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The fully frustrated Ising model in infinite dimensions

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Abstract. We solve, subject to the validity of some reasonable assumptions, the 'fully frustrated' Ising model in the limit of infinite dimensions using an extension of the TAP theory for spin glasses. In contrast to the TAP theory of the infinite-range spin glass, an infinite summation of diagrams is required to recover the Gibbs free energy for this model. The model undergoes a first-order transition. The method used to solve the model should have many applications to other physical problems.

1. Introduction

Frustration and disorder are the two key features of the spin glass. In trying to disentangle the relative importance of these two elements, it is natural to consider models in which only one of them is present. In this paper, we will study the 'fully frustrated' Ising model on a d-dimensional hypercubic lattice, a model which was introduced by Villain in its two-dimensional form [1] and extended to arbitrary dimension by Derrida *et al* in two papers [2, 3]. This is a model which incorporates strong frustration without disorder. Numerical simulations by Diep *et al* [4] established that this model undergoes a phase transition into an ordered phase in three dimensions. Whether the transition is of first or second order in that case is still somewhat unclear [5].

For many models in statistical physics, the limit of infinite spatial dimensions is particularly simple—it usually serves as a limit in which 'mean-field theory' is exact. In [3] the infinite-dimensional limit for the 'fully frustrated' Ising model on a hypercubic lattice was considered, but they were only able to solve for the free energy in the high-temperature phase. In this paper, we give an exact solution (subject to some very reasonable assumptions) for the free energy of this model in the infinite-dimensional limit for both low- and high-temperature phases, and we show that the two phases are separated by a first-order transition. It is very interesting that in this infinite-dimensional theory, in contrast to the theory of the Ising ferromagnet in infinite dimensions, spins can be influenced by very distant spins through large loops. We believe that the method we use to solve this model is also interesting in its own right, and should have many applications for other physical models.

We consider a Hamiltonian for Ising spins located on a hypercubic lattice

$$H = -\sum_{(ij)} J_{ij} S_i S_j. \qquad (1)$$

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A 'fully frustrated' Ising model is one in which every plaquette (elementary loop of four spins) is frustrated—i.e. the product of the four bonds in the loop is negative [6]. We consider the model in which every bond has the same magnitude (although they will differ in sign) which is scaled as $|J_{ij}| = 1/\sqrt{d}$. This scaling ensures that the critical temperature and ground-state energy density are O(1). Notice that this scaling is the same as the scaling of the spin glass and different from the $1/d$ scaling appropriate for ferromagnets.

A fully frustrated hypercubic lattice can be constructed in any dimension using a recursive procedure [2]. One first constructs a fully frustrated d-dimensional lattice. One stacks the d-dimensional lattices on top of each other to make a $(d+1)$-dimensional lattice. Then one flips the signs of all the bonds in every other d-dimensional lattice. Because every bond is flipped, those d-dimensional lattices are still fully frustrated. Finally, one connects adjacent d-dimensional lattices with ferromagnetic bonds. As the adjacent lattices have bonds of opposite sign, connecting them with ferromagnetic bonds insures that every plaquette in the $(d+1)$th dimension is also frustrated. The procedure can be started using the one-dimensional ferromagnetic chain.

In [3] the high-temperature free energy of the infinite-dimensional fully frustrated Ising model was found by an indirect argument—they solved the fully frustrated spherical model exactly, and then showed that the high-temperature expansion in infinite dimensions scaled in a simple way with n, where n is the number of the components of spins. The free energy that they found was

$$-\frac{\beta F}{N} = \ln 2 + \frac{-1+\sqrt{1+8\beta^2}}{4} - \frac{1}{4}\ln\left(\frac{1+\sqrt{1+8\beta^2}}{2}\right) \tag{2}$$

where β is the inverse temperature and N is the total number of spins.

