

$\pm J$ Ising model on Archimedean $(4, 8^2)$ lattices

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Abstract

We report results on ground state properties for a $\pm J$ Ising model defined on the Archimedean $(4, 8^2)$ lattice. The sublattice method is adapted to this system. By means of combinatorics and probability analysis, weight functions are obtained allowing to calculate properties such as frustrated plaquette distribution, frustration length, energy per bond, and fractional content of unfrustrated bonds; these analytic expressions are presented as functions of x (concentration of ferromagnetic bonds). On the other hand, these parameters are also calculated by an exact numerical algorithm applied to a large number of samples for increasing size N (number of spin sites) and values of x in the range $[0.0, 1.0]$. Analytical and numerical results tend to agree, which makes these two techniques complementary to each other. Finally, comparison is made to results previously reported for other Archimedean lattices.

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1. Introduction and theory

The Edwards–Anderson model was proposed as a simple way to understand the basic of spin-glasses [1]. Other frustrated systems can also be considered in a similar way [2]. In particular the crucial role played by frustrated plaquettes was recognized very early [3] and has proven to be a key element to make progress in the understanding of frustration in all kind of lattices. Present work is an application of this line of thought to the $(4, 8^2)$ lattice in the notation of Grünbaum and Shephard [4] as illustrated in Fig. 1(a). Sites represent positions for spins. Bonds between neighboring sites can be ferromagnetic (F) with a probability x or antiferromagnetic (AF) with a probability $(1 - x)$; in a particular sample this assignment is at random but remains frozen. The minimum circuit formed by bonds is called a plaquette; in the present case there are as many square plaquettes (SL) as octagonal plaquettes (OL). A plaquette is frustrated or *curved* if it is formed by an odd number of AF bonds.

The probability that a SL is curved is given by $\varphi_c^{SL}(x) = 4x(1 - x)^3 + 4x^3(1 - x)$, taking into consideration the 4 possible orientations in the lattice [5]. A similar analysis can be done to find φ_c^{OL} , the probability that an OL is curved. Then, the weighted probability that any plaquette is curved can be put as [5]

$$\varphi_c(x) = 2x(1 - x)(3 - 14x + 46x^2 - 96x^3 + 128x^4 - 96x^5 + 32x^6), \quad (1)$$

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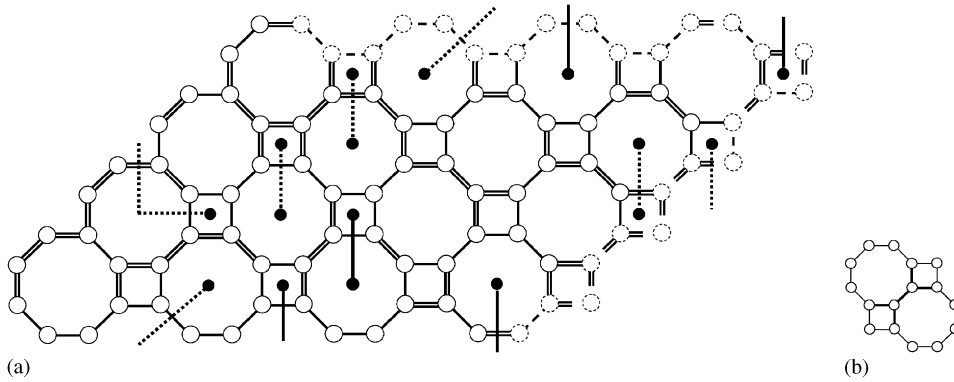


Fig. 1. (a) One illustrative sample for $(4, 8^2)$ lattices of size $N = 64$. Single (double) line represents a(n) ferromagnetic (antiferromagnetic) exchange interaction, periodic boundary conditions are used (dashed lines on the upper and right boundaries). Black circles mark curved plaquettes. One possible double ground state (out of 6) is given by means of frustration segments (dashed and solid lines, where the last ones correspond to rigid frustrations [7]); (b) sublattice or cell formed by two square plaquettes and two octagonal plaquettes.

