Antiferromagnetic Ising model saturation field entropies: ladders and kagome lattice

Vipin Kerala Varma
Bethe Center for Theoretical Physics,
Universität Bonn, Germany

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Saturation field entropies of antiferromagnetic Ising models on quasi one-dimensional lattices (ladders) and the kagome lattice are calculated. The former is evaluated exactly by constructing the corresponding transfer matrices, while the latter calculation uses Binder’s algorithm for efficiently and exactly computing the partition function of over 1300 spins to give $S_{\text{kag}}/k_B = 0.393589(6)$.

Antiferromagnetic Ising models can harbour a macroscopic number of degenerate ground states at zero external field on frustrated lattices like the triangular lattice, kagome lattice, pyrochlore lattice, to name a few. An extensive entropy may survive, albeit with different values, even for infinitesimal fields on certain lattices; as the field is varied, a strongly enhanced peak in the entropy develops just before the field-induced spin-ordering sets in; this substantial peak occurs because, at this field strength, a large number of non-neighbouring spins may be flipped against the field without a cost in energy. In fact, such residual saturation entropies $S_{\text{sat}}$ persist in quantum spin models (anisotropic Heisenberg models), although with different values from the Ising limits, and for different reasons pertaining to the existence of localized magnons.

Our results are summarized in Table II. In Section I, residual saturation entropies of related quasi one-dimensional lattices or ladders (Fig. 1(a)) are exactly computed; of which, ladder $L_1$ will be used to build up the kagome lattice (Fig. 1(b)). For the kagome lattice, approximate values of $S_{\text{sat}}$ may be deduced from calculations for spin ice on the pyrochlore lattice in a $(111)$ field; results of Monte Carlo simulations, series expansion techniques and the Bethe approximation were found to be comparable for the saturation entropy. In Section II, we elucidate a procedure for obtaining a more accurate estimate of this value through (a) transfer matrix methods, and equivalently (b) the solution of appropriate difference equations that generate the partition function. Finally in Section III, we provide a considerably improved estimate of $S_{\text{sat}}$ for the kagome lattice using Binder’s algorithm. With which we may exactly calculate the partition function of a system of over, in our case, 1300 Ising spins at the saturation field with the expenditure of modest computational resources. We point out that it is only for the Ising kagome lattice, among other two dimensional lattices, that the zero field entropy exceeds the saturation field entropy.

The antiferromagnetic Ising models we investigate are described by the Hamiltonian

$$\mathcal{H} = \sum_{<i,j>} \sigma_i \sigma_j - h_c \sum_i \sigma_i,$$  \hspace{1cm} (1)

on an $N$ site lattice with $|h_c| = z$, the nearest neighbour of neighbours. This is the saturation field beyond which ordering sets in. The variables $\sigma_i = \pm 1$ which we represent by up and down spins, and the interaction between nearest neighbours is denoted by the angular brackets, setting the energy scale of the problem. The boundary conditions are chosen to be either free or periodic. Although the number of allowed states for a given finite system will differ depending on the boundary conditions, the dominant multiplicative degeneracy of the system as $N \to \infty$ will reflect the bulk property. It will then be a question of computational convenience whether free or periodic boundary conditions be chosen.

I. LADDERS

In this section we describe the transfer matrix procedure to calculate the partition function $\Omega_m$ of a ladder with $m$ unit cells, such that no up spin may neighbour another; the space of such configurations is denoted as $C_m$ which comprises the degenerate ground states at $h_c$ for $L_1$ and $L_2$. We illustrate the idea with the case of ladder $L_3$ where a unit cell is taken to be a simple triangle; this will be relevant while building up the kagome lattice from this ladder. We emphasize that, for this particular ladder $L_3$, the configurations in $C_m$ do not con-

![FIG. 1: (a) Quasi one-dimensional lattices (ladders) $L_1, L_2, L_3$. $L_2$ in a triangular lattice pattern reproduces the kagome lattice. (b) Kagome lattice with unit cell labelled A, B, C.](image-url)
TABLE I: Partition function in configuration space $C_m$ for $m$–site (cell) Ising chain (ladder $L_3$) with periodic and free boundary conditions; values for $m = 1, 2, 3, 4$ (which exclude the boundary spins/cells for free boundaries) are indicated.