2. The method of solution

The method that we use to solve this model in its low-temperature phase is an extension of the theory that Thouless *et al* [7] (TAP) developed for the infinite-range spin glass. Plefka [8] had previously derived the TAP equations using the same formalism, but he did not exploit the formalism to extend the TAP equations. Our extension of the TAP theory should have many applications, and has already been used to derive $1/d$ expansions valid in the low-temperature phase for both ferromagnets [9] and spin glasses [10]. It should be recalled that previous $1/d$ expansions for those problems [11–13] were valid only in the high-temperature phase. A closely related formalism was used twenty years ago by Gaunt and Baker to study the Ising ferromagnet in its low-temperature phase [14].

To illustrate the generality of the method used, we will consider, for the time being, an Ising model in which the bonds J_{ij} are *arbitrary* and can connect any two spins. We will specialise to the 'fully frustrated' hypercubic J_{ij} bond matrix later. We construct a Gibbs free energy which depends on the magnetisation at every site i:

$$-\beta G(\beta, m_i) = \ln \operatorname*{Tr}_{\{S_i\}} \exp\left(\beta \sum_{(ij)} J_{ij}S_iS_j + \sum_i \alpha_i(\beta)(S_i - m_i)\right). \tag{3}$$

The Lagrange multipliers $\alpha_i(\beta)$ fix the magnetisation at each site i to their thermal expectation values: $m_i \equiv \langle S_i \rangle$, where the meaning of the $\langle\ \rangle$ brackets is that if we have some operator O, then

$$\langle O \rangle \equiv \frac{\mathrm{Tr}_{\{S_i\}} O \exp[\beta \sum_i J_{ij} S_i S_j + \sum_i \alpha_i(\beta)(S_i - m_i)]}{\mathrm{Tr}_{\{S_i\}} \exp[\beta \sum_i J_{ij} S_i S_j + \sum_i \alpha_i(\beta)(S_i - m_i)]}. \tag{4}$$

Note that the Lagrange multipliers $\alpha_i(\beta)$ explicitly depend on the inverse temperature.

Since m_i is fixed equal to $\langle S_i \rangle$ for any temperature β, it is, in particular, equal to $\langle S_i \rangle$ when $\beta = 0$, which means that

$$m_i = \langle S_i(\beta = 0) \rangle = \frac{\mathrm{Tr}\, S_i \exp(\alpha_i(0) S_i)}{\mathrm{Tr} \exp(\alpha_i(0) S_i)} = \tanh[\alpha_i(0)]. \tag{5}$$

Now we expand $-\beta G(\beta, m_i)$ around $\beta = 0$ using a Taylor expansion:

$$-\beta G(\beta, m_i) = -\beta G(\beta)\bigg|_{\beta=0} - \beta \frac{\mathrm{d}(\beta G)}{\mathrm{d}\beta}\bigg|_{\beta=0} - \frac{\beta^2}{2} \frac{\mathrm{d}^2(\beta G)}{\mathrm{d}\beta^2}\bigg|_{\beta=0} - \ldots \tag{6}$$

where we have temporarily suppressed the dependence of G on m_i. From the definition of $-\beta G(\beta, m_i)$ given in equation (3) we find that

$$-\beta G(\beta, m_i)\bigg|_{\beta=0} = \sum_i \ln[\cosh(\alpha_i(0))] - \alpha_i(0) m_i. \tag{7}$$

Using equation (5), we recover

$$-\beta G(\beta, m_i)\bigg|_{\beta=0} = \sum_i -\{\tfrac{1}{2}(1+m_i)\ln[\tfrac{1}{2}(1+m_i)] + \tfrac{1}{2}(1-m_i)\ln[\tfrac{1}{2}(1-m_i)]\} \tag{8}$$

which is the entropy of non-interacting Ising spins constrained to have magnetisations m_i. Considering, next, the first derivative in equation (5), we find that

$$-\beta \frac{\mathrm{d}(\beta G(m_i))}{\mathrm{d}\beta}\bigg|_{\beta=0} = \beta \left\langle \sum_{(ij)} J_{ij} S_i S_j \right\rangle_{\beta=0} + \beta \frac{\mathrm{d}\alpha_i}{\mathrm{d}\beta}\bigg|_{\beta=0} \langle S_i - m_i \rangle_{\beta=0}. \tag{9}$$