$$H = \sum_{i < j}^N J_{ij} S_i S_j$$

is the Ising Hamiltonian for this system, where $J_{ij} = J (-J)$ for AF (F) interactions, with $J > 0$; the sum runs over all pairs of nearest neighbors; S_i is the spin of the i th site. A state is an ordered set of the N spins. Not all local fields can be simultaneously satisfied which leads to frustration [3,6]. The ground state energy can be found joining frustrated plaquettes in pairs by means of frustration segments minimizing the number of frustrated bonds. The frustration length A is the total number of frustrated bonds adding the contribution of the v frustration segments. The average frustration segment is $\lambda = A/v = 2A/P_c$, where P_c is the total number of curved plaquettes. The total energy is expressed as $E = -B + 2A$, where B is the total number of bonds. The ground state energy E_g is obtained by finding A_g , the absolute minimum frustration length (subscript g refers to ground level). The ground energy per bond is simply given by

$$\varepsilon_g = -1 + \frac{2A_g}{B} = -1 + \frac{P_c \lambda_g}{B} = -1 + \frac{P \wp_c \lambda_g}{B} = -1 + \frac{\wp_c \lambda_g (C - 2)}{C}, \tag{2}$$

where P is the total number of plaquettes and C is the coordination number. C is 3 for $(4, 8^2)$ lattices. The sample illustrated in Fig. 1(a) corresponds to $N = 64$, with $B = 96$, for the case $x = 0.5$. The 16 frustrated plaquettes are depicted by a black circle. The 8 segments for one possible ground state are shown as lines joining pair of plaquettes. Solid lines mark those segments that are present in all 6 ground states (periodic boundary conditions are imposed). For this example $v = 8$; $A_g = 9$ yielding $\lambda_g = \frac{9}{8}$; $\wp_c = P_c/P = \frac{16}{32} = 0.5$. All of which leads to $\varepsilon_g = -1 + (0.5 \times 1.125)/3 = -0.8125$.

The diluted lattice [8] is formed by the D bonds that do not frustrate in any ground state. The fraction of unfrustrated bonds is $h_g = D/B$.

All ground state properties can be calculated in terms of probability distributions by using a sublattice or cell. We restrict ourselves to $\lambda_g(x)$, $\varepsilon_g(x)$ and $h_g(x)$, obtaining their analytic expressions. Combinatorics is used to assign a statistical weight to each plaquette configuration. We pick here a cell formed by 2 plaquettes of each kind as can be seen in Fig. 1(b). The pairing of plaquettes within the proposed cell minimize energy following simple rules: (a) frustration segments up to length 2 are considered; (b) for an even number of plaquettes they pair within the cell only; (c) for an odd number of plaquettes the last one is paired towards the outside minimizing energy.

Each possible plaquette distribution will be labelled by j , with degeneracy α_j . The probability of producing such plaquette distribution will be denoted as ψ_j and is obtained by weighting all bond distributions leading to the j th plaquette distribution with σ_j frustration segments, and λ_{gj} as the average segment. All of this

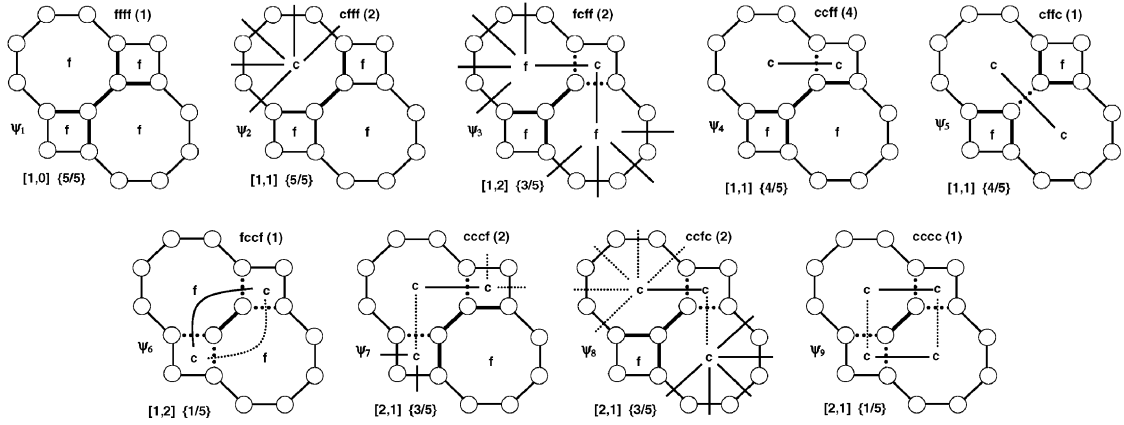


Fig. 2. The 9 different plaquette configurations for $(4, 8^2)$ lattices.

