Magnetisation and Entropy of a One-Dimensional $\pm J$ Ising Model in a Uniform Magnetic Field

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An approximation scheme related to the averaging procedure over finite fragments of the lattice was proposed. The magnetisation and entropy were calculated numerically. The correctness of this approximation scheme was analysed against the magnetic field and temperature.

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1. Introduction

Properties of the systems with a frozen disorder need to be averaged thermodynamically over both the spin states and the distribution of random exchange integrals or random fields. The systems can be studied by a number of methods representing three categories [1]. The first comprises the mean field methods, for which the averaging over disorder is included in the method. Thanks to this approach, it has been possible to describe in detail the infinite-range spin glasses [2]. The methods of the second category treat the averaging over disorder as a problem of secondary importance and apply the theory of error techniques to assess the reliability of results. This category is dominated by all kinds of computer simulations for finite systems. The methods of the third category assume that the Boltzmann averaging and that over the atomic disorder are of the same importance and the main difference between them is that a number of methods have been proposed to perform the former, while not many to deal with the latter. However, in view of this assumption the solutions are possible only in the ground state or when a given system behaves as a set of finite subsystems (as a result of dilution or infinite value of the fields).

This paper representing the third category, is a continuation of our earlier works [3, 4]. The first of them presents a method of linear equations whose application permits a reduction of the physical problem of determination of thermodynamical quantities of systems with quenched disorder to a mathematical question of solving a set of linear equations. In [4] this method

has been generalised over ordered systems in nonzero temperatures. The present paper is a continuation of the two above-mentioned ones and gives a method of generalisation of the same approach over disordered systems. As the method is based on the invariance of the vector of state, it becomes approximate for the systems devoid of translational invariance. The physical meaning of the approximation is that the properties of the whole system are approximated on the basis of the properties of a small fragment of the lattice. The approximation presented here allows the analysis of the applied-field dependence of both the magnetisation and the entropy for nonzero temperatures.

2. Description of the system studied

The subject of our interest is a one-dimensional system described by the following Hamiltonian:

$$\mathcal{H} = -\sum_i J_{i,i+1} S_i S_{i+1} - H \sum_i S_i \tag{1}$$

with $S_i = \pm 1$. The random exchange integrals $J_{i,i+1}$ assume the value of J with the probability $1-p$, and $-J$ with the probability p. This model has been studied for about 30 years. At nonzero temperatures and for finite systems this model has been studied by Fernández [5] and Puma and Fernández [6]. However, so far only for the ground state the exact expressions for physical quantities have been found by Brandt and Gross [7], Derrida et al. [8] and Williams [9]. The chain system can be described by the two transition matrices $\boldsymbol{f}$ and $\boldsymbol{a}$ for ferromagnetic and antiferromagnetic bonds, respectively

$$\boldsymbol{f} = \left[\begin{array}{cc} \mathrm{e}^{K+B} & \mathrm{e}^{-K} \\ \mathrm{e}^{-K} & \mathrm{e}^{K-B} \end{array} \right] (1-p), \qquad \boldsymbol{a} = \left[\begin{array}{cc} \mathrm{e}^{-K+B} & \mathrm{e}^{K} \\ \mathrm{e}^{K} & \mathrm{e}^{-K-B} \end{array} \right] p, \tag{2}$$

where $K = \beta J$, $B = \beta H$.

