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Thermodynamic integration method applied to $\pm J$ Ising lattices

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Abstract

Square lattices with Ising spins at the sites and $\pm J$ exchange interactions between nearest neighbors are one of the realizations of the Edwards–Anderson model originally proposed to mimic spin glasses. Such systems produce a complex configuration space due to frustration originated in local competing fields. Reaching exact results for physical parameters is limited to the ground states of small systems. Due to this complexity it is unavoidable to use numerical methods subject to controlled error to attempt a good approximation for large enough systems. Here we make use of the thermodynamic integration method to obtain energy and remnant entropy for lattices 20×20 with variable concentration x of ferromagnetic bonds. It turns out that both energy and entropy reach their minima at $x = 0.0$ and 1.0 growing towards the symmetric point $x = 0.5$ in a similar way, leading to an almost linear relationship between entropy and energy.

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1. Introduction

The thermodynamic integration method (TIM) [1] has been applied to calculate ground state properties for $\pm J$ Edwards–Anderson systems [2–5] with equal amount of ferromagnetic (F) and antiferromagnetic (AF) interactions. Recent results show that good accuracy can be obtained when sources of errors are treated separately which allows to grow in system size [6]. In the present paper we focus on square lattices of 400 spins (20×20), varying the concentration x of ferromagnetic bonds in the interval [0.0,1.0], namely between a pure AF and a pure F system, going over several intermediate situations. The aim is to calculate and discuss two main ground state properties as functions of x: ground state energy per bond and associated remnant entropy per bond.

Frustrated systems, like $\pm J$ Ising lattices under consideration, are complex systems due to randomness and frustration leading to high ground state energies and large degeneracies. Exact calculations based on exhaustive scanning of the whole ground manifold (GM) are limited to small systems only [7–11]. To get results for larger systems (over a 100 spins say), approximate methods have to be invoked. One such method is TIM, which become more reliable after error sources are kept under control.

In the next section, we briefly review the method and its main characteristics; additionally, systems are also defined reminding their most relevant known properties. In Section 3 we present and discuss the results. Finally, the last section is devoted to conclusions.

2. Methodology and systems

The way TIM is applied to systems with complex configuration space was recently presented in the literature [6], so we merely sketch here the main considerations for its use.

The starting point is the usual equation from the thermodynamics:

$$\frac{1}{T} = \left(\frac{\partial S}{\partial U}\right)_N , \tag{1}$$

where T is the absolute temperature, U is the total internal energy, S is the entropy and N is the total number of active centers in the sample. By integrating the above equation, it is possible to obtain the remnant entropy per bond, $S_i(N)$ [6]:

$$S_i(N) = \frac{\ln 2^N}{2N} + \int_{\infty}^{0} U_i(N,t)\,\mathrm{d}\left(\frac{1}{t}\right) = \frac{\ln 2}{2} + I_i(N) , \tag{2}$$

where $U_i(N,t)$ is the mean energy at temperature t and the subindex indicates the ith sample. Here we have made use of the fact that for any Ising system formed by N

spins we have

$$\lim_{T\to\infty} S(N,T) = \ln 2^N . \tag{3}$$

In the present application, we deal with square lattices, with Ising spins at the sites and exchange interactions or bonds to nearest neighbors that can be either F in proportion x, or AF in proportion $(1-x)$. Size will be 400, all in square arrays of 20 spins along each direction. For each concentration x, a total of $M = 500$ independent samples were prepared (each sample is a random distribution of F and AF bonds). Concentration x was varied within the interval [0.0,1.0]. Then, a total of 22,500 samples were numerically calculated handling the sources of error as already reported in literature [6]. Additionally, a finer variation of x was done for the interval [0.0,0.2] to discuss and compare with analytic expressions valid for local fields in the way presented below.

Each spin is subjected to different possible local fields due to competition among random F and AF interactions. Not all interactions can be simultaneously satisfied and some of them remain frustrated even in the ground states. Frustration raises energy and increases degeneracy making even ground state characterization a very difficult problem. Ground state degeneracy is associated to remnant entropy which is one of the aims of the present calculation.