is combined to write

$$A_g = \sum_j \alpha_j \psi_j \sigma_j \lambda_{gj}; \quad v_g = \sum_j \alpha_j \psi_j \sigma_j; \quad \lambda_g = \frac{\sum_j \alpha_j \psi_j \sigma_j \lambda_{gj}}{\sum_j \alpha_j \psi_j \sigma_j}.$$

The ground state energy per bond is obtained from Eq. (2) where $\wp_c(x)$ is given by Eq. (1) and λ_g was obtained in previous equation. To obtain an expression for $h_g(x)$ we pay attention to the 5 inner bonds in the cell (thicker bonds in Fig. 2). Each plaquette configuration yields a value for this parameter which will be denoted by \tilde{h}_j . Then, by making use of the statistical weights, we can write $h_g(x) = \sum_j \alpha_j \psi_j \tilde{h}_j$.

Alternatively, we will obtain and report exact numerical results [9] considering average values over 500 samples for each concentration x on lattices of size 64; a total of 10 500 samples were exactly solved.

2. Discussion, results and conclusions

In Fig. 2 we present the 9 possible plaquette configurations ψ_1 through ψ_9 with the following labelling: at the center of each plaquette we indicate whether it is curved: *c* or *flat*: *f*; in the upper right corner we give the configuration and its multiplicity (α_j); in the lower left sector we give the number of frustration segments of each possible length: $[\sigma_j, \lambda_{gj}]$; this is followed by the ratio of the configurational fraction of unfrustrated bonds $D_j/5$. Criteria (a)–(c) were strictly observed [10]. Combining Table 1 and previous equation we get

$$\lambda_g(x) = \frac{2\psi_2 + 4\psi_3 + 4\psi_4 + \psi_5 + 2\psi_6 + 4\psi_7 + 4\psi_8 + 2\psi_9}{\psi_1 + 2\psi_2 + 2\psi_3 + 4\psi_4 + \psi_5 + \psi_6 + 4\psi_7 + 4\psi_8 + 2\psi_9}. \quad (3)$$

Then, $\varepsilon_g(x)$ is easily obtained from a combination of Eqs. (2), (1) and (3). Making use of the expression for $h_g(x)$ given above and Table 1 we find

$$h_g(x) = \frac{5\psi_1 + 10\psi_2 + 6\psi_3 + 16\psi_4 + 4\psi_5 + \psi_6 + 6\psi_7 + 6\psi_8 + \psi_9}{5}.$$

In Fig. 3 we plot functions $\lambda_g(x)$, $h_g(x)$ and $\varepsilon_g(x)$, where we also include discrete results obtained by numerical calculations on samples for $N = 64$. The overall correspondence is good, especially in the central part of the range.

For the case of λ_g a disagreement is shown towards the extremes of the range which can be attributed to the truncation of the contributions so $\lambda \leq 2$ (an ever larger disagreement was obtained by considering a smaller cell). However, the expected particular values $\lambda_g(0.0) = \lambda_g(1.0) = 0.0$ are recovered by both the analytic expression and the numerical calculations. As for all lattices with plaquettes formed by an even number of bonds $\lambda_g(x)$ turns out to be symmetric with respect to $x = 0.5$. A better agreement is seen for $h_g(x)$. Actually,