3. Magnetisation

In order to generate systems with random ferromagnetic and antiferromagnetic bonds we construct the matrix

$$\boldsymbol{M} = \left[\begin{array}{cc} \boldsymbol{f} & \boldsymbol{a} \\ \boldsymbol{f} & \boldsymbol{a} \end{array} \right]. \tag{3}$$

It is a 2×2 dimensional matrix whose elements are the matrices $\boldsymbol{f}$ and $\boldsymbol{a}$. The matrix has the same rows, which will also be the property of the matrix $\boldsymbol{M}^n$ containing the partition functions for the systems composed of n ferromagnetic and n antiferromagnetic bonds. If these systems are components of a greater system, in the first row of the matrix the partition functions are preceded by the matrix $\boldsymbol{f}$ and in the second by the matrix $\boldsymbol{a}$. The matrix $\boldsymbol{M}$ treated as a 4×4 dimensional matrix of scalars has two nonzero eigenvalues λ_+ and λ_- in terms of which a partition function can be expressed as [10]:

$$Z_n = \mathrm{Tr}\boldsymbol{M}^N = \lambda_+^N + \lambda_-^N \xrightarrow[N \to \infty]{} \lambda_+^N. \tag{4}$$

The result in the thermodynamic limit has two interpretations. Keeping only λ_+ we assume that the system is infinite. On this assumption the partition function gets factorised and there is one λ_+ factor per bond, which means that the mean energy or magnetisation per a site are intensive quantities.

Taking the higher eigenvalue of $\lambda = \lambda_+$ we find the right and left eigenvectors, respectively

$$\boldsymbol{M}|\boldsymbol{Y}\rangle = \lambda|\boldsymbol{Y}\rangle \quad \text{and} \quad \langle\boldsymbol{X}|\boldsymbol{M} = \lambda\langle\boldsymbol{X}|, \tag{5}$$

with the normalisation condition

$$\langle\boldsymbol{X}|\boldsymbol{Y}\rangle = 1. \tag{6}$$

The matrix $\boldsymbol{M}$ can be expressed as a sum of two $\boldsymbol{ff}$ and $\boldsymbol{aa}$ matrices, where

$$\boldsymbol{ff} = \begin{bmatrix} \boldsymbol{f} & 0 \\ \boldsymbol{f} & 0 \end{bmatrix}, \qquad \boldsymbol{aa} = \begin{bmatrix} 0 & \boldsymbol{a} \\ 0 & \boldsymbol{a} \end{bmatrix}. \tag{7}$$

Although the vectors $\langle\boldsymbol{X}|$ and $|\boldsymbol{Y}\rangle$ are the eigenvectors of the matrix $\boldsymbol{M}$, they are not eigenvectors of $\boldsymbol{aa}$ or $\boldsymbol{ff}$. Therefore, $\lambda = \langle\boldsymbol{X}|\boldsymbol{M}|\boldsymbol{Y}\rangle$ is a partition function of a single bond, but $\lambda_{\mathrm{f}} = \langle\boldsymbol{X}|\boldsymbol{ff}|\boldsymbol{Y}\rangle$ and $\lambda_{\mathrm{a}} = \langle\boldsymbol{X}|\boldsymbol{aa}|\boldsymbol{Y}\rangle$ are not the partition functions of a ferromagnetic or antiferromagnetic bond.

In the process of anneal averaging, the system assumes the states most convenient not only with respect to spin variables but also with respect to the concentration and positions of antiferromagnetic exchange integrals. We have one factor normalising the probability λ, irrespective of whether it comes from the Boltzmann factors or the probabilities of ferromagnetic and antiferromagnetic integrals. When for each arrangement of exchange integrals separately we determine the normalising factor, then we deal with the quench averaging. However, as long as we do not normalise the probability and calculate only the partition functions, we do not choose any type of averaging.

Let us now describe an approach, called in the following the quench approach, which permits obtaining a quenched system (free energy averaging) from an anneal system (partition function averaging). The approach is based on imposing that the competition between ferromagnetic and antiferromagnetic bonds is forbidden. To realise this imposition, the matrices $\boldsymbol{f}$ and $\boldsymbol{a}$ are rewritten in the forms

$$\boldsymbol{f} = (1 - p)\{\lambda_{\mathrm{f}_+}|\psi_+\rangle\langle\psi_+| + \lambda_{\mathrm{f}_-}|\psi_-\rangle\langle\psi_-|\},$$