| Boundary | Ising chain | Ladder $L_3$ |
|----------|-------------|--------------|
| Periodic | $(\frac{1 + \sqrt{3}}{2})^m + (\frac{1 - \sqrt{3}}{2})^m = 1, 3, 4, 7, \ldots$ | $(2 + \sqrt{3})^m + (2 - \sqrt{3})^m = 4, 14, 52, 194, \ldots$ |
| Free | $\frac{1}{\sqrt{2}} [(\frac{1 + \sqrt{3}}{2})^{m+2} - (\frac{1 - \sqrt{3}}{2})^{m+2}] = 2, 3, 5, 8, \ldots$ | $\frac{1}{\sqrt{2}} [(2 + \sqrt{3})^{m+1} - (2 - \sqrt{3})^{m+1}] = 4, 15, 56, 209, \ldots$ |

Of the transfer matrix over the conditions, the total number of states is given by the trace where a zero entry indicates the aforementioned disallowed states on the chain. Following Metcalf and Yang, the third of these states may not follow the second of these states on the chain. Following Metcalf and Yang, the transfer matrix for the present case may be defined as

$$M_{L_3} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix},$$

where a zero entry indicates the aforementioned disallowed sequence of states. Under periodic boundary conditions, the total number of states is given by the trace of the transfer matrix over the $m$ cells. That is

$$\Omega_m^{\text{PBC}} = \text{Tr}[(M_{L_3})^m] = (2 + \sqrt{3})^m + (2 - \sqrt{3})^m. \quad (2)$$

Note that the trace automatically disallows the reverse of condition (b) i.e. $C_1(2)$ not following $C_1(3)$ through the chain ends; thus the non-Hermiticity of $M_{L_3}$ poses no issues.

We treat the boundary conditions on a more general footing by solving for the characteristic polynomial of $M_L$, to give $\lambda^2(\lambda^2 - 4\lambda + 1) = 0$, from which the difference equation relating the partition function $\Omega_m$ of $m$–cell ladders may be readily read off as

$$\Omega_m = 4\Omega_{m-1} - \Omega_{m-2}, \quad (3)$$

for both periodic and free boundary conditions, for each of which we merely have to set different initial conditions in Eqn. (3). The partition functions of $C_m$ with both boundary conditions are compared with that of the Ising linear chain at saturation in Table I.

The entropy per cell is then given by the logarithm of the dominant contribution to $\Omega_m$. With this, we may obtain the saturation entropies of all the illustrated ladders in Fig. 1(a). The values and the generating difference equations are tabulated in Table II. For ladders $L_1$ and $L_2$, the computed values are indeed the saturation field entropies. The addition of diagonal bonds, in proceeding from the former to the latter, clearly reduces the residual entropy associated per lattice site.

II. KAGOME LATTICE

The kagome lattice, a section of which is illustrated in Fig. 1(b), may be thought of as ladder $L_3$ repeated in a two dimensional triangular lattice pattern, with a ‘site’ now being a simple triangle labelled $A, B, C$ in the figure. Before proceeding with the calculations, we can provide upper and lower bounds for the kagome lattice’s entropy at the very outset. For the lower bound, following the arguments in Ref. [9], there must be more entropy per site than the triangular lattice because the increased connectivity of the latter serves to restrict the configuration space: we have already seen the reduction in entropy, while constructing $L_2$ from $L_1$, from the addition of diagonal bonds. As regard an upper bound, following similar reasoning, clearly the kagome lattice cannot support more configurations than the ladder $L_3$ from which it is built. Therefore we get the inequality

$$0.3332427 \ldots < S_{\text{kagome}} < 0.4389859 \ldots \quad (4)$$

where the lower bound, the saturation entropy for the Ising triangular lattice, is known exactly through the solution of the hard-hexagon model.\textsuperscript{12}

We adopt 2 approaches for estimating the convergence of the entropy as a function of system size. The first follows the transfer matrix and linear scaling method of Metcalf and Yang,\textsuperscript{15} for which we also provide an alternative reformulation; and the second is the ratios method of Milošević et al.\textsuperscript{14}

In Fig. 2(a) we illustrate how free and periodic boundary conditions are effected for an $m \times n = 2 \times 2$ kagome system. The black (dark) bonds indicate the underlying equivalent triangular lattice; this transformation to a triangular lattice makes the remainder of the analysis tractable.

