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How to expand around mean-field theory using high-temperature expansions

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Abstract. High-temperature expansions performed at a fixed-order parameter provide a simple and systematic way to derive and correct mean-field theories for statistical mechanical models. For models like spin glasses which have general couplings between spins, we show that these expansions generate the Thouless-Anderson-Palmer (TAP) equations at low order. We explicitly calculate the corrections to TAP theory for these models. For ferromagnetic models, we show that our expansions can easily be converted into $1/d$ expansions around mean-field theory, where d is the number of spatial dimensions. Only a small finite number of graphs need to be calculated to generate each order in $1/d$ for thermodynamic quantities like free energy or magnetization. Unlike previous $1/d$ expansions, our expansions are valid in the low-temperature phases of the models we consider. We consider alternative ways to expand around mean-field theory besides $1/d$ expansions. In contrast to the $1/d$ expansion for the critical temperature, which is presumably asymptotic, these schemes can be used to devise convergent expansions for the critical temperature. They also appear to give convergent series for thermodynamic quantities and critical exponents. We test the schemes using the spherical model, where their properties can be studied using exact expressions.

1. Introduction

High-temperature expansions have long provided an extremely important tool in the study of lattice spin systems [1]. Our goal in this paper is to demonstrate that high-temperature expansions that are performed at a fixed-order parameter (like the magnetization for a ferromagnet) also have a very close relationship with 'mean-field' theories, and can in fact be used to systematically generate corrections to mean-field theories. The basic idea of our work, which curiously does not appear to have been recognized before, is actually very simple: in constructing a high-temperature expansion for the magnetization-dependent free energy $A(\beta, m)$ of a ferromagnet, one recovers the ordinary mean-field theory with just the first two terms in the expansion, and higher-order terms will give systematic corrections.

Many of the problems and ideas described here have a long history, and some of our description merely puts old results in a different light. Nevertheless, we have found that these new perspectives can be very useful—so to whet the reader's appetite, it may be worthwhile to outline briefly those new results that we have obtained by looking at old problems in a different way:

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(i) In section 2, we show how one can very simply derive TAP-like [2] equations for models with arbitrary coupling between spins, and we demonstrate how to systematically obtain corrections to those TAP equations. Although the TAP equations have been rederived by a number of authors [3-6], nobody has previously obtained the corrections which become important for any short-ranged and finite-dimensional model.

(ii) In section 3, we apply these TAP equations to the Ising ferromagnet on a d-dimensional hypercubic lattice, and show that the corrections can be organized into a $1/d$ expansion around mean-field theory. Previous $1/d$ expansions for thermodynamic quantities like the free energy [7] were only valid in the high-temperature phase, but we obtain expansions for thermodynamic quantities like the magnetization which are valid in the low-temperature phase. To obtain a given order in $1/d$ using this technique, only a small finite number of graphs need to be computed.

(iii) Unfortunately, $1/d$ expansions for critical temperatures are believed to be at best asymptotic (for a review see [8]). Indeed, their asymptotic nature has been proven for the ferromagnetic spherical model on a hypercubic lattice [9]. The TAP-like equations that we derive for the ferromagnet suggest natural expansions around mean-field theory which are different from $1/d$ expansions. In section 4, we explain these expansions and show that they apparently converge (or can easily be turned into convergent series) for the critical temperature and thermodynamic quantities, even below the upper critical dimension. We use exact expressions for the spherical model to study the convergence properties of these schemes in more detail.

While it has been known for a long time that high-temperature expansions at a fixed-order parameter can give useful information at temperatures even below the critical temperature [10], we believe that the power and scope of such techniques have been very much under-appreciated. We have already applied these approaches to obtain new results for models about which much less is known than for the ferromagnet. In particular, combining these methods with the replica method we have obtained expansions to $O(1/d^2)$ for thermodynamic quantities including the order parameter for the spin glass on a hypercubic lattice [11]. We have also used these techniques to solve the fully frustrated Ising model in the limit of infinite dimensions [12]. Finally, we have found that a very similar approach can be used to construct mean-field theories (which can be systematically corrected) for quantum models such as the Hubbard model [13]. We believe, in general, that these techniques can be useful for a very wide range of problems, and that they give valuable insights into how mean-field theories work. One of the main purposes of this paper is to explore the limitations and successes of these methods for the well-understood case of the classical ferromagnet, as a point of comparison for other models and problems.

2. The TAP equations and beyond

We begin by considering an Ising model in which the bonds J_{ij} are arbitrary and can connect any two spins. The Hamiltonian is

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

We construct a free energy which depends on the magnetization at every site i:

$$-\beta A(\beta, m_i) = \ln \operatorname*{Tr}_{\{S_i\}} \exp\left(\beta \sum_{(ij)} J_{ij} S_i S_j + \sum_i \lambda_i(\beta)(S_i - m_i)\right). \tag{2}$$

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

$$\langle O \rangle \equiv \frac{\mathrm{Tr}_{\{S_i\}}\, O \exp(\beta \sum_i J_{ij} S_i S_j + \sum_i \lambda_i(\beta)(S_i - m_i))}{\mathrm{Tr}_{\{S_i\}} \exp(\beta \sum_i J_{ij} S_i S_j + \sum_i \lambda_i(\beta)(S_i - m_i))}. \tag{3}$$

Note that the Lagrange multipliers $\lambda_i(\beta)$ explicitly depend on the inverse temperature. Eventually, we will require that $\partial A/\partial m_i = 0$, which combined with the constraint that $m_i = \langle S_i \rangle$, ensures that $\lambda_i(\beta) = 0$ at the minimum of A.

Since m_i is fixed equal to $\langle S_i \rangle$ for any inverse temperature β, it is in particular equal to $\langle S_i \rangle$ when $\beta = 0$, which gives us the important relation

$$m_i = \langle S_i \rangle_{\beta=0} = \frac{\mathrm{Tr}\, S_i \exp(\lambda_i(0) S_i)}{\mathrm{Tr} \exp(\lambda_i(0) S_i)} = \tanh(\lambda_i(0)). \tag{4}$$

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

$$-\beta A(\beta) = -\beta A(\beta)|_{\beta=0} - \left.\frac{\partial(\beta A)}{\partial \beta}\right|_{\beta=0} \beta - \left.\frac{\partial^2(\beta A)}{\partial \beta^2}\right|_{\beta=0} \frac{\beta^2}{2} - \dots \tag{5}$$

where we have temporarily suppressed the dependence of A on m_i. From the definition of $-\beta A(\beta, m_i)$ given in equation (2) we find that

$$-\beta A(\beta, m_i)|_{\beta=0} = \sum_i \ln[\cosh(\lambda_i(0))] - \lambda_i(0) m_i. \tag{6}$$

At this point, we can choose to work with either the variables m_i or the variables $\lambda_i(0)$, which are directly related to the m_i through equation (4). We will choose to eliminate the $\lambda_i(0)$† and thereby recover

$$-\beta A(\beta, m_i)|_{\beta=0} = -\sum_i \frac{1+m_i}{2} \ln\left(\frac{1+m_i}{2}\right) + \frac{1-m_i}{2} \ln\left(\frac{1-m_i}{2}\right) \tag{7}$$

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

$$-\beta \left.\frac{\partial(\beta A)}{\partial \beta}\right|_{\beta=0} = \beta \left\langle \sum_{(ij)} J_{ij} S_i S_j \right\rangle_{\beta=0} + \beta \langle S_i - m_i \rangle_{\beta=0} \left.\frac{\partial \lambda_i}{\partial \beta}\right|_{\beta=0}. \tag{8}$$