$$\boldsymbol{a} = p\{\lambda_{\mathrm{a}_+}|\phi_+\rangle\langle\phi_+| + \lambda_{\mathrm{a}_-}|\boldsymbol{\phi}_-\rangle\langle\phi_-|\}, \tag{8}$$

where λ_{f_+} and λ_{f_-} are the higher and the lower eigenvalues of the ferromagnetic matrix, corresponding to the normalised eigenvectors $|\psi_+\rangle$, $|\psi_-\rangle$, respectively. Analogously for the antiferromagnetic bond we have λ_{a_+}, λ_{a_-} and $|\phi_+\rangle$, $|\phi_-\rangle$. If we divide the matrix component proportional to λ_{f_+} by λ_{f_+} and the component proportional to λ_{f_-} by λ_{f_-}, and perform the same procedure for the antiferromagnetic bond, the modified matrix $\boldsymbol{fm}$ becomes

$$\boldsymbol{fm} = (1-p)\{|\psi_+\rangle\langle\psi_+| + |\psi_-\rangle\langle\psi_-|\} \tag{9}$$

and the modified matrix $\boldsymbol{am}$ takes the form

$$\boldsymbol{am} = p\{|\phi_+\rangle\langle\phi_+| + |\phi_-\rangle\langle\phi_-|\}. \tag{10}$$

From these two matrices we can create a modified matrix $\boldsymbol{Mm}$, satisfying the condition

$$\langle\boldsymbol{X}|\boldsymbol{Mm}|\boldsymbol{Y}\rangle = 1. \tag{11}$$

In order to determine the magnetisation let us note that for the state $|\psi_+\rangle$ the mean spin value is $s_{\mathrm{f}} = \sinh B/\sqrt{\sinh^2 B + \mathrm{e}^{-4K}}$, while for the state $|\psi_-\rangle$ it is $-s_{\mathrm{f}}$. Similarly, for the antiferromagnetic bond for the state $|\phi_+\rangle$ $s_{\mathrm{a}} = \sinh B/\sqrt{\sinh^2 B + \mathrm{e}^{4K}}$, while for the state $|\phi_-\rangle$ it is $-s_{\mathrm{a}}$. Let us define now two matrices:

$$\boldsymbol{fs} = (1-p)\{|\psi_+\rangle s_{\mathrm{f}}\langle\psi_+| - |\psi_-\rangle s_{\mathrm{f}}\langle\psi_-|\},$$

$$\boldsymbol{as} = p\{|\phi_+\rangle s_{\mathrm{a}}\langle\phi_+| - |\phi_-\rangle s_{\mathrm{a}}\langle\phi_-|\} \tag{12}$$

and construct from them the matrix $\boldsymbol{S}$:

$$\boldsymbol{S} = \left[\begin{array}{cc} \boldsymbol{fs} & \boldsymbol{as} \\ \boldsymbol{fs} & \boldsymbol{as} \end{array}\right] \tag{13}$$

and now we can determine the magnetisation per site as

$$\langle s\rangle = \langle\boldsymbol{X}|\boldsymbol{S}|\boldsymbol{Y}\rangle. \tag{14}$$

Numerical values of $\langle s\rangle$ have been found for $p = 1/2$, $1/kT = 100$, $|J| = 1$ and are presented in Fig. 1, curve (a). The temperature for which they have
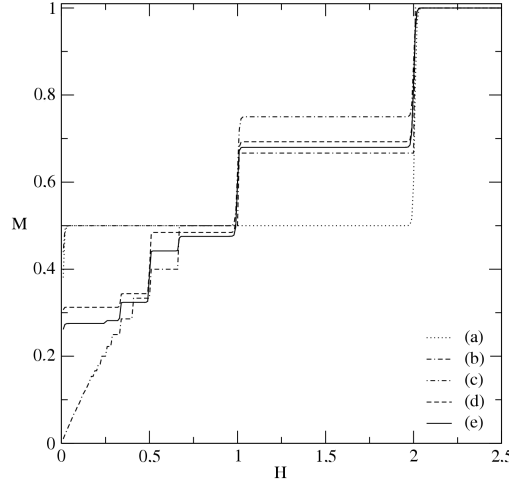