At $\beta = 0$, the spin-spin correlation functions factorise, so we find that

$$-\beta \frac{\mathrm{d}(\beta G(m_i))}{\mathrm{d}\beta}\bigg|_{\beta=0} = \beta \sum_{(ij)} J_{ij} m_i m_j. \tag{10}$$

Continuing to the second derivative in the Taylor expansion, we find, after a short computation, that

$$\frac{-\beta^2}{2} \frac{\mathrm{d}^2(\beta G(m_i))}{\mathrm{d}\beta^2}\bigg|_{\beta=0} = \frac{\beta^2}{2} \sum_{(ij)} J_{ij}^2 (1 - m_i^2)(1 - m_j^2) \tag{11}$$

which is the famous Onsager reaction term in the TAP equations. To compute (11), one needs to use the Maxwell relation:

$$-\frac{\mathrm{d}\alpha_i}{\mathrm{d}\beta}\bigg|_{\beta=0} = -\frac{\mathrm{d}^2(\beta G(m_i))}{\mathrm{d}\beta\, \mathrm{d}m_i}\bigg|_{\beta=0} = \sum_j J_{ij} m_j. \tag{12}$$

The Taylor expansion can be continued to arbitrarily high order. To order β^4, one finds that

$$
\begin{aligned}
-\beta G(\beta, m_i) = & -\sum_i \{\tfrac{1}{2}(1+m_i)\ln[\tfrac{1}{2}(1+m_i)]+\tfrac{1}{2}(1-m_i)\ln[\tfrac{1}{2}(1-m_i)]\}+\beta\sum_{(ij)} J_{ij}m_im_j \\
& +\frac{\beta^2}{2}\sum_{(ij)} J_{ij}^2(1-m_i^2)(1-m_j^2)+\frac{2\beta^3}{3}\sum_{(ij)} J_{ij}^3 m_i(1-m_i^2)m_j(1-m_j^2) \\
& +\beta^3\sum_{(ijk)} J_{ij}J_{jk}J_{ki}(1-m_i^2)(1-m_j^2)(1-m_k^2) \\
& -\frac{\beta^4}{12}\sum_{(ij)} J_{ij}^4(1-m_i^2)(1-m_j^2)(1+3m_i^2+3m_j^2-15m_i^2m_j^2) \\
& +2\beta^4\sum_{(ijk)} J_{ij}^2J_{jk}J_{ki}m_i(1-m_i^2)m_j(1-m_j^2)(1-m_k^2) \\
& +\beta^4\sum_{(ijkl)} J_{ij}J_{jk}J_{kl}J_{li}(1-m_i^2)(1-m_j^2)(1-m_k^2)(1-m_l^2)+\ldots.
\end{aligned}
\tag{13}
$$

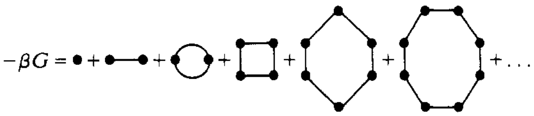
The notation (ij), (ijk) or $(ijkl)$ means one should sum over all distinct pairs, triplets or quadruplets of pins.

The Taylor expansion which is being described is clearly a high-temperature expansion (directly in β rather than $\tanh(\beta)$) at a fixed (site-dependent) magnetisation m_i. Setting $m_i=0$, one recovers from equation (13) the ordinary high-temperature expansion of the Ising model. From a diagrammatic point of view, there are two changes that occur in the expansion of the free energy when $m_i \neq 0$: (i) new diagrams appear corresponding to terms like $\Sigma J_{ij}m_im_j$; (ii) diagrams which appeared even for $m_i=0$ are modified to have new weights associated with the magnetisations at the vertices. Although we were not able to prove it, we believe that the only non-zero diagrams in this generalised expansion are 'strongly irreducible'—i.e. even removing a vertex does not split the diagram into two pieces. We found this to be true by direct calculation for relatively low-order diagrams, and we also note that if it were not true, non-strongly irreducible diagrams would also modify the TAP theory of the infinite-range spin glass.