At $\beta = 0$, the spin–spin correlation functions factorize so we find that

$$-\beta \left.\frac{\partial(\beta A)}{\partial \beta}\right|_{\beta=0} = \beta \sum_{(ij)} J_{ij} m_i m_j. \tag{9}$$

This is of course the 'mean-field' energy for a ferromagnetic model and, together with the zeroth-order term given in equation (7), gives the standard mean-field theory which becomes exact when, for example, all the J_{ij}s are equal, positive and infinite-ranged [14]. Continuing to the second derivative in the Taylor expansion, we find, after a short computation (see appendix 1), that

$$-\frac{\beta^2}{2} \left.\frac{\partial^2(\beta A)}{\partial \beta^2}\right|_{\beta=0} = \frac{\beta^2}{2} \sum_{(ij)} J_{ij}^2 (1 - m_i^2)(1 - m_j^2) \tag{10}$$

† When applying this formalism to other models, it is sometimes more convenient to eliminate the m_i, in particular if equation (4) is difficult to invert.

which is the famous Onsager reaction term in the TAP equations [2]. When added to the zeroth- and first-order terms, the TAP term gives a free energy that is presumably exact for J_{ij}s that are infinite-ranged but of random sign. In appendix 1, we present a formalism that we have found useful for computing this term and higher-order terms in the Taylor expansion.

The Taylor expansion presented here was pursued to second order in [5], thus recovering the ordinary TAP equations. But it can in fact be continued to arbitrarily high order. To $O(\beta^4)$, one finds that

$$\begin{aligned}-\beta A(\beta, m_i) = &-\sum_i \frac{1+m_i}{2}\ln\left(\frac{1+m_i}{2}\right)+\frac{1-m_i}{2}\ln\left(\frac{1-m_i}{2}\right)+\beta\sum_{(ij)} J_{ij}m_im_j \\ &+\frac{\beta^2}{2}\sum_{(ij)} J_{ij}^2(1-m_i^2)(1-m_j^2)+\frac{2\beta^3}{3}\sum_{(ij)} J_{ij}^3 m_i(1-m_i^2)m_j(1-m_j^2) \\ &+\beta^3\sum_{(ijk)} J_{ij}J_{jk}J_{ki}(1-m_i^2)(1-m_j^2)(1-m_k^2) \\ &-\frac{\beta^4}{12}\sum_{(ij)} J_{ij}^4(1-m_i^2)(1-m_j^2)(1+3m_i^2+3m_j^2-15m_i^2m_j^2) \\ &+2\beta^4\sum_{(ijk)} J_{ij}^2J_{jk}J_{ki}m_i(1-m_i^2)m_j(1-m_j^2)(1-m_k^2) \\ &+\beta^4\sum_{(ijkl)} J_{ij}J_{jk}J_{kl}J_{li}(1-m_i^2)(1-m_j^2)(1-m_k^2)(1-m_l^2)+\ldots \qquad (11)\end{aligned}$$

The notation (ij), (ijk) or $(ijkl)$ means that one should sum over all distinct pairs, triplets or quadruplets of spins. In figure 1, we write equation (11) in a diagrammatic shorthand notation. Each bond represents a βJ_{ij} term, while the vertices represent functions of the m_is. Unfortunately, these diagrams are only a shorthand, for we have not succeeded in deriving a full set of Feynman rules which would give us the vertex weights.

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) magnetization m_i. Setting $m_i = 0$, one recovers from equation (11) the ordinary high-temperature expansion of the zero-field free energy of the Ising model [15]. From a diagrammatic

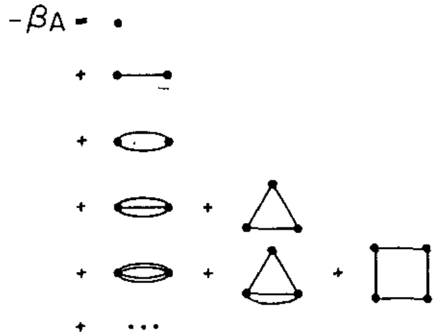

Figure 1. A diagrammatic representation of the magnetization-dependent free energy to $O(\beta^4)$ of an Ising model with arbitrary couplings between spins. Each bond represents a βJ_{ij}, while the vertices represent functions (given explicitly in equation (11)) of the site-dependent magnetizations m_i.

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 $\Sigma J_{ij} m_i m_j$; (ii) diagrams which appeared even for $m_i = 0$ are modified to have new weights associated with the magnetizations at the vertices.

The only non-zero diagrams in this generalized expansion for the Ising model are 'strongly irreducible'—that is, removing a vertex does not split the diagram into two pieces. This property implies that the only diagrams which contribute to the free energy of the Ising model on a Bethe lattice are those connecting just two sites i and j (see figure 2). In appendix 2, we use this fact to simply derive the exact solution of the ferromagnet on the Bethe lattice from the exact solution of the one-dimensional ferromagnetic chain in a magnetic field, and then use our exact solutions to compute all two-site diagrams for the ferromagnet (which we give explicitly up to $O(\beta^7)$).

Figure 2. Two-site diagrams which can be computed from the one-dimensional solution of the Ising model.

On the other hand, one should be aware that the property of 'strong irreducibility' does not necessarily hold for other models. For example, for the quantum Heisenberg ferromagnet, non-strongly irreducible diagrams contribute even in the high-temperature phase [16]. A more subtle counter-example is found in the case of the free energy of the spin glass averaged over disorder (using the replica method), for which one finds that non-strongly irreducible diagrams do not contribute in the high-temperature phase, but do contribute in the low-temperature phase [11].

The expansion represented in equation (11) will be very useful for any model in which the magnetization is inhomogeneous. One interesting example is the study of domain walls in the ferromagnet, which can be modelled by imposing magnetizations of different signs at distant boundaries. Equation (11) will give corrections to the standard mean-field theory of that problem.

3. 1/*d* expansions for the ferromagnet

In this section, we show that the 'extended' TAP-like equations of section 2 can be used to obtain new results even for the well-studied Ising ferromagnet on a hypercubic lattice. In particular, these equations can be converted into $1/d$ expansions that are valid in the low-temperature phase for any thermodynamic quantity of interest.

We work with the Hamiltonian

$$H = -J \sum_{(ij)} S_i S_j = -\frac{1}{2d} \sum_{(ij)} S_i S_j \tag{12}$$

where now only nearest-neighbour sites on the d-dimensional hypercubic lattice interact. We have chosen the conventional scaling $J = 1/(2d)$ so that the energy density of the lowest-energy state will always be $E/N = -1$, irrespective of dimension. With this scaling, it is clear that we can organize diagrams of our extended TAP equations into the order at which they first contribute to a $1/d$ expansion for $-\beta A$. In figure 3, we

$$-\frac{\beta A}{N} = -\left[\frac{1+m}{2}\ln\frac{1+m}{2} + \frac{1-m}{2}\ln\frac{1-m}{2}\right]$$
$$+\frac{\beta}{2d}\, d\, m^2$$
$$+\frac{1}{2}\left(\frac{\beta}{2d}\right)^2 d\,(1-m^2)^2$$
$$+\frac{2}{3}\left(\frac{\beta}{2d}\right)^3 d\, m^2(1-m^2)^2$$
$$+\left(\frac{\beta}{2d}\right)^4 \frac{d(d-1)}{2}\,(1-m^2)^4$$
$$-\frac{1}{12}\left(\frac{\beta}{2d}\right)^4 d\,(1-m^2)^2(1+6m^2-15m^4)$$
$$+2\left(\frac{\beta}{2d}\right)^5 2d(d-1)\, m^2(1-m^2)^4$$
$$+\left(\frac{\beta}{2d}\right)^6\left[d(d-1)+\frac{8}{3}d(d-1)(d-2)\right](1-m^2)^6$$