Fig. 1.   Magnetisation per spin as a function of magnetic field at $1/kT = 100$, for the concentration of antiferromagnetic integrals of $p = 1/2$ and for $|J| = 1$; (a) quench approximation, (b) ground state, (c) single-site approximation, (d) four-site approximation, (e) seven-site approximation.

been found is so low that it can be assumed that the numerical values of an arbitrary thermodynamical quantity do not differ significantly from their ground state values, so Fig. 1, curve (b) presents the magnetisation in the ground state calculated for $p = 1/2$ (Eq. (22) [9]). As follows from Fig. 1, curve (b), only for high fields the approximation can be treated as reliable. To find out to which degree the quench approach follows from the assumed description of the probabilities (division of the transfer matrices by their eigenvalues) and to which degree it follows from the fact that only one bond is considered, another single-site approach has been proposed. The partition function for a single bond can be written in the form

$$\lambda = \langle \boldsymbol{X}_1 | \boldsymbol{f} | \boldsymbol{Y}_1 \rangle + \langle \boldsymbol{X}_2 | \boldsymbol{f} | \boldsymbol{Y}_1 \rangle + \langle \boldsymbol{X}_1 | \boldsymbol{a} | \boldsymbol{Y}_2 \rangle + \langle \boldsymbol{X}_2 | \boldsymbol{a} | \boldsymbol{Y}_2 \rangle, \tag{15}$$

where $\langle \boldsymbol{X} | = \langle \boldsymbol{X}_1, \boldsymbol{X}_2 |$, $| \boldsymbol{Y} \rangle = | \boldsymbol{Y}_1, \boldsymbol{Y}_2 \rangle$ and $| \boldsymbol{Y}_1 \rangle = | \boldsymbol{Y}_2 \rangle$.

The two-dimensional vectors $\langle \boldsymbol{X}_1 |$ and $\langle \boldsymbol{X}_2 |$ correspond to the cases when the directly preceding bond is ferromagnetic and antiferromagnetic, respectively. Introducing the notation

$$\boldsymbol{mf} = \frac{\mathrm{d}}{\mathrm{d}B} \boldsymbol{f} \quad \text{and} \quad \boldsymbol{ma} = \frac{\mathrm{d}}{\mathrm{d}B} \boldsymbol{a}. \tag{16}$$

We get magnetisation m from the formula

$$m = (1 - p)^2 \frac{\langle \boldsymbol{X}_1 | \boldsymbol{mf} | \boldsymbol{Y}_1 \rangle}{\langle \boldsymbol{X}_1 | \boldsymbol{f} | \boldsymbol{Y}_1 \rangle} + p(1 - p) \frac{\langle \boldsymbol{X}_2 | \boldsymbol{mf} | \boldsymbol{Y}_1 \rangle}{\langle \boldsymbol{X}_2 | \boldsymbol{f} | \boldsymbol{Y}_1 \rangle}$$

$$+ p(1 - p) \frac{\langle \boldsymbol{X}_1 | \boldsymbol{ma} | \boldsymbol{Y}_2 \rangle}{\langle \boldsymbol{X}_1 | \boldsymbol{a} | \boldsymbol{Y}_2 \rangle} + p^2 \frac{\langle \boldsymbol{X}_2 | \boldsymbol{ma} | \boldsymbol{Y}_2 \rangle}{\langle \boldsymbol{X}_2 | \boldsymbol{a} | \boldsymbol{Y}_2 \rangle} \tag{17}$$