A. Transfer matrix: linear scaling

For a two dimensional lattice the transfer matrices are constructed as follows from the one dimensional building chains\textsuperscript{9}, which in our case are the $L_3$ ladders. The matrix element $M_{i,j}$ is set to 0 if the state $j$ of an
FIG. 2: (a) Free and periodic boundary conditions for the kagome lattice using an $m \times n = 2 \times 2$ system. Upper figure shows FBC: grey (light) triangles indicate spins aligned with the field, red (circled) triangles have finite degeneracies, black (dark) lines indicate the bonds constituting the triangular lattice. Bottom figure shows PBC with grey (dashed) lines indicating the imposition of periodicity. The partition function for each case and the segment of the equivalent triangular lattice (right) are also indicated. (b) Scaling of residual saturation entropy, in units of $k_B$, on the Ising kagome lattice as function of number of triangles for two different scaling and boundary conditions. $m$ denotes the number of unit cell triangles on each ladder, and the number of such ladders $n = 100$.

$m$-cell ladder cannot follow state $i$ on an adjacent $m$-cell ladder; otherwise the matrix element is 1. Clearly the matrix is of size $\Omega_m \times \Omega_m$, which already for $m = 6$ gives a little over 7 million matrix elements in $M$. The partition function is then given as before by $\Omega_{m,n} = \text{Tr}[M^n]$ for the $m \times n$ system; as we will see, typically $n = 100$ gives a good estimate up to three to four decimal places for the entropy. To obtain the entropy per $m$-cells, it is assumed that every new ladder added to the finite system multiplies the system’s degeneracy by a constant factor of $\alpha$, so that

$$\log \Omega_{m,n} = n \log \alpha + C_{m,n},$$

(5)
gives the entropy per $m$ cells as $\log \alpha$, where the $C_{m,n}$ denote the correction terms. It is expected that these terms decrease for increasing $m, n$ values. Thus the procedure is to calculate $\Omega_{m,n}$ and use the linear fit against $n$ to extract the entropy. We show in Fig. 2(b) with full and dashed red lines the convergence of the entropy as the number of triangles is varied for periodic and free boundary conditions. Note that the trace operation automatically imposes periodic boundary conditions along the $n$-direction. Moreover we have checked for a system with free boundary conditions along the $n$-direction as well (using Binder’s algorithm in Section III) that the values obtained, and hence the convergence trends, are essentially the same. And as observed in Ref. [13] for other lattices, free boundary conditions does not give rapid convergence using Eqn. 5. As noted in the previous section (see Eqn. 3 or Table II for instance), the degeneracies may also be generated by solving difference equations on the lattice subject to appropriate initial values. For the kagome lattice, a difference equation for each $m$ is obtained and solved to obtain identical results as in Fig. 2(b). However this alternative and equivalent approach to Metcalf and Yang’s procedure of matrix multiplication followed by the trace operation retains, at the present time, no computational gain because determining the characteristic polynomial of a matrix is about as hard as matrix multiplication with today’s algorithms.

B. Transfer matrix: ratios

In the ratio method, the correction terms $C_{m,n}$ are substantially reduced by using a sequence of estimators for the entropy as:

$$S_{m,n} = \log \left( \frac{\Omega_{m+1,n+1}}{\Omega_{m,n}} \right).$$

(6)

For relatively large $m$ and $n$ values each added chain will multiply the system’s degeneracy by a factor of $\alpha = \beta^{3m}$, where $\beta$ is the factor associated with each site. Thus Eqn. 6 is seen to give the residual entropy per cell with considerable diminution of the correction terms. As plotted in Fig. 2(b) with the dotted and dashed-dotted black lines, the use of Eqn. 6 provides faster convergence for the entropy compared to Eqn. 5; in contrast to Eqn. 5, Eqn. 6 seems better suited for free
We have seen in the preceding section that free boundary conditions along with Eqn. 6 provide a rapidly convergent sequence for the entropy. The main limitation was however the calculation of $\Omega_{m,n}$ for large \{m, n\} values. This may be achieved by employing Binder’s algorithm towards an exact evaluation of the partition function of finite lattice systems\cite{Binder}. To briefly recapitulate, the partition function of a system of size \{m, n\} is expressed in terms of the degeneracies $\gamma_{m,n}(i)$ of the $n^{th}$ ladder in its $i^{th}$ state. Then clearly