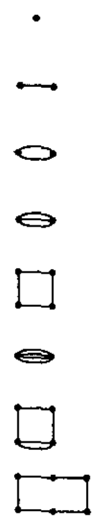

Figure 3. The magnetization-dependent free energy of the Ising ferromagnet on a hypercubic lattice, including all terms which contribute to $O(1/d^3)$.

organize all the diagrams which are necessary to compute corrections to $O(1/d^3)$, giving next to each diagram its contribution to $-\beta A$. It is rather easy to understand the organization—take, for instance, the square diagram in figure 3. Clearly each bond gives one order of $J \sim 1/d$, but there exist $d(d-1)/2 \sim d^2$ such squares on the lattice, so we find that the square diagram first contributes at $O(d^2/d^4) = O(1/d^2)$. Note that the first two terms in the high-temperature expansion are the dominant terms in $1/d$, which justifies the well-known fact that the standard mean-field theory becomes exact for the ferromagnet in the limit $d \to \infty$. For more complicated models, such as 'fully frustrated' models, a different scaling of J with d is necessary, and higher-order terms in the high-temperature expansion also contribute even in the limit $d \to \infty$ [12].

It should be recalled that a certain class of diagrams, namely those that connect just two sites i and j (see figure 2), can be conveniently obtained from the exact solution of the one-dimensional chain or Bethe lattice at a fixed magnetization. We compute these diagrams in detail in appendix 2. Another class of diagrams which are especially easy to compute are the 'ring' diagrams shown in figure 4. The contributions of these diagrams to the magnetization-dependent free energy can be obtained by multiplying the contribution of the corresponding $m = 0$ high-temperature diagram by a factor of $(1-m^2)$ for each vertex.

Armed with the expansion of the free energy to order $1/d^3$ given in figure 3, one can construct $1/d$ expansions for any thermodynamic quantity one wants, in both the high- and low-temperature phases. We begin by considering the critical temperature T_c which separates the two phases. If we expand $-\beta A$ in powers of m, then T_c is given

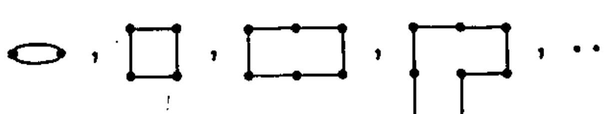

Figure 4. The 'ring diagrams'.

as usual by the temperature at which the m^2 coefficient vanishes. Thus we find

$$T_c = 1 - \frac{1}{2d} - \frac{1}{3d^2} - \frac{13}{24d^3} - \ldots \tag{13}$$

in agreement with previously obtained results [7].

Next we consider the $1/d$ expansion for the magnetization itself. It is best to work at a fixed-scale inverse temperature $b \equiv \beta/\beta_c$. By minimizing the free energy with respect to m, we find

$$m(b) = m_0(b) + \frac{m_1(b)}{d} + \frac{m_2(b)}{d^2} + \ldots \tag{14}$$

where

$$\begin{aligned} &m_0 = \tanh(bm_0) \qquad m_1 = \frac{b}{2} m_0(1 - m_0^2) \\ &m_2 = \frac{m_1}{1 - b(1 - m_0^2)} \left(\frac{7}{6} - \frac{b}{2} - \frac{b^2}{6}(1 - m_0^2)(1 - 3m_0^2) - \frac{b^3}{2}(1 - m_0^2)^3 \right). \end{aligned} \tag{15}$$

Clearly we can substitute these results back into the free energy and thereby recover $1/d$ expansions for the internal energy or specific heat that are valid throughout the low-temperature phase.

In the rest of the paper, we will generally choose to work near T_c, not because we are forced to, but simply because our expressions then become much less unwieldy. Working near T_c also lets us make use of high-temperature series expansions available in the literature to obtain somewhat higher-order $1/d$ expansions both above and below T_c. The reason is that, to obtain results to dominant order in $t = (T_c - T)/T$, it is sufficient to consider the expansion of the free energy near $m = 0$ up to $O(m^4)$:

$$-\beta A(\beta, m) = A_0(\beta) + A_2(\beta) m^2 + A_4(\beta) m^4 + \ldots \tag{16}$$

$A_2(\beta)$ and $A_4(\beta)$ are related to the derivatives of the free energy in a field $F(\beta, h)$ by the relations

$$A_2(\beta) = -\frac{\beta}{2\chi} \qquad A_4(\beta) = -\frac{\beta}{24\chi^4} \frac{\partial^4 F}{\partial h^4}\bigg|_{h=0} \tag{17}$$

where

$$\chi(\beta) = -\frac{\partial^2 F}{\partial h^2}\bigg|_{h=0}. \tag{18}$$

The high-temperature series for $A_2(\beta)$ and $A_4(\beta)$ are available [17] for arbitrary dimensionality up to order β^9:

$$\begin{aligned} A_2(\beta) = &-\frac{1}{2} + \frac{1}{2}\beta - \frac{1}{4d}\beta^2 + \frac{1}{12d^2}\beta^3 - \left(\frac{1}{8d^2} - \frac{5}{48d^3}\right)\beta^4 + \left(\frac{1}{8d^3} - \frac{29}{240d^4}\right)\beta^5 \\ &- \left(\frac{1}{4d^3} - \frac{61}{96d^4} + \frac{139}{360d^5}\right)\beta^6 + \left(\frac{5}{16d^4} - \frac{5}{6d^5} + \frac{5251}{10080d^6}\right)\beta^7 \\ &- \left(\frac{27}{32d^4} - \frac{133}{32d^5} + \frac{4271}{640d^6} - \frac{54205}{16128d^7}\right)\beta^8 \\ &+ \left(\frac{53}{48d^5} - \frac{173}{32d^6} + \frac{4949}{576d^7} - \frac{3113459}{725760d^8}\right)\beta^9 + \ldots \end{aligned} \tag{19}$$

$$A_4(\beta) = -\frac{1}{12}+\frac{1}{8d}\beta^2-\frac{1}{6d^2}\beta^3+\left(\frac{3}{16d^2}-\frac{5}{96d^3}\right)\beta^4-\left(\frac{1}{2d^3}-\frac{5}{12d^4}\right)\beta^5$$
$$+\left(\frac{5}{8d^3}-\frac{71}{64d^4}+\frac{379}{720d^5}\right)\beta^6-\left(\frac{15}{8d^4}-\frac{55}{12d^5}+\frac{1963}{720d^6}\right)\beta^7$$
$$+\left(\frac{189}{64d^4}-\frac{815}{64d^5}+\frac{24223}{1280d^6}-\frac{294697}{32256d^7}\right)\beta^8$$
$$-\left(\frac{53}{6d^5}-\frac{251}{6d^6}+\frac{4711}{72d^7}-\frac{588379}{18144d^8}\right)\beta^9+\ldots. \tag{20}$$

(The expansions for $A_0(\beta)$ are given in [7].) We can now use $A_2(\beta_c)=0$ to obtain [7] the expansion of β_c to $O(1/d^4)$:

$$\beta_c = 1+\frac{1}{2d}+\frac{7}{12d^2}+\frac{1}{d^3}+\frac{93}{40d^4}+\ldots. \tag{21}$$