The numerical procedure for evaluating the thermodynamical quantities corresponding to a given sample is the following:

(a) A concentration x is set.
(b) A random sample is generated.
(c) A dummy temperature t is chosen.
(d) The average energy, $U_i(t)$, is measured by means of a Monte Carlo process.
(e) t is varied at small intervals and process (d) is repeated.
(f) A curve $U_i(t)$ versus $1/t$ is constructed in the whole range of temperature.
(g) The integral I_i from Eq. (2) corresponds to the area under this curve between $t = \infty$ down to $t = 0$. Then entropy $S_i(N)$ can be readily calculated according to this expression.

By iterating this procedure for M samples, we obtain $S_M \equiv \langle S_i(N)\rangle$. Then concentration x is varied and previous procedure starts at point (a) above, so the function $S_M(x)$ is generated to any desired degree of continuity. Additionally, the method is capable of determining $U_M(x)$, the averaged energy over M samples as a function of the concentration x.

Independently of previous numeric approach, analytic local field calculations can be done in the limits of $x \to 0.0$ and $x \to 1.0$. The former case means that all bonds are AF except a very few ones with a negligible probability of being neighbors to each other. Then such F bonds are frustrated, which leads to

$$U_M(x \to 0.0) = \frac{-2N(1-x) + 2Nx}{2N} = -1 + 2x . \tag{4}$$

Equivalently for the case $x \to 1.0$, we get

$$U_M(x \to 1.0) = -1 + 2(1 - x)\,. \tag{5}$$

For these two extremes the remnant entropy can be calculated using this local field approximation in the following way. Let us suppose that the first few free spins n (those that can be flipped without energy change) are scattered through the lattice, independent of each other. Then the degeneracy associated to their random orientation is $w = 2^n$ and the expression for the remnant entropy per bond is given by

$$S_M(x) = \frac{\ln(2^n)}{2N} = n\frac{\ln(2)}{2N}\,. \tag{6}$$

To have a free spin it is necessary that two of bonds converging onto it are frustrated and the other two are satisfied, which means a weight $x^2(1-x)^2$ in either extreme. There are 6 geometrical distributions of bonds fulfilling this condition. Then the total number of free spins can be approximately given by

$$n(x \to 0.0) = n(x \to 1.0) = 6Nx^2(1-x)^2\,, \tag{7}$$

which immediately leads to

$$S_M(x \to 0.0) = S_M(x \to 1.0) = x^2(1-x)^2\ln(8)\,. \tag{8}$$

Upon combining Eqs. (4), (5) and (8), we get the relationship:

$$S_M(U_M \to -1.0) = (1 - U_M^2)^2\frac{\ln 8}{16}\,. \tag{9}$$

3. Results and discussion

The dependence of the ground energy per bond as a function of the concentration of F bonds x is shown in Fig. 1 for lattice size 20×20. Results of numerical simulations, corresponding to 500 samples for each concentration x are shown by

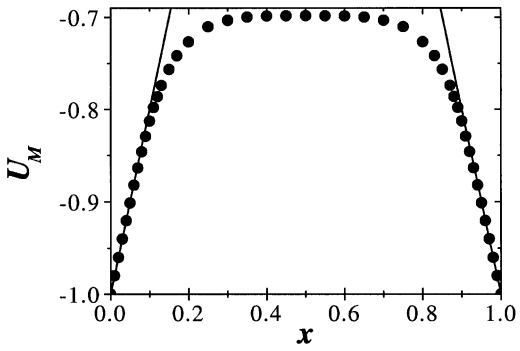

Fig. 1. Ground energy per bond as a function of the concentration of F bonds x, for size 20×20. Circles represent average results after numeric simulation over 500 samples for each x value. Solid lines correspond to the approximate expressions valid at the extremes of the interval.