$$
\Omega_{m,n} = \sum_i \gamma_{m,n}(i). \tag{7}
$$

Now the degeneracies of an added ladder for the \{n, m + 1\} system may be recursively computed by

$$
\gamma_{m,n+1}(i) = \sum_{i'} \gamma_{m,n}(i'), \tag{8}
$$

with the summation running over only those values of $i'$ such that state $i$ may be adjacent to it. With this, we have computed the partition function of over 1300 spins with modest computational effort. For instance, we are able to reproduce up to 10 digits in the residual saturation field entropy value for the square lattice using twenty 10-rung $L_1$ ladders. Using Eqns. 6-8 we compute $S_{6,50}$, $S_{7,50}$ and $S_{8,50}$ to give six stable digits for the kagome lattice saturation field entropy

$$
S_{\text{kag.}}/k_B = 0.393589(6). \tag{9}
$$

We compare this with low temperature Monte Carlo simulation results and the Bethe approximation for pyrochlore spin ice which, at the saturation field, may be described by a two-dimensional network of Ising pseudospin kagome lattice\cite{Takayama}. Scaling the saturation field results of Isakov et al. by a factor of $4/3$ (because the corner spin in the pyrochlore tetrahedron is considered frozen giving a high temperature entropy per site of only $\log(2)$), we obtain the relevant results to be

$$
S_{\text{kag.}}^{\text{MC}}(T/J = 0.15) \approx 0.397, \quad S_{\text{kag.}}^{\text{Bethe}} \approx 0.38772.
$$

## III. BINDER’S ALGORITHM

We have considered the degenerate space of states of a few Ising ladders and the Ising kagome lattice at the saturation external field. For the ladders, by a simple redefinition of a site, the residual entropy may be exactly computed. We treat the generation of states for periodic and free boundary conditions on a general footing by use of difference equations.

For the kagome lattice, we are able to provide six stable digits for the residual entropy by calculating the exact partition function of over 1300 spins using Binder’s algorithm implemented on a standard computer. Our accurate result compares reasonably with approximate results from low temperature Monte Carlo simulations and the Bethe approximation for an equivalent system. We believe that by constructing appropriate ladders the residual saturation field entropies of geometrically complex lattices, like the pyrochlore, may be similarly computed with more ease after their transformation to standard lattice structures.

The primary results are summarized in Table II.

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| Lattice        | Difference equation | Entropy                                  |
|----------------|---------------------|------------------------------------------|
| $L_1$          | $x_n = 7x_{n-1} - 7x_{n-2} + x_{n-3}$ | $\frac{1}{4} \log (3 + 2\sqrt{2}) = 0.440686 \ldots$ |
| $L_2$          | $x_n = 5x_{n-1} - 2x_{n-2} + x_{n-3}$ | $\frac{1}{3} \log (2 + \sqrt{3}) = 0.438985 \ldots$ |
| $L_3$          | $x_n = 4x_{n-1} - x_{n-2}$          | $0.393589(6)$                            |
| Kagome        | -                   |                                          |

For the kagome lattice, we are able to provide six stable digits for the residual entropy by calculating the exact partition function of over 1300 spins using Binder’s algorithm implemented on a standard computer. Our accurate result compares reasonably with approximate results from low temperature Monte Carlo simulations and the Bethe approximation for an equivalent system. We believe that by constructing appropriate ladders the residual saturation field entropies of geometrically complex lattices, like the pyrochlore, may be similarly computed with more ease after their transformation to standard lattice structures.

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### Table II: Residual entropies per site, in units of $k_B$, in the configuration space $C_m$ for the lattices in Figure 1. The difference equations for the ladders are independent of the boundary conditions but the total number of states changes for each finite segment.

| Lattice | Difference equation | Entropy |
|---------|---------------------|---------|
| $L_1$   | $x_n = 7x_{n-1} - 7x_{n-2} + x_{n-3}$ | $\frac{1}{4} \log (3 + 2\sqrt{2}) = 0.440686 \ldots$ |
| $L_2$   | $x_n = 5x_{n-1} - 2x_{n-2} + x_{n-3}$ | $\frac{1}{3} \log (2 + \sqrt{3}) = 0.438985 \ldots$ |
| $L_3$   | $x_n = 4x_{n-1} - x_{n-2}$          | $0.393589(6)$ |
| Kagome  | -                   |          |
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