Minimizing the free energy $A(\beta, m)$ with respect to the magnetization gives m near β_c:

$$m=\sqrt{\frac{(\beta_c-\beta)A_2'(\beta_c)}{2A_4(\beta_c)}}. \tag{22}$$

Substituting in our results from equations (19) and (20) we find

$$\frac{m}{\sqrt{3t}}=1+\frac{1}{2d}+\frac{25}{24d^2}+\frac{49}{16d^3}+\frac{68551}{5760d^4}+\ldots. \tag{23}$$

Note that in a $1/d$ expansion, we always have the classical mean-field critical exponent $\beta=\frac{1}{2}$; only the amplitude is corrected. For the specific heat, we find

$$\frac{C}{N}=\frac{3}{2}+\frac{1}{d}+\frac{2}{d^2}+\frac{17}{3d^3}+\frac{221}{10d^4}+\ldots \tag{24}$$

at temperatures just below T_c, and

$$\frac{C}{N}=\frac{1}{4d}+\frac{5}{8d^2}+\frac{23}{12d^3}+\frac{349}{48d^4}+\ldots \tag{25}$$

just above T_c. Again our results are qualitatively like the classical mean-field behaviour, with a simple discontinuity in the specific heat. In the next section, we will discuss schemes which enable one to expand around mean-field theory, and at the same time understand non-classical critical behaviour.

4. Convergent expansions around mean-field theory

An unfortunate feature of $1/d$ expansions is that they are generally asymptotic, although proving that can be very difficult. Gerber and Fisher did succeed in proving that the $1/d$ expansion for T_c of the ferromagnetic spherical model is asymptotic [9]. For this exactly soluble model [18], the explicit expression for β_c for arbitrary dimensionality is $J\beta_c = W_d(0)$, where the function $W_d(z)$ is defined by

$$W_d(z)=\frac{1}{2}\int\frac{d^dk}{(2\pi)^d}\,\frac{1}{z+\Sigma_{n=1}^d(1-\cos(k_n))}. \tag{26}$$

From this expression, it was proven in [9] that the coefficients $|B_m|$ in the $1/d$ expansion

$$J\beta_c(d) = \sum_{m=1}^{\infty} \frac{B_m}{d^m} \tag{27}$$

grow as $(m!)c^m b_m$, with $|b_m|^{1/m} \to 1$ and $c \approx 1.2$. On the other hand, Abe [19] has found a rearrangement of the $1/d$ expansion which can be proven convergent down to the lower critical dimension. We will show here that Abe's rearrangement (and others of the same kind) actually arises from a very natural alternative expansion around mean-field theory. This alternative expansion can be used for the Ising model (or for any n-component spin model) and for any thermodynamic quantity.

Our alternative expansions rely on the observation that the two first terms in the high-temperature expansion of $-\beta A(\beta, m)$ at fixed m give mean-field theory, while higher-order terms give corrections. Any scheme in which we introduce some parameter λ and scale the higher-order terms by increasing powers of λ, while keeping the first two terms as a zeroth order, will give an expansion around mean-field theory. One possible scaling (the 'λ scheme'), in which the power of λ equals the number of lines for the higher-order diagrams (or equivalently, the power of β), is depicted in figure 5(a). Another, slightly different scaling (the 'μ scheme') is shown in figure 5(b). As we shall see, the μ series are generally better behaved while the λ scheme corresponds precisely to Abe's rearrangement for the spherical model and has a natural physical interpretation which we will describe shortly. The parameter-dependent free energies defined through these scalings are (defining $\hat{A}(\beta, m) \equiv -\beta A(\beta, m)$)

$$\begin{aligned} \hat{A}(\beta, m; \lambda) &= \hat{A}(\beta\lambda, m) + \beta(1-\lambda)\left.\frac{\partial \hat{A}}{\partial \beta}\right|_{\beta=0} \\ \hat{A}(\beta, m; \mu) &= \frac{1}{\mu}\hat{A}(\beta\mu, m) + \left(1 - \frac{1}{\mu}\right)\hat{A}(\beta = 0, m). \end{aligned} \tag{28}$$

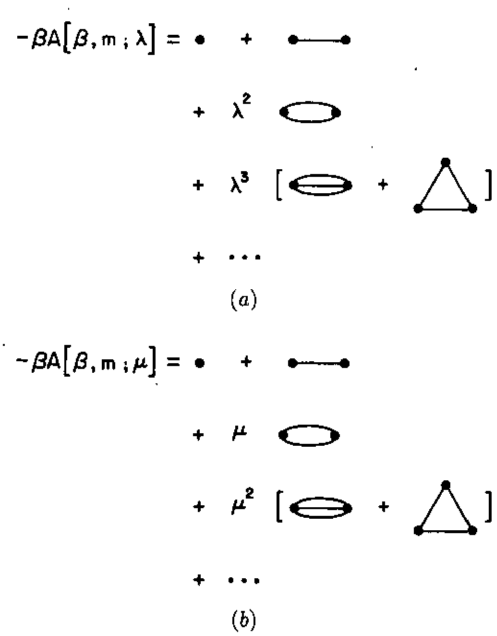

Figure 5. (a) A diagrammatic representation of the λ scheme. (b) A diagrammatic representation of the μ scheme.

Clearly, organizing the high-temperature expansion of $-\beta A$ using $1/d$ is just one of many ways to expand around mean-field theory, and the above schemes are simply rearrangements of the $1/d$ series. What might have been unexpected is that these simple rearrangements can dramatically improve convergence properties.

The λ expansion actually has a very natural physical interpretation as an expansion in the fluctuations of the local field felt by a spin ($h_i = \sum J_{ij} S_j$) with respect to the 'mean' field ($\langle h_i \rangle = \sum J_{ij} m_j$). This can most easily be seen by starting with the exact equation of motion [20] obeyed by m_i:

$$m_i = \langle \tanh(\beta h_i) \rangle_H \tag{29}$$

where the notation $\langle \rangle_H$ means the thermal expectation value with respect to the Hamiltonian H. We can decompose the local field into a mean field plus a fluctuation δh_i scaled by the parameter λ:

$$h_i^\lambda = \langle h_i \rangle + \lambda \delta h_i \qquad \delta h_i = \sum_{j(i)} J_{ij}(S_j - m_j). \tag{30}$$

Let us also decompose the Hamiltonian into a mean-field, independent spin Hamiltonian H_0 plus fluctuations:

$$H_0 = -\sum_{(ij)} J_{ij}(S_i m_j + S_j m_i - m_i m_j) \tag{31}$$

$$\begin{aligned} H_\lambda &= H_0 - \lambda \sum_{(ij)} J_{ij}(S_i - m_i)(S_j - m_j) \\ &= H_0 - \lambda \sum_i (S_i - m_i)\delta h_i. \end{aligned} \tag{32}$$

Of course, the equations of motion are simply

$$m_i^\lambda = \langle S_i \rangle_\lambda = \langle \tanh(\beta h_i^\lambda) \rangle_{H_\lambda}. \tag{33}$$

If $\lambda = 0$, we have mean-field theory, while the full original model is recovered at $\lambda = 1$. Now one can easily convince oneself using perturbation theory in λ that the solutions m_i^λ of equation (33) are given by the minimization of the scaled potential $A(\beta, m_i; \lambda)$; i.e. they satisfy

$$\left.\frac{\partial}{\partial m_i} A(\beta, m_i; \lambda)\right|_{m_i = m_i^\lambda} = 0. \tag{34}$$

Thus the λ scheme is truly an expansion in the fluctuations around the mean local field.