and the corresponding plot is presented in Fig. 1, curve (c). Although these two single-site approximations give different results in the fields $H \in (1, 2)$, the values of the ground state magnetisation are between the values predicted by the two approximations and they can be treated as reasonable in this range of fields. Unfortunately, it is not the case for low fields, although for them the approximations give identical results, therefore analogous calculations have been performed for four and seven bonds; the results are given in Fig. 1, curves (d) and (e). The plots are only insignificantly different, and for the fields $H > 0.25$ their values well approximate the values obtained for the ground state. Similar calculations have been performed for higher temperatures. Figures 2 and 3 present the magnetisation versus the magnetic field for $p = 1/2$, $|J| = 1$ for $1/kT$ of 10 and 1. Analogously as for $1/kT = 100$, the single-site approximations are weak, while the quenched approximation in high temperatures becomes unacceptable. Moreover, with increasing temperature the differences between the predictions of the approximations, being consequences of the size of the cluster considered, decrease.

All the calculations have been made using the vectors $\langle \boldsymbol{X} | = \langle \boldsymbol{X}_1, \boldsymbol{X}_2 |$, so only two cases were taken into account: of the directly preceding bond being ferromagnetic or antiferromagnetic. As the task of determination of magnetisation has proved to be a many-bond problem, thus besides taking into account clusters
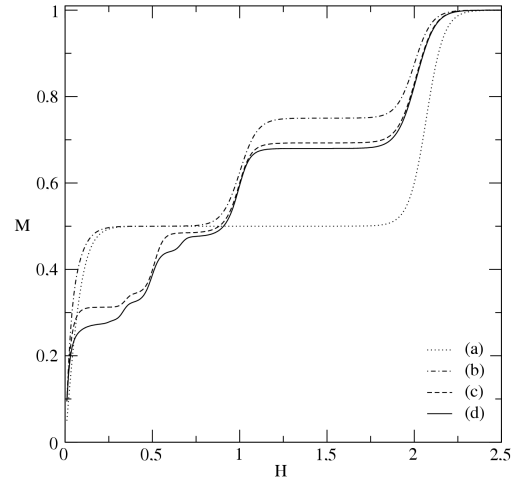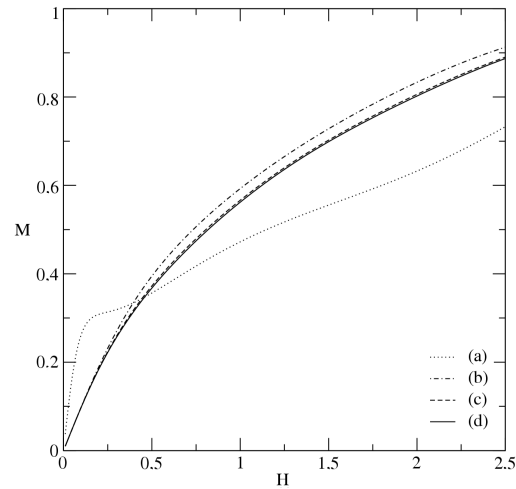
Fig. 2.   Magnetisation per spin as a function of magnetic field at $1/kT = 10$, for the concentration of antiferromagnetic integrals of $p = 1/2$ and for $|J| = 1$; (*a*) quench approximation, (*b*) single-site approximation, (*c*) four-site approximation, (*d*) seven-site approximation.

Fig. 3.   Magnetisation per spin as a function of magnetic field at $1/kT = 1$, for the concentration of antiferromagnetic integrals of $p = 1/2$ and for $|J| = 1$; (*a*) quench approximation, (*b*) single-site approximation, (*c*) four-site approximation, (*d*) seven-site approximation.

