spin conditioned only on its nearest neighbors $H[\sigma_i|\sigma_{nn}]$, given that the AFIM Hamiltonian only includes nearest neighbor interactions. The localized entropy r describes how much of the entropy density h is localized to that single spin and not shared with its neighbors. It is now natural to then define a quantity called the *bound entropy entropy*[1] given by

$$b = h - r, \tag{5}$$

which describes what fraction of a given spin's total entropy is shared with its neighbors and, by extension, the rest of the lattice.

There are two final entropic quantities that will be considered in this paper. The first is the *total correlation density*[1] given by

$$\rho = H[\boldsymbol{\sigma}_0] - h. \tag{6}$$

Note that this quantity goes to zero in the limit that $T \to \infty$ and $h \to H[\boldsymbol{\sigma}_0]$. Therefore, it make sense to think of ρ as a measure of how much structure is present in a spin system. Lastly, we define the *enigmatic entropy density*[1]

$$q = \rho - b. \tag{7}$$

This quantity is more challenging to interpret than the others, but can be roughly described as a measure of structure not captured by the entropy density h. FIG 4. provides a useful visualization displaying how these five

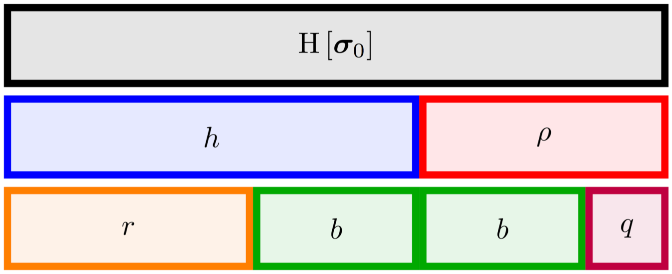

FIG. 4. Entropic Decomposition[1]

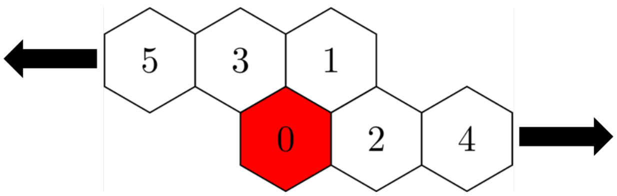

FIG. 5. Neighborhood template about a site σ_0.

entropic quantities are related to each other.

IV. METHOD

The entropic quantities described in the previous section are estimated using a representative samples of probable lattice configurations generated using a Monte Carlo simulations. The Monte Carlo simulations used in this work modeled a 32×32 TAFIM using Metropolis-Hasting accept-reject criteria to decide whether or note to flip a spin. All estimates of entropic quantities were calculated using a saved sample of $10,000$ lattice configurations at a given temperature. In the case of zero external field a configuration was saved every 10 sweeps through the lattice, while with a non-zero external field of $B = 1$ a configuration was saved every 100 sweeps through the lattice.

It is now possible to estimate h using the method outlined in Ref [3]: by constructing a neighborhood template about a selected spin σ_0 in such a way that as this template grows infinitely large it splits the lattice in half, it has been shown that

$$h = \lim_{M\to\infty} H[\sigma_0|\sigma_1, \sigma_2, \ldots, \sigma_M]$$
$$h = \lim_{M\to\infty} \big[H[\sigma_0, \sigma_1, \ldots, \sigma_M] - H[\sigma_1, \ldots, \sigma_M]\big], \tag{8}$$

where M is the size of the neighborhood template. For a system like the AFIM that only has nearest-neighbor interactions this limit converges very rapidly. In fact, by constructing a template of only five spins about a given lattice sites, as shown in FIG. 5, it is already possible to very accurately estimate the entropy density h using the 10,000 sampled lattice configurations. It is similarly possible to directly calculate estimates for $H[\boldsymbol{\sigma}_0]$ and r using the saved configurations. At this point ρ, b and q can be calculated by taking differences.

V. RESULTS AND DISCUSSION

Studying the entropic properties of the TAFIM is interesting because it is a frustrated lattice with finite non-zero entropy at zero temperature.