We now describe how to generate convergent expansions for the critical temperature. It follows from equations (28) and from the fact that $A_2(\beta) = -\frac{1}{2} + \beta/2 + O(\beta^2)$ that the coefficient of m^2 in the expansion of $-\beta A(\beta, m; \lambda)$ and $-\beta A(\beta, m; \mu)$ are, respectively:

$$A_2(\beta; \lambda) = \frac{2A_2(\beta\lambda) + \beta(1-\lambda)}{2} \qquad A_2(\beta; \mu) = \frac{2A_2(\beta\mu) + (1-\mu)}{2\mu}. \tag{35}$$

Thus, for $0 \leqslant \lambda, \mu \leqslant 1$, these magnetization-dependent potentials have a second-order phase transition at a critical inverse temperature $\beta_c(\lambda)$ or $\beta_c(\mu)$ given by the solution of

$$A_2(\lambda\beta_c(\lambda)) + \frac{(1-\lambda)\beta_c(\lambda)}{2} = 0 \qquad 2A_2(\mu\beta_c(\mu)) + (1-\mu) = 0. \tag{36}$$

From these equations and the high-temperature series for A_2 (which can be inferred from the inverse susceptibility), we can obtain an expansion in powers of λ or μ for β_c. For the spherical model, $A_2(\beta)$ is given by

$$A_2(\beta) = -\frac{\beta}{2d} W_d^{-1}\left(\frac{\beta}{2d}\right) \tag{37}$$

so we obtain for $\beta_c(\lambda)$ the result

$$\beta_c(\lambda) = \frac{2d}{\lambda} W_d\left(d\left(\frac{1}{\lambda}-1\right)\right) = \int \frac{d^dk}{(2\pi)^d}\left(1-\frac{\lambda}{d}\sum_{n=1}^{d}\cos(k_n)\right)^{-1} \tag{38}$$

and thus the series

$$\beta_c(\lambda) = \sum_{m=0}^{\infty} \lambda^{2m} C_{2m}(d) \tag{39}$$

where

$$C_{2m}(d) = \frac{1}{d^{2m}} \int \frac{d^dk}{(2\pi)^d}\left(\sum_{n=1}^{d}\cos(k_n)\right)^{2m}. \tag{40}$$

For $\lambda = 1$, this is precisely Abe's rearrangement [19] of the $1/d$ series for β_c, which he has proven to be convergent for dimensions larger than two, which is the lower critical dimension for the spherical model. Indeed, the asymptotic behaviour of C_{2m} for large m is [19]

$$C_{2m} \sim 2^{1-d}\left(\frac{d}{\pi m}\right)^{d/2}. \tag{41}$$

The first eight coefficients of the λ series for β_c are given in [19]. In table 1, we give the first 12 terms in the μ series for β_c, which can easily be obtained from an expansion of W_d. For the μ case, no general expression of the coefficients like that given in equation (40) can be derived, which makes the proof of convergence at $\mu = 1$ problematic. However, convergence for any $d > 2$ is strongly supported by the coefficients in table 1 and the arguments given below. Actually, the μ series are, in practice, even better behaved than the λ series†, so we will concentrate exclusively on the μ series in the following development.

For the Ising model with arbitrary dimensionality, we can use the high-temperature expansion of $A_2(\beta)$ given in equation (19) to compute the series for $\beta_c(\mu)$ to $O(\mu^8)$. This series is given in table 1. For the square lattice ($d = 2$), the longest available high-temperature series for the susceptibility [17] can be converted into expansions for $\beta_c(\mu)$ up to order μ^{19}. We find

$$\begin{aligned}\beta_c(\mu) = 1 &+ 0.25\mu + 0.0833333\mu^2 + 0.0625\mu^3 + 0.04375\mu^4 + 0.030599\mu^5 \\ &+ 0.0237165\mu^6 + 0.019165\mu^7 + 0.0158149\mu^8 + 0.133331\mu^9 \\ &+ 0.0114299\mu^{10} + 0.00993522\mu^{11} + 0.00873751\mu^{12} \\ &+ 0.00775816\mu^{13} + 0.00694619\mu^{14} + 0.00626492\mu^{15} + 0.00568658\mu^{16} \\ &+ 0.00519072\mu^{17} + 0.00476189\mu^{18} + 0.00438817\mu^{19} + \dots\end{aligned} \tag{42}$$

† For example, in contrast to the spherical case, the Ising series for $\beta_c(\lambda)$ includes odd power terms. The coefficients alternate in sign and grow (albeit regularly) in amplitude, compared with the Ising series for $\beta_c(\mu)$ which has only positive coefficients that decrease very regularly.

Table 1. The coefficients D_i in the series $\beta_c(\mu)=\Sigma D_i\mu^i$ for the spherical and Ising models of arbitrary dimensionality d.

Spherical model	
D_0	1
D_1	$\frac{1}{2d}$
D_2	$\frac{1}{2d^2}$
D_3	$\frac{1}{4d^2}+\frac{1}{4d^3}$
D_4	$\frac{3}{4d^3}-\frac{1}{4d^4}$
D_5	$\frac{1}{2d^3}+\frac{1}{16d^4}-\frac{1}{16d^5}$
D_6	$\frac{9}{4d^4}-\frac{15}{4d^5}+\frac{2}{d^6}$
D_7	$\frac{27}{16d^4}-\frac{81}{32d^5}+\frac{89}{64d^6}-\frac{3}{64d^7}$
D_8	$\frac{155}{16d^5}-\frac{35}{d^6}+\frac{3041}{64d^7}-\frac{1389}{64d^8}$
D_9	$\frac{31}{4d^5}-\frac{1823}{64d^6}+\frac{2817}{64d^7}-\frac{1919}{64d^8}+\frac{461}{64d^9}$
D_{10}	$\frac{849}{16d^6}-\frac{5155}{16d^7}+\frac{101721}{128d^8}-\frac{890}{d^9}+\frac{46711}{128d^{10}}$
D_{11}	$\frac{1415}{32d^6}-\frac{8969}{32d^7}+\frac{199391}{256d^8}-\frac{575483}{512d^9}+\frac{836817}{1024d^{10}}-\frac{241175}{1024d^{11}}$
Ising model	
D_0	1
D_1	$\frac{1}{2d}$
D_2	$\frac{1}{3d^2}$
D_3	$\frac{1}{4d^2}$
D_4	$\frac{1}{2d^3}-\frac{3}{10d^4}$
D_5	$\frac{1}{2d^3}-\frac{11}{16d^4}+\frac{17}{48d^5}$
D_6	$\frac{13}{8d^4}-\frac{7}{2d^5}+\frac{113}{56d^6}$
D_7	$\frac{27}{16d^4}-\frac{173}{32d^5}+\frac{431}{64d^6}-\frac{185}{64d^7}$
D_8	$\frac{359}{48d^5}-\frac{1531}{48d^6}+\frac{2269}{48d^7}-\frac{3275}{144d^8}$

An examination of the coefficients in table 1 and equation (42) strongly suggests that the μ expansions for β_c are convergent at $\mu=1$, even for the Ising model. First of all, the functional form of $\beta_c(\mu)$ near $\mu=1$ can be connected to the behaviour of $A_2(\beta)$ just above the critical temperature. One expects that $A_2(\beta)\sim(\beta_c-\beta)^\gamma$, where γ is the critical exponent of the susceptibility. Substituting this behaviour into equation (36), we find

$$\beta_c(\mu\to 1^-)-\beta_c\sim(1-\mu)^{1/\gamma}. \tag{43}$$

Of course, $\gamma>1$ for $d<4$ and $\gamma=1$ for $d>4$. Inspection of the coefficients given above suggests that the (positive) coefficients of the series for $\beta_c(\mu)=\Sigma\, D_m\mu^m$ decay as a power law, so, from equation (43), we expect that $D_m\sim m^{-(1+1/\gamma)}$ as $m\to\infty$ for any dimension less than four and greater than the lower critical dimension. For the spherical model, $\gamma=2/(d-2)$ for $d<4$, so the asymptotic form of the C_m coefficients of the $\beta_c(\lambda)$ given in equation (41) is also consistent with these conjectures. The one-dimensional Ising model for which $A_2(\beta)=(e^{-2\beta J})/2$ (see appendix 2) and therefore

$$\beta_c(\mu)=-\frac{\ln(1-\mu)}{2\mu} \tag{44}$$

is also a trivial illustration of this behaviour, with $1/\gamma=0$.