of increasing size, we should also reduce the mixing of states $\langle \boldsymbol{X} |$ by specifying not only its nearest left neighbour but also next nearest one. Therefore, the matrix $\boldsymbol{M}$ has been replaced by

$$\mathcal{M} = \begin{bmatrix} \boldsymbol{ff} & \boldsymbol{fa} & \boldsymbol{af} & \boldsymbol{aa} \\ \boldsymbol{ff} & \boldsymbol{fa} & \boldsymbol{af} & \boldsymbol{aa} \\ \boldsymbol{ff} & \boldsymbol{fa} & \boldsymbol{af} & \boldsymbol{aa} \\ \boldsymbol{ff} & \boldsymbol{fa} & \boldsymbol{af} & \boldsymbol{aa} \end{bmatrix}. \tag{18}$$

Using this matrix we get new eigenvectors related to the eigenvalues λ^2 through the following equations:

$$\mathcal{M}|\mathcal{Y}\rangle = \lambda^2|\mathcal{Y}\rangle, \qquad \langle\mathcal{X}|\mathcal{M} = \lambda^2\langle\mathcal{X}|, \qquad \langle\mathcal{X}|\mathcal{Y}\rangle = 1. \tag{19}$$

These vectors are used for the calculation of magnetisation at $1/kT = 100$, $|J| = 1$, $p = 1/2$ for the four-bond clusters and they were compared with the results of the earlier calculations for the four-dimensional vectors $\langle\boldsymbol{X}|$ and $|\boldsymbol{Y}\rangle$, shown in Fig. 4. As follows from the figure, although the clusters remember the subsequent neighbours, this effect is much smaller than that related to the size of the cluster. For practical reasons further calculations were performed assuming the Markov character of the chain, i.e. that the state of a given site is determined by the neighbouring bond only.
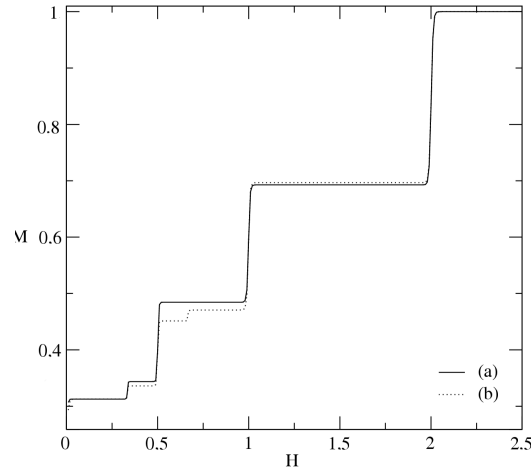

Fig. 4. Magnetisation per spin as a function of magnetic field at $1/kT = 100$, $p = 1/2$, $|J| = 1$, taking into account four bonds in a cluster when (*a*) the vectors of state are four-dimensional, (*b*) the vectors of state are eight-dimensional.

In order to compare the performance of this approximation for different concentrations of the antiferromagnetic bonds p, the magnetisation values obtained for $1/kT = 100$, $|J| = 1$, three concentrations and clusters of seven bonds have been tabulated, see Fig. 5. The same figure also presents the magnetisation values in the ground state for the same concentrations. Besides the field value, the accuracy of the approximation depends on the concentration p (the higher p the
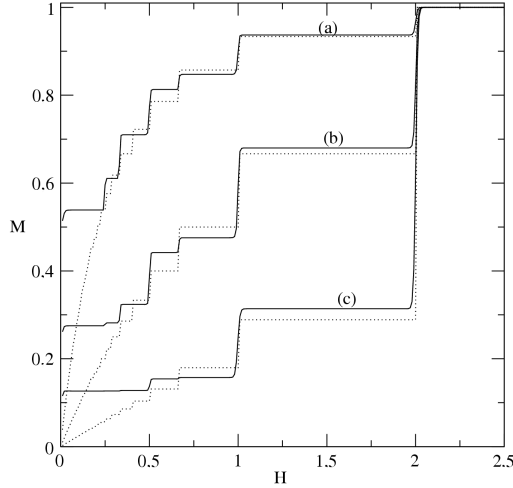
Fig. 5.   Magnetisation per spin as a function of magnetic field at $1/kT = 100$ and $|J| = 1$ (solid line) and for the ground state (dotted line) for three concentrations $p = 0.2$ (a), $p = 0.5$ (b), and $p = 0.8$ (c).