Table 1

Weight coefficients of power in terms $x^{19-i}(1-x)^i$ ($i = 0-19$) for plaquette distribution functions ψ_j ($j = 1-9$) corresponding to Fig. 2

i	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
ψ_1	1	0	22	67	250	762	1582	3030	4844	5826	5826	4844	3030	1582	762	250	67	22	0	1
ψ_2	0	5	9	84	268	664	1680	3108	4604	5962	5962	4604	3108	1680	664	268	84	9	5	0
ψ_3	0	2	10	56	248	736	1680	3144	4744	5764	5764	4744	3144	1680	736	248	56	10	2	0
ψ_4	0	1	11	62	242	722	1694	3158	4730	5764	5764	4730	3158	1694	722	242	62	11	1	0
ψ_5	0	1	27	62	242	770	1582	3030	4858	5812	5812	4858	3030	1582	770	242	62	27	1	0
ψ_6	0	0	6	42	214	762	1806	3170	4638	5746	5746	4638	3170	1806	762	214	42	6	0	0
ψ_7	0	0	4	44	228	748	1764	3212	4708	5676	5676	4708	3212	1764	748	228	44	4	0	0
ψ_8	0	0	12	68	236	708	1708	3172	4716	5764	5764	4716	3172	1708	708	236	68	12	0	0
ψ_9	0	0	2	46	242	734	1722	3254	4778	5606	5606	4778	3254	1722	734	242	46	2	0	0

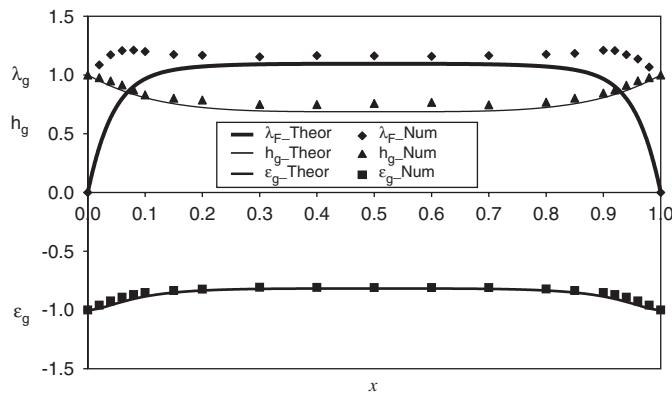


Fig. 3. Average frustration segment, fractional content of diluted lattice and average energy per bond for $(4, 8^2)$ lattices. Analytic results are represented by curves while average values over exact numerical results are given by symbols.

as the size of the lattices used in the numerical simulations grow a better agreement is obtained. Again, the expected extreme cases $h_g(0.0) = h_g(1.0) = 1.0$ are obtained. What is most interesting is that the general fashion is basically the same for numerical and analytic results, which is a strong support for the method of the sublattice. Finally, the agreement for $\epsilon_g(x)$ is excellent, which is again a good argument in favor of the method of the sublattice to give the functional dependence of physical parameters for frustrated lattices. The extreme cases $\epsilon_g(0.0) = \epsilon_g(1.0) = -1.0$ are obtained quite naturally.

A scaling analysis (not shown here) was done for parameters $\lambda_g(0.5)$, $h_g(0.5)$ and $\epsilon_g(0.5)$, after considering 500 samples for 7 sizes from $N = 36$ to 144. The extrapolated values in the thermodynamic limit are: $\lambda_g(0.5) = 1.09$, $h_g(0.5) = 0.74$ and $\epsilon_g(0.5) = -0.82$. For comparison we also give the analytic values for these parameters which are 1.09, 0.69 and -0.82 , respectively.

The main conclusion is the validation of the method of the sublattice to obtain analytic expressions for physical magnitudes even in the case of non-homogeneous lattices like the $(4, 8^2)$. The truncation affects directly $\lambda_g(x)$, but the effect is less pronounced for $h_g(x)$ and $\epsilon_g(x)$. This is encouraging to extend this method to any nonhomogeneous lattice and even in three-dimensions where this method has not been explored. The agreement between numerical and simulated results is better in the central part of the range, for $0.2 < x < 0.8$ say, where values and curvatures are well depicted. The agreement in the case of the energy per bond is good over the entire range. Physical parameters $\epsilon_g(0.5)$ and $h_g(0.5)$ show a strong correlation with C which allows a comparison with a similar behavior for other lattices, like the hexagonal one, also with $C = 3$, where it has been found that $h_g(0.5) = 0.75$ and $\epsilon_g(0.5) = -0.82$ which are close to the values for the $(4, 8^2)$ lattice reported here and far from lattices with even coordination number [10].

Acknowledgments

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