It is interesting to try to construct a function $1/\gamma(\mu)$ that has an expansion in powers of μ which converges at $\mu=1$ towards the true $1/\gamma$ for any dimension greater than the lower critical dimension. This can be achieved, for example, by choosing

$$\frac{1}{\gamma(\mu)}=1-(1-\mu)\frac{d}{d\mu}\ln\left(\frac{d}{d\mu}(\mu\beta_c(\mu))\right). \tag{45}$$

Using equation (43), it is clear that, with this definition, $\gamma(\mu)\to\gamma$ as $\mu\to 1^-$. In table 2, we give the first several terms in the μ series for $1/\gamma(\mu)$ for the spherical and Ising models in arbitrary dimensionality. It is amusing to see how these series rearrange a $1/d$ series which gives $1/\gamma=1$ to all orders. For the square lattice Ising model, we find

$$\begin{aligned}\frac{1}{\gamma}=0.5+0.25\mu-0.25\mu^2+0.0625\mu^3+0.0351563\mu^4-0.0117188\mu^5\\ -0.00390625\mu^6-0.00195312\mu^7-0.00125122\mu^8\\ -0.0000686646\mu^9-0.00062561\mu^{10}-0.00064373\mu^{11}\\ -0.000277162\mu^{12}-0.000252455\mu^{13}-0.000281595\mu^{14}\\ -0.000230975\mu^{15}-0.000194763\mu^{16}-0.00017929\mu^{17}\\ -0.000162608\mu^{18}-0.000146673\mu^{19}+\dots\end{aligned} \tag{46}$$

These series all appear to be convergent. Simply truncating the series for the square lattice Ising model, we obtain $1/\gamma=0.575$, which should be compared to the exact value $1/\gamma=0.5714\dots$. Of course, our $\gamma(\mu)$ should not be interpreted as the critical exponent of any model, and is merely a mathematical construction. Suzuki's 'power series coherent anomaly method' to obtain critical exponents is based on rather similar ideas [21].

Table 2. The coefficients E_i in the series $1/\gamma(\mu) = \Sigma E_i \mu^i$ for the spherical and Ising models of arbitrary dimensionality d.

Spherical model	
E_0	$1-\frac{1}{d}$
E_1	$\frac{1}{d}-\frac{2}{d^2}$
E_2	$-\frac{1}{d^2}+\frac{1}{2d^3}$
E_3	$\frac{3}{d^2}-\frac{23}{2d^3}+\frac{17}{2d^4}$
E_4	$-\frac{4}{d^3}+\frac{87}{8d^4}-\frac{53}{8d^5}$
E_5	$\frac{15}{d^3}-\frac{743}{8d^4}+\frac{1373}{8d^5}-\frac{187}{2d^6}$
E_6	$-\frac{21}{d^4}+\frac{467}{4d^5}-\frac{3313}{16d^6}+\frac{1783}{16d^7}$
E_7	$\frac{189}{2d^4}-\frac{3389}{4d^5}+\frac{43149}{16d^6}-\frac{57289}{16d^7}+\frac{3273}{2d^8}$
E_8	$-\frac{132}{d^5}+\frac{38361}{32d^6}-\frac{63321}{16d^7}+\frac{349269}{64d^8}-\frac{164263}{64d^9}$
E_9	$\frac{1395}{2d^5}-\frac{271261}{32d^6}+\frac{642427}{16d^7}-\frac{5883635}{64d^8}+\frac{3208259}{32d^9}-\frac{2604713}{64d^{10}}$
E_{10}	$-\frac{955}{d^6}+\frac{101805}{8d^7}-\frac{1051235}{16d^8}+\frac{5170441}{32d^9}-\frac{47642085}{256d^{10}}+\frac{20085029}{256d^{11}}$
Ising model	
E_0	$1-\frac{1}{d}$
E_1	$\frac{1}{d}-\frac{1}{d^2}$
E_2	$-\frac{2}{d^2}+\frac{2}{d^3}$
E_3	$\frac{3}{d^2}-\frac{8}{d^3}+\frac{5}{d^4}$
E_4	$-\frac{9}{d^3}+\frac{225}{8d^4}-\frac{153}{8d^5}$
E_5	$\frac{15}{d^3}-\frac{643}{8d^4}+\frac{1083}{8d^5}-\frac{70}{d^6}$
E_6	$-\frac{189}{4d^4}+\frac{2213}{8d^5}-\frac{3997}{8d^6}+\frac{1081}{4d^7}$
E_7	$\frac{189}{2d^4}-\frac{6395}{8d^5}+\frac{19617}{8d^6}-\frac{12715}{4d^7}+\frac{2863}{2d^8}$

Finally, μ series can be derived for the spontaneous magnetization. We now need the coefficient of m^4 in $-\beta A$, which can be obtained from equations (28):

$$A_4(\beta;\mu)=\frac{1}{\mu}A_4(\beta\mu)-C\left(1-\frac{1}{\mu}\right) \tag{47}$$

where $C=\frac{1}{4}$ for the spherical model and $C=\frac{1}{12}$ for the Ising model (more generally, $C=n/4(n+2)$ for the O(n) model). Defining t_μ by

$$t_\mu=\frac{\beta-\beta_c(\mu)}{\beta_c(\mu)} \tag{48}$$

we can generate expansions for $m/\sqrt{t_\mu}$ by minimizing the free energy as usual. For the spherical model, we find, for any μ,

$$\frac{m}{\sqrt{t_\mu}}=1 \tag{49}$$

near T_c, which corresponds precisely to the exact result. (The critical exponent β is unchanged for the spherical model for $d<4$.) For the Ising model, we give the μ series for $m/\sqrt{3t_\mu}$ to $O(\mu^8)$ in table 3. We believe it to be convergent at $\mu=1$ for $d>4$. We expect that the series diverges at $\mu=1$ for $d<4$ because A_4 should diverge like $(T_c-T)^{\gamma-2\beta}$ near T_c, where β now signifies the critical exponent for the magnetization: $m\sim(T_c-T)^\beta$. From equation (43), we find that

$$\frac{m(\mu\to 1^-)}{\sqrt{t_\mu}}\sim(1-\mu)^{(2\beta-1)/2\gamma}. \tag{50}$$

Table 3. The coefficients F_i in the series $m/\sqrt{3t_\mu}=\Sigma F_i\mu^i$ near T_c for the Ising model of arbitrary dimensionality d.