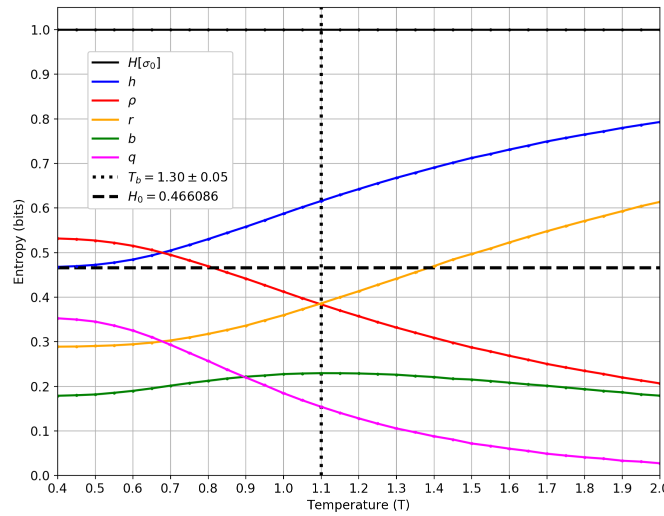

FIG. 6. Frustrated Antiferromagnetic Ising Model on a Triangular Lattice

FIG [6] shows how the different entropic quantities vary as a function of temperature; it is worth noting that, as expected, $h \to H_0$ as $T \to 0$. It is also obvious that in this limit the localized entropy density r is larger than the bound entropy density b. This intuitively makes sense as the largest portion of the zero-temperature entropy H_0 should be associated with the spin-symmetry of the frustrated "third" spin in a triangle, where the energy of the lattice does not change regardless of its orientation. Another interesting feature is that the bound entropy b is non-monotonic as a function of temperature, with an apparent maximum at $T_b = 1.30 \pm 0.05$. The fact that this behavior has a maximum at a finite temperature even in the absence of a phase transition is puzzling. An analysis of the $1D$ Ferromagnetic Ising Model in Ref. [1] similarly found that b has a maximum value at a finite temperature T_b even though there is no phase transition.

Next we consider the AFIM on a triangular lattice in the presence of an external field $B = 1$. Recall that in the presence of an external field the system is no longer frustrated and has a second-order finite temperature phase transition from a paramagnetic phase to the $(\sqrt{3}\times\sqrt{3})$ phase. By studying the behavior of the specific heat c_v and magnetic susceptibility χ as a function of temperature at $B = 1$, shown in FIG. 7, we