3. Specialising to the fully frustrated case

Let us now specialise to a fully frustrated hypercubic lattice with bonds $J_{ij}=\pm 1/\sqrt{d}$. In the limit of infinite dimensionality, and assuming that only strongly irreducible diagrams contribute, we find a very drastic simplification in the number of high-temperature diagrams which contribute to the free energy. In fact, the only diagrams which survive are those corresponding to the zeroth, first and second derivatives calculated above and diagrams in which the vertices are arranged in a closed loop (see figure 1). The loop diagrams are all O(1) because each bond in the loop contributes a factor of $1/\sqrt{d}$ but if the loop consists of b bonds, then there are $O(d^{b/2})$ such loops on the lattice. It is obvious that other strongly irreducible diagrams will always be of lower order than the loop diagrams. Note that by setting all $m_i=0$, we recover from the loop diagrams the term-by-term expansion around $\beta=0$ of the free energy in the high-temperature phase given by equation (2) above.

To extend these high-temperature results into the low-temperature phase we need to make the following reasonable assumption: that in the limit as the number of spatial



$$= -\sum_i \left(\frac{1+m_i}{2}\right)\ln\left(\frac{1+m_i}{2}\right)+\left(\frac{1-m_i}{2}\right)\ln\left(\frac{1-m_i}{2}\right)$$

$$+\beta\sum_{(ij)} J_{ij}m_im_j+\frac{\beta^2}{2}\sum_{(ij)} J_{ij}^2(1-m_i^2)(1-m_j^2)$$

$$+\beta^4\sum_{(ijkl)} J_{ij}J_{jk}J_{kl}J_{li}(1-m_i^2)(1-m_j^2)(l-m_k^2)(1-m_l^2)+\ldots.$$

Figure 1. The Gibbs free energy of the 'fully frustrated' Ising model on a hypercubic lattice in the limit of infinite dimensions.

dimensions approaches infinity, the equilibrium squared magnetisation at each site will become uniform. We believe that this assumption is reasonable because each site is *a priori* identical and feels the field caused by many other sites. Note that we are only assuming that the *squared* magnetisation, not the magnetisation itself, is uniform.

Given this assumption, extending the high-temperature results into the low-temperature phase is rather simple. The 'ln 2' in equation (2) becomes the entropy of spins fixed to a given site-dependent magnetisation. One needs to add a $\Sigma J_{ij}m_im_j$ term. Using the uniformity of the squared magnetisation, we can write $m_i=\sqrt{q}\varepsilon_i$, where $\varepsilon_i=\pm1$ and q is the squared magnetisation. Finally, the loop diagrams can be handled by noting that in the high-temperature phase the infinite summation of these diagrams yielded the expression in equation (2). One can easily show that in the low-temperature phase the only modification of the loop diagrams is that every factor of β should be replaced by a factor of $\beta(1-q)$. Thus we can again sum the loop diagrams and find the Gibbs free energy:

$$\frac{-\beta G(q,\varepsilon_i)}{N} = -\{\tfrac{1}{2}(1+\sqrt{q})\ln[\tfrac{1}{2}(1+\sqrt{q})]+\tfrac{1}{2}(1-\sqrt{q})\ln[\tfrac{1}{2}(1-\sqrt{q})]\}+\frac{\beta q}{N}\sum_{(ij)} J_{ij}\varepsilon_i\varepsilon_j$$
$$+\frac{[1+8\beta^2(1-q)^2]^{1/2}-1}{4}-\frac{1}{4}\ln\left(\frac{1+[1+8\beta^2(1-q)^2]^{1/2}}{2}\right). \tag{14}$$