F_0	1
F_1	$\frac{1}{2d}$
F_2	$\frac{7}{24d^2}$
F_3	$\frac{3}{4d^2}-\frac{9}{16d^3}$
F_4	$\frac{9}{8d^3}-\frac{5729}{5760d^4}$
F_5	$\frac{5}{2d^3}-\frac{571}{96d^4}+\frac{8167}{2304d^5}$
F_6	$\frac{225}{32d^4}-\frac{1143}{64d^5}+\frac{10551473}{967680d^6}$
F_7	$\frac{189}{16d^4}-\frac{9845}{192d^5}+\frac{1773637}{23040d^6}-\frac{10355671}{276480d^7}$
F_8	$\frac{4697}{96d^5}-\frac{59739}{256d^6}+\frac{16947623}{46080d^7}-\frac{85143368147}{464486400d^8}$

The main significance of this result is that it can be used to derive series for the critical exponent β as we previously did for γ.

In conclusion, we believe that high-temperature expansions performed at a fixed-order parameter provide a simple, systematic and reliable way to derive mean-field theories and their corrections. This method combines the advantages of high-temperature expansions and mean-field theories to yield a quantitatively precise understanding of phases with a non-zero-order parameter. The method is not at all limited to classical spin systems: it can be applied to any model for which a transition from a 'trivial' disordered phase to an ordered phase occurs at some initially small parameter is varied. That parameter need not be the inverse temperature: for quantum systems, one can use the strength of the interaction between particles or any other parameter which, when zero, gives a solvable problem. Indeed, as mentioned in the introduction, we have already been able to apply this method to problems as diverse as spin glasses [11], fully frustrated models [12] and the Hubbard model [13]. Given the ubiquitous importance of mean-field theories and the recurrent (often unanswered) questions about the effect of fluctuations around mean-field theory, we expect this method to have many more useful applications.

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Note added in proof. The reason why simple vertex rules do not exist for the expansion in equation (11) and figure 1 can be understood in the framework of the 'linked cluster expansion' (see, for example, [23]). In a linked cluster expansion, one can derive simple diagrammatic rules for the free energy functional expressed in terms of an infinite set of 'renormalized semi-invariants'. Our expansion for $A(\beta, m_i)$ uses only the first invariant (the physical magnetization), replacing all higher-order ones by their values at the extremum in terms of the m_i's. It is this elimination procedure which is responsible for the non-factorized terms in equation (11), appearing first at order β^4.

Appendix A

In this appendix, we present a formalism that we have found useful for computing the high-temperature expansion of a (possibly) inhomogeneous Ising model at fixed site-dependent magnetization. The formalism can easily be extended to many other models. We will use the same notation as was introduced in section 2. This formalism may appear rather primitive to the reader, but we nevertheless feel that it is useful to present it as it stands, for it enabled us to systematically calculate the previously unknown corrections to the TAP equations.

We begin by introducing the very useful operator U as follows:

$$U \equiv H - \langle H \rangle - \sum_i \frac{\partial \lambda_i(\beta)}{\partial \beta}(S_i - m_i). \tag{A1.1}$$

With this definition in hand, it is easy to work out that the derivative of the thermal expectation value of any operator O is simply given by

$$\frac{\partial\langle O\rangle}{\partial\beta}=\left\langle\frac{\partial O}{\partial\beta}\right\rangle-\langle OU\rangle. \tag{A1.2}$$

We have introduced the Lagrange multipliers $\lambda_i(\beta)$ to fix the magnetization $m_i=\langle S_i\rangle$ independent of β. The fact that the magnetization does not depend on β results in some interesting identities for U. First, we obtain the trivial identity

$$\langle U\rangle=0. \tag{A1.3}$$

Next, using equation (A1.2), we find that

$$\frac{\partial\langle S_i\rangle}{\partial\beta}=-\langle US_i\rangle=-\langle U(S_i-m_i)\rangle=0. \tag{A1.4}$$

Consider now the derivatives of U with respect to β. Using all our previous results, we find

$$\begin{aligned}\frac{\partial U}{\partial\beta}&=\langle HU\rangle-\sum_i\frac{\partial^2\lambda_i}{\partial\beta^2}(S_i-m_i)\\&=\langle U^2\rangle-\sum_i\frac{\partial^2\lambda_i}{\partial\beta^2}(S_i-m_i).\end{aligned} \tag{A1.5}$$

Taking a second derivative and again using our previous results, we obtain

$$\begin{aligned}\frac{\partial^2 U}{\partial\beta^2}&=2\left\langle U\frac{\partial U}{\partial\beta}\right\rangle-\langle U^3\rangle-\sum_i\frac{\partial^3\lambda_i}{\partial\beta^3}(S_i-m_i)\\&=-\langle U^3\rangle-\sum_i\frac{\partial^3\lambda_i}{\partial\beta^3}(S_i-m_i).\end{aligned} \tag{A1.6}$$

Consider now the derivatives of the magnetization-dependent free energy that we are interested in computing. The first derivative is given by

$$\frac{\partial(\beta A)}{\partial\beta}=\langle H\rangle-\sum_i\frac{\partial\lambda_i}{\partial\beta}\langle S_i-m_i\rangle=\langle H\rangle. \tag{A1.7}$$

Using the relations derived above, we can easily calculate successively higher derivatives. Thus we find

$$\begin{aligned}\frac{\partial^2(\beta A)}{\partial\beta^2}&=\langle HU\rangle=-\langle U^2\rangle\\ \frac{\partial^3(\beta A)}{\partial\beta^3}&=\langle U^3\rangle-2\left\langle U\frac{\partial U}{\partial\beta}\right\rangle=\langle U^3\rangle\\ \frac{\partial^4(\beta A)}{\partial\beta^4}&=-\langle U^4\rangle+3\left\langle U^2\frac{\partial U}{\partial\beta}\right\rangle=-\langle U^4\rangle+3\langle U^2\rangle^2-3\sum_i\frac{\partial^2\lambda_i}{\partial\beta^2}\langle U^2(S_i-m_i)\rangle\\ \frac{\partial^5(\beta A)}{\partial\beta^5}&=\langle U^5\rangle-10\langle U^2\rangle\langle U^3\rangle-3\sum_i\frac{\partial^3\lambda_i}{\partial\beta^3}\langle U^2(S_i-m_i)\rangle+7\sum_i\frac{\partial^2\lambda_i}{\partial\beta^2}\langle U^3(S_i-m_i)\rangle\\&\quad+6\sum_i\sum_j\frac{\partial^2\lambda_i}{\partial\beta^2}\frac{\partial^2\lambda_j}{\partial\beta^2}\langle U(S_i-m_i)(S_j-m_j)\rangle.\end{aligned} \tag{A1.8}$$

The results obtained so far are true for any β. We now derive results that hold at $\beta=0$ by exploiting the fact that spin-spin correlation functions always factorize at

$\beta=0$. We will denote quantities evaluated at $\beta=0$ with a 0 subscript, i.e. $\langle O\rangle_0 \equiv \langle O\rangle_{\beta=0}$. First we find that

$$\left.\frac{\partial(\beta A)}{\partial\beta}\right|_0 = \langle H\rangle_0 = -\left\langle \sum_{(ij)} J_{ij} S_i S_j \right\rangle_0 = -\tfrac{1}{2}\sum_i\sum_j J_{ij} m_i m_j. \tag{A1.9}$$

We now use equation (A1.9) to derive the Maxwell relation

$$\left.\frac{\partial\lambda_i}{\partial\beta}\right|_0 = \left.\frac{\partial^2(\beta A)}{\partial m_i \partial\beta}\right|_0 = -\sum_{j(\neq i)} J_{ij} m_j. \tag{A1.10}$$