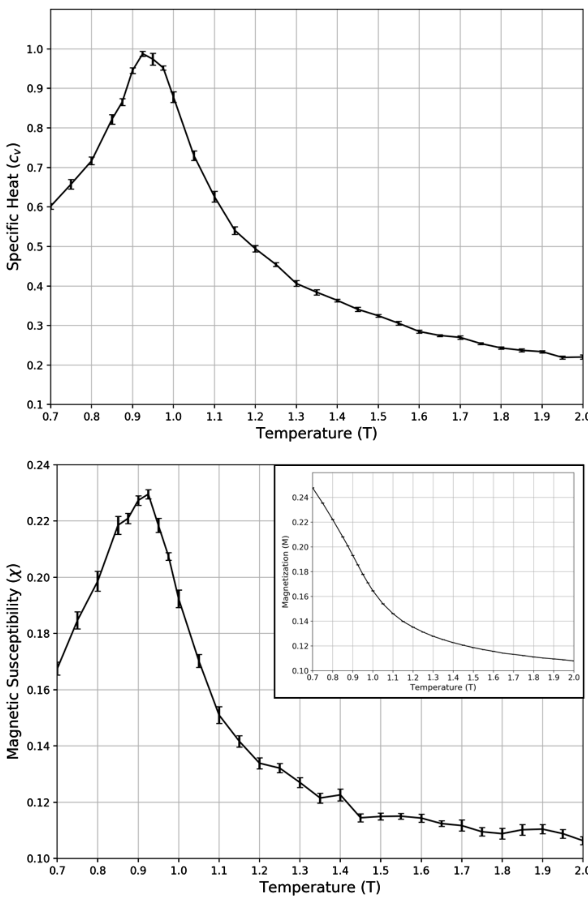

FIG. 7. Specific Heat and Magnetic Susceptibility vs. Temperature for $B = 1$

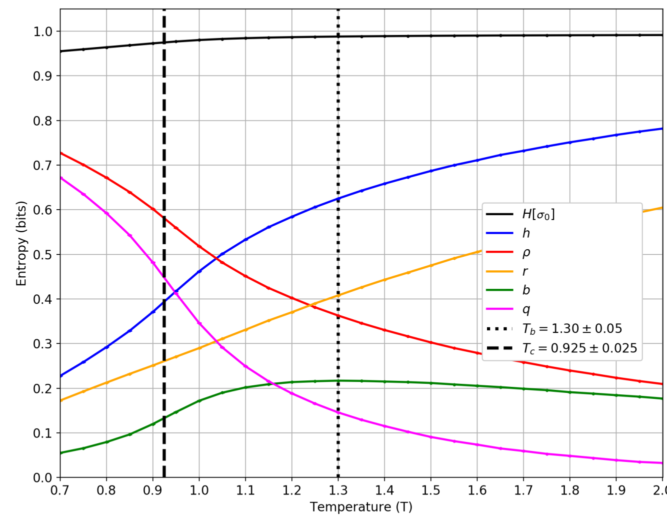

FIG. 8. For $B = 1$

see that the critical temperature is $T_c = 0.925 \pm 0.025$, which is in good agreement with the phase diagram displayed in FIG. 3.

Now let us consider how the entropy of the triangular AFIM varies with temperature in the presence of an external field, keeping in mind that for $B \neq 0$ that $h \to 0$ as $T \to 0$. As observed previously when $B = 0$, FIG. 8 shows that once again $r > b$, although both of these value now approach zero as the temperature goes to zero. It is also the case that b is once more non-monotonic with a maximum value at a finite temperature $T_b = 1.30 \pm 0.05$. This result is puzzling as one might expect that T_b and T_c should equal each other, even though it is clearly the case that $T_b > T_c$. An analysis of the Ferromagnetic Ising Model on a square lattice in two-dimensions (FIM) in Ref. [1] also found that $T_b > T_c$. However, that analysis showed that ρ and q are both maximized at T_c for the FIM. That is clearly not the case for the triangular AFIM with an external field: both ρ and q monotonically decrease with increasing temperature. The reason for this difference is that the isolated spin entropy provides a hard upper bound for both ρ and q in the FIM where $m \to 0$ and $H[\boldsymbol{\sigma}_0] \to 0$ as $T \to 0$ for $T < T_c$. For the TAFIM in an external field as $T \to 0$ then $m \to \frac{1}{3}$ and $H[\boldsymbol{\sigma}_0] \to 0.918$ bits; note that the behavior of $H[\boldsymbol{\sigma}_0]$ in FIG. 8 appears consistent with this bound.

VI. CONCLUSION

Having described the decomposition of a classical spins system's thermodynamic entropy density h into a local entropy density r and bound entropy density b, it is found that for the frustrated TAFIM as $T \to 0$ and $h \to H_0$ that $r > b$. Moreover, both with and without an applied external field B the bound entropy has a maximum value at a finite temperature denoted T_b. In the case of an external field $B = 1$, for which there is a finite temperature phase transition at T_c, we see that $T_b > T_c$. This result is consistent with a similar analysis of the FIM.[1] However, unlike the FIM where both ρ and q are maximized at T_c, for the triangular AFIM in an external field both these quantities decrease monotonically with increasing temperature.

The different entropic quantities studied in this paper give valuable insight into structural dynamics of spatially extended classical spin systems. However, there is clearly a need for further investigation. There is no clear understanding of what underlying dynamic determines the temperature T_b at which the bound entropy density b is maximized. Another possible extension of the work presented in this paper would be to replace $H[\boldsymbol{\sigma}_0]$ in the entropic decomposition outlined in this paper with the slightly modified quantity

$$H[\boldsymbol{\sigma}_0|\boldsymbol{S}] = \sum_{\alpha} H[\boldsymbol{\sigma}_0|S_\alpha] \tag{9}$$

where sum runs over distinct sub-lattices. The reason this slightly modified definition would be interesting to study is that unlike the isolated spin entropy $H[\boldsymbol{\sigma}_0]$ defined in this paper, $H[\boldsymbol{\sigma}_0|\boldsymbol{S}] \to 0$ as $T \to 0$ even in the case of antiferromagnetic order.

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