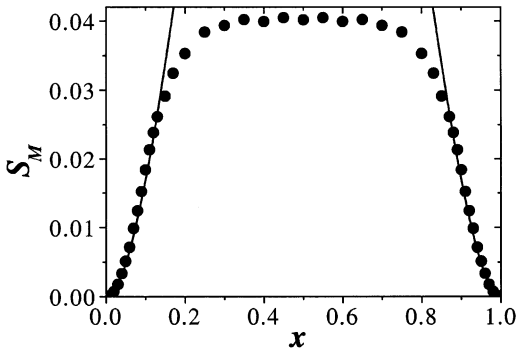

Fig. 2. Remnant entropy per bond as function of x following the same approach used in Fig. 1.

means of circles, while the analytic expressions based on local field approximations valid for the extreme values of x are presented by solid lines following Eqs. (4) and (5). As it can be noticed, the result is -1.0 in both extremes, where no frustration is present. As x departs from the extreme values, energy raises linearly at the beginning curving then to form a plateau, with the value $U_M(x) \approx -0.7$ in the range [0.25,0.75]. This result is similar to the exact one obtained for $x = 0.5$ in a previous work [6]. It is also consistent with extensive approximate numerical calculations that focus precisely on the value $U_M(0.5) = -0.703$ of this parameter, leaving other physical features out of consideration to tackle larger sizes [12].

Entropy results obtained by numerical analysis using TIM are shown by symbols in Fig. 2, where we also present the approximate analytic results based on local fields, Eq. (8), by means of solid lines. As it can be seen, remnant entropy goes to 0.0 at the extremes of the interval for x, which is the expected value for both the singlet ferromagnetic and antiferromagnetic states. From these extreme values, remnant entropy grows (quadratically in the onset of the variation) towards the center of the interval, showing a plateau with the value $S_i(x) \approx 0.04$ for the interval [0.25,0.75], which is in good agreement with elaborate calculations done at the point $x = 0.5$ [6,13–18].

In Fig. 3 we plot $S_M(U_M)$. It can be seen that the numerical results (symbols) tend to a linear function towards the center of the interval, departing from the dependence found in Eq. (9). However, if a closer examination is done for really small values of x, such polynomial dependence is revealed as it is shown in the inset of Fig. 3, where it is seen that notorious deviations between the approximate expression given by Eq. (9) and numerical results occur for $x > 0.07$ or $x < 0.93$, corresponding to concentrations at which free spins are not longer independent of each other.

4. Concluding remarks

The variation of the ground energy per bond $U_M(x)$ for $\pm J$ Ising lattices is reported by means of an improved Monte Carlo simulation designed for the accurate

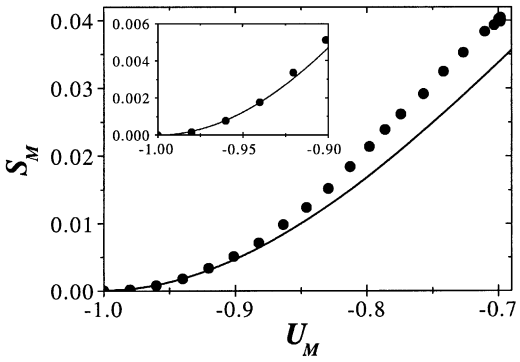

Fig. 3. Remnant entropy as a function of the ground energy.

use of the TIM [6]. Numerical calculations and approximate analytic expressions based on local fields agree well in the range $x<0.07$ and $x>0.93$. Results in the range $0.25<x<0.75$ are very little sensitive to x. In particular, at $x=0.5$ (by far the most popular case treated in the literature) we recover the values $U_M(x)\approx -0.7$ and $S_M(x)\approx 0.04$ found by other methods [6,12–18].

The ratio $S_M(x)/U_M(x)$ provides a very interesting insight as it is found that a linear relationship dominates towards the center of the interval, where both magnitudes tend to be constant. However, towards the extremes of the interval, a polynomial relationship holds as it is predicted from the approximation where free frustrated bonds are independent of each other, while, at the same time, free spins are independent of each other. To our knowledge results for remnant entropy reported here, namely $S_M(x)$, correspond to those in which simultaneously the following conditions are met: largest lattice size (20×20), largest variation of concentration in the interval (45 different values of x were tried in the interval) and largest number of samples for each concentration of x (500 independent randomly prepared samples). This makes the values and tendencies reported here very reliable.

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