Substituting equation (A1.11) into equation (A1.1), we find the very useful result

$$U_0 = -\sum_{(ij)} J_{ij}(S_i - m_i)(S_j - m_j) = -\sum_l J_l Y_l \tag{A1.11}$$

where we have introduced the *link* operators $J_l = J_{ij}$ and $Y_l = (S_i - m_i)(S_j - m_j)$. For the Y_l operators, we easily obtain

$$\begin{aligned}
&\langle Y_l\rangle_0 = 0 \\
&\langle Y_l(S_i - m_i)\rangle_0 = 0 \\
&\langle Y_k Y_l\rangle_0 = (1-m_i^2)(1-m_j^2)\delta_{kl}.
\end{aligned} \tag{A1.12}$$

Given the form of the U_0 operators and equations (A1.8), it is easy to convince oneself that only *connected* diagrams will contribute to the Taylor expansion for the free energy. For example, using equations (A1.8) and (A1.12), we compute

$$\begin{aligned}
\left.\frac{\partial^2(\beta A)}{\partial\beta^2}\right|_0 &= -\langle U^2\rangle_0 \\
&= -\sum_{l_1 l_2} J_{l_1} J_{l_2} \langle Y_{l_1} Y_{l_2}\rangle_0 \\
&= -\sum_{(ij)} J_{ij}^2 (1-m_i^2)(1-m_j^2)
\end{aligned} \tag{A1.13}$$

which gives us the TAP-Onsager term.

From equation (13) we obtain the new Maxwell relation

$$\left.\frac{\partial^2\lambda_i}{\partial\beta^2}\right|_0 = \left.\frac{\partial^3(\beta A)}{\partial m_i \partial\beta^2}\right|_0 = 2m_i \sum_{j(\neq i)} J_{ij}^2 (1-m_j^2). \tag{A1.14}$$

In general, we will be able to compute derivatives of λ_i with respect to β by using Maxwell relations obtained from previous results.

To compute the next derivative of the free energy, we need $\langle Y_{l_1} Y_{l_2} Y_{l_3}\rangle_0$ which is only non-zero if either $l_1 = l_2 = l_3$, in which case we find that

$$\langle Y_l^3\rangle_0 = 4m_i m_j (1-m_i^2)(1-m_j^2) \tag{A1.15}$$

or if l_1, l_2 and l_3 are three links in a triangle, in which case we find that

$$\langle Y_{l_1} Y_{l_2} Y_{l_3}\rangle_0 = (1-m_i^2)(1-m_j^2)(1-m_k^2) \tag{A1.16}$$

where i, j and k are the three sites included in the triangle. Using these results, we obtain

$$\left.\frac{\partial^3(\beta A)}{\partial\beta^3}\right|_0 = \langle U^3\rangle_0$$
$$= -\sum_{l_1 l_2 l_3} J_{l_1} J_{l_2} J_{l_3} \langle Y_{l_1} Y_{l_2} Y_{l_3}\rangle_0$$
$$= -4\sum_{(ij)} J_{ij}^3 m_i(1-m_i^2) m_j(1-m_j^2)$$
$$-6\sum_{(ijk)} J_{ij} J_{jk} J_{ki}(1-m_i^2)(1-m_j^2)(1-m_k^2). \qquad \text{(A1.17)}$$

Higher derivatives of βA can be obtained by a continuation of these procedures. The only new feature is that the Maxwell relations like equation (A1.14) must be used. With some labour, one can compute the next derivative and verify equation (11) in section 2.

Appendix 2

In this appendix, we use the exact solution of the one-dimensional Ising model in a field to compute the exact magnetization-dependent free energy of the ferromagnetic Ising model on the Bethe lattice. We then use these results to calculate the contribution to the free energy of any homogeneous ferromagnetic model from diagrams which connect just two sites i and j (see figure 2). These calculations are possible because the property of strong irreducibility implies that only two-site diagrams contribute to the Ising model on a chain or on a Bethe lattice.

We begin by considering an Ising model in a fixed field h. The Hamiltonian is

$$H = -J\sum_{i=1}^{N} S_i S_{i+1} - h\sum_{i=1}^{N} S_i. \qquad \text{(A2.1)}$$

Using standard transfer matrix techniques, the field-dependent free energy per spin is given in the thermodynamic limit by

$$-\frac{\beta F}{N} = \beta J + \ln[\cosh(\beta h) + \sqrt{\sinh^2(\beta h) + \mathrm{e}^{-4\beta J}}]. \qquad \text{(A2.2)}$$

The magnetization per spin is

$$m = \frac{\sinh(\beta h)}{\sqrt{\sinh^2(\beta h) + \mathrm{e}^{-4\beta J}}}. \qquad \text{(A2.3)}$$

Inverting this relation, and substituting in the resulting expression for the field in terms of the magnetization, we obtain the magnetization-dependent free energy:

$$-\frac{\beta A}{N} = \ln\left[\mathrm{e}^{\beta J}\left(1 + \frac{m^2}{1-m^2}\mathrm{e}^{-4\beta J}\right)^{1/2} + \frac{\mathrm{e}^{-\beta J}}{\sqrt{1-m^2}}\right] - m\sinh^{-1}\left(\frac{m}{\sqrt{1-m^2}}\mathrm{e}^{-2\beta J}\right). \qquad \text{(A2.4)}$$

At $\beta = 0$, this reduces to the standard result for the entropy of non-interacting spins constrained to have magnetization m:

$$-\frac{\beta A(\beta=0)}{N} = -\left[\frac{1+m}{2}\ln\left(\frac{1+m}{2}\right) + \frac{1-m}{2}\ln\left(\frac{1-m}{2}\right)\right]. \qquad \text{(A2.5)}$$

To generalize from the chain to the Bethe lattice with coordination number q, we note that while the $\beta = 0$ piece of the free energy depends only on non-interacting sites, the rest of the free energy comes from the interaction of two adjacent sites. Since there are $q/2$ adjacent sites per spin, we find

$$A(q,\beta)=A(q=2,\beta=0)+\frac{q}{2}(A(q=2,\beta)-A(q=2,\beta=0)). \qquad \text{(A2.6)}$$

This is the exact magnetization-dependent free energy of the ferromagnet on the Bethe lattice, as can be checked by comparison with the results derived by more conventional combinatorial arguments [22]. Expanding this result in powers of β, we find

$$\begin{aligned}-\frac{\beta A}{N}=-\bigg[&\frac{1+m}{2}\ln\left(\frac{1+m}{2}\right)+\frac{1-m}{2}\ln\left(\frac{1-m}{2}\right)\bigg]\\&+\frac{q}{2}\bigg[\beta J m^2+\frac{\beta^2J^2(1-m^2)^2}{2}+\frac{2\beta^3J^3m^2(1-m^2)^2}{3}\\&-\frac{\beta^4J^4(1-m^2)^2(1+6m^2-15m^4)}{12}\\&+\frac{2\beta^5J^5m^2(1-m^2)^2(1-18m^2+21m^4)}{15}\\&+\frac{\beta^6J^6(1-m^2)^2(1+120m^4-420m^6+315m^8)}{45}\\&+\frac{4\beta^7J^7m^2(1-m^2)^2(1-180m^2+1410m^4-2700m^6+1485m^8)}{315}+\dots\bigg].\end{aligned} \qquad \text{(A2.7)}$$

Since each line in a diagram corresponds to one power of βJ, it is easy to match the terms in equation (A2.7) with the appropriate two-site diagrams.

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