worse the accuracy). This observation suggests that the quality of the approximation can be described by the antiferromagnetic clusters in the ground state, as for high fields $H \in (1, 2)$ only such clusters comprise downwards spins. Although the exact expression in the ground state demands taking into account the infinite antiferromagnetic chains, within the formalism accepted the assumption of a finite number of bonds does not lead to significant errors. With a decreasing field value, the length of the chains that have to be considered increases and includes also ferromagnetic bonds besides the antiferromagnetic ones [9]. This increase in the length of the chains deteriorates the quality of the approximation, but the thermal excitations break the spins ordering and thus improve the quality of the approximation by finite clusters. In the ground state the magnetisation shows discontinuities for the fields $H = 2I/r$ (r is an integer), whereas at the same points the entropy shows spikes, therefore, the performance of this approximation was also studied for the entropy.

4. Entropy

We consider first the single-bond approximation. The probability of the spin state of the bond is defined when the sign of the preceding bond is known. If we denote by $p(j)$ the probability of occurrence of a pair of bonds, and by $w(i, j)$ the density of probability of the pair of spins of the other bond, the entropy per spin can be described as

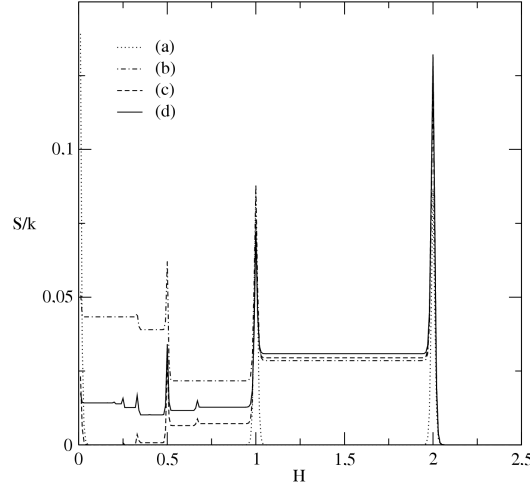$$S/k = -\frac{1}{2} \sum_{j=1}^{4} p(j) \sum_{i=1}^{4} w(i, j) \ln[w(i, j)]. \tag{20}$$

Fig. 6. Entropy per spin as a function of magnetic field at $1/kT = 100$, $p = 1/2$ and $|J| = 1$, in (a) single-site approximation, (b) four-site approximation, (c) seven-site approximation, (d) ten-site approximation.

The entropy per spin values calculated in the single-bond approximation for $1/kT = 100$, $|J| = 1$ and $p = 1/2$ versus H are presented in Fig. 6. The plot shows three spikes for the fields 0, 1, 2, but the first of them has no physical interpretation as it is generated by the finite cluster (a single bond). To improve the results, analogous calculations have been performed for four-, seven- and ten-site clusters (see Fig. 6, curves (b)–(d)). Analysis of the quality of the results is almost the same as for magnetisation. The difference is that the magnetisation in the ground state is expressed by the power series whose coefficients do not depend on the size of the cluster, while for the entropy they show a logarithmic dependence on the cluster size (Eq. (29) in [9]), which deteriorates the accuracy of results.

5. Concluding remarks

For low fields the single-site approximations give the same results of magnetisation, so it can be concluded that the source of errors is of the cluster nature of spin glass, as has been shown numerically for a three-dimensional model $\pm J$ [11]. The system considered does not show a Markov type behaviour, although deviations from it are insignificant. For high fields the multi-spin approximations are acceptable even in low temperatures, which indicates a possibility of applying this approximation when studying the lattice in which the frustration is a result of a competition, since the exchange integrals are of the same or comparable magnitude.

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