Now we minimise G over the ε_i, to find an effective free energy which is valid in our restricted subspace in which all the squared magnetisations are identical:

$$\frac{-\beta G(q)}{N} = -\{\tfrac{1}{2}(1+\sqrt{q})\ln[\tfrac{1}{2}(1+\sqrt{q})]+\tfrac{1}{2}(1-\sqrt{q})\ln[\tfrac{1}{2}(1-\sqrt{q})]\}-e\beta q$$
$$+\frac{[1+8\beta^2(1-q)^2]^{1/2}-1}{4}-\frac{1}{4}\ln\left(\frac{1+[1+8\beta^2(1-q)^2]^{1/2}}{2}\right) \tag{15}$$

where e is the ground-state energy density of the model.

One can solve the model for any value of e, but the studies in [2] of the ground-state energy density as a function of dimension motivate the choice $e=-1$. They found in [2] that the ground-state energy density of any n-component spin model on a fully frustrated lattice in any dimension was bounded below by -1. For all $n>1$, this bound could be achieved in any dimension, but for $n=1$, there is a possibly tighter bound caused by the Ising nature of the spins. On the other hand, the Ising model empirically achieved the tighter bound for all dimensions tested (up to $d=7$) and the tighter bound approaches -1 in the limit of infinite dimensions.

To solve the model, we minimise this free energy as a function of the squared magnetisation. We find (for $e=-1$) two phases, separated by a first-order transition at $\beta_c \simeq 0.982$. In the high-temperature phase, $q=0$. In the low-temperature phase

$$q = \tanh^2\left(2\beta\sqrt{q} - \frac{\sqrt{q}\{[1+8\beta^2(1-q)^2]^{1/2}-1\}}{2(1-q)}\right). \tag{16}$$

The energy density is given by

$$\frac{U}{N} = \frac{\mathrm{d}}{\mathrm{d}\beta}\left(\frac{\beta G}{N}\right) = -q - \frac{[1+8\beta^2(1-q)^2]^{1/2}-1}{4\beta}. \tag{17}$$

At the transition, $q_c \simeq 0.778$, so the latent heat density is $L \simeq 0.326$. The results will be qualitatively similar for all ground-state energy densities e such that $-1 \leqslant e < -1/\sqrt{2}$. For $e \geqslant -1/\sqrt{2}$, the stable state at very low temperatures is actually paramagnetic, but such a value of e seems extremely unlikely given the results of [2].

One might also note that the free energy given in equation (15) only has a finite radius of convergence (in β) for any value of q, and in fact the high-temperature expansion is not convergent at the equilibrium temperature for any value of q, including $q=0$.

All these results are rather different than the corresponding results for the infinite-range (or infinite-dimensional [10]) Ising spin glass. For the spin glass, the transition is third order, with only a cusp in the specific heat at T_c [7]. Another difference is that at very low temperatures, the spin-glass order parameter has temperature dependence such that $1-q \sim T^2$ [7], while in the fully frustrated case, the order parameter approaches unity exponentially at low temperatures.

4. Discussion

Some comments are in order. First, it is interesting to see that the frustration in this model causes the mean-field theory to have such a high degree of reactivity that an infinite summation of diagrams is necessary to recover the free energy. This feature is connected to the $1/\sqrt{d}$ scaling of the bonds and is likely to appear in other non-trivial models. For example, in the Hubbard model, the scaling of the electron hopping term t_{ij} in high dimensions is also $1/\sqrt{d}$ [15], so one can expect that to recover the free energy in the limit of infinite dimensions, another infinite summation of loop diagrams will be necessary (in this case the loops correspond to the electron hopping around a loop).

Secondly, the method used to solve this model is of very great generality. In the case at hand, the model was of sufficient complexity that even the solution in infinite dimensions was non-trivial. In other models where the infinite-dimensional mean-field theory is known, the higher-order terms in the high-temperature expansion at fixed magnetisation will give $1/d$ corrections to mean-field theory [9]. Since mean-field theory is used so widely in physics, it is obviously of interest to have such a simple method of calculating the corrections in finite dimensions.

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