How to Compute Loop Corrections to Bethe Approximation

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Abstract

We introduce a method for computing corrections to Bethe approximation for spin models on arbitrary lattices. Unlike cluster variational methods, the new approach takes into account fluctuations on all length scales.

The derivation of the leading correction is explained and applied to two simple examples: the ferromagnetic Ising model on d-dimensional lattices, and the spin glass on random graphs (both in their high-temperature phases). In the first case we rederive the well-known Ginzburg criterion and the upper critical dimension. In the second, we compute finite-size corrections to the free energy.

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1 Introduction

Mean field approximations are the among the most frequently used tools in Statistical Physics. Among them, Bethe approximation (BA) [1] allows to treat with reasonable accuracy a large variety of lattice models. Recently it has been successfully applied (in an algorithmic form) to problems of inference [2–4], communications [5], and combinatorial optimization [6]. Often in these cases the underlying lattice has few or no short loops, and BA (which is exact on trees) can become exact in the thermodynamic limit.

BA can be systematically improved using Kikuchi [7] or cluster variational methods (CVM). These approaches take into account 'exactly' of correlations up to some finite range r and their complexity grows exponentially with r. Because of this feature, they are unsuited for understanding the effect of long length scale fluctuations. Furthermore, in lattices without short loops, no improvement is obtained unless r is very large (which is of course unfeasible).

For models on d-dimensional lattices, mean field can be also regarded as the zeroth order term in a $1/d$ expansion.[1] Such an expansion is however close in spirit to CVM, in that it keeps into account only the effect of short loops in the lattice [8].

In the field-theoretical setting [9, 10], mean field approximation is usually derived by retaining only tree-level Feynman diagrams. The usual loop expansion improves systematically over such an approximation by taking into account of fluctuations on all length scales order-by-order in a properly defined coupling parameter. When resummed using renormalization-group ideas, it gives an accurate description of many critical phenomena.

Often a simple (and correct) field-theoretical formulation of the problem is hard to derive. This is the case, for instance, of problems with quenched disorder, where one usually invoke the replica trick for averaging over the disorder [10]. Also, field theoretical methods are usually unreliable for computing non-universal quantities. These can be on the other hand important for some of the applications (inference, communications, optimization) mentioned above. In this paper we present an approach for computing corrections to BA coming from fluctuations on all length scales.

To be concrete, we shall focus on spin models with pairwise interactions on general graphs, with Hamiltonian

$$E(\sigma) = -\sum_{(ij)\in\mathcal{G}} J_{ij}\sigma_i\sigma_j - \sum_{i=1}^{N} H_i\sigma_i\,. \tag{1.1}$$

Here $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is a graph with vertex set $\mathcal{V} = \{1, \dots, N\}$ and edges $\mathcal{E} \ni (i, j)$, $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$. The set of neighbors of the site i is noted ∂i. We shall use the letters $a, b, \dots$ to denote generic edges, and, whenever necessary write $(i_a, j_a) = a$. Finally, for any set of vertices $A \in \mathcal{V}$, $\sigma_A \equiv \{\sigma_i : i \in A\}$. Several families of graphs and choices of the couplings J_{ij}, H_i will be considered in Section 3, but for the time being we shall remain completely general.

The Bethe approximation for such a model [11] is better described by introducing a field $h_i^{(j)}$ for each directed link $i \to j$ of $\mathcal{G}$. Such fields are required to satisfy the

[1] Generally, BA takes into account exactly also the first $1/d$ correction.

equations

$$h_i^{(j)} = H_i + \sum_{l\in\partial i\setminus j} u_{J_{ij}}(h_l^{(i)})\, , \qquad u_J(h) \equiv \frac{1}{\beta}\,\text{atanh}[\tanh(\beta J)\tanh(\beta h)]\, . \tag{1.2}$$

Once a solution of these equations is found, one can use the fields $h_i^{(j)}$ to estimate the thermal average of local operators. For instance

$$\langle\sigma_i\rangle \overset{\text{Bethe}}{=} \frac{1}{w_i}\sum_{\sigma=\pm 1}\sigma\,\exp(\beta H_i\sigma)\prod_{j\in\partial i}\frac{e^{\beta u(J_{ij},h_j^{(i)})\sigma}}{2\cosh(\beta u(J_{ij},h_j^{(i)}))}\, , \tag{1.3}$$

$$w_i = \sum_{\sigma=\pm 1}\exp(\beta H_i\sigma)\prod_{j\in\partial i}\frac{e^{\beta u(J_{ij},h_j^{(i)})\sigma}}{2\cosh(\beta u(J_{ij},h_j^{(i)}))}\, . \tag{1.4}$$

The basic approximation involved in derived these equations is the following. Consider a spin σ_i and set its interaction with the neighbors to 0: $J_{ij} = 0$ for all $j \in \partial i$ (in other words σ_i is 'removed' from the system). Now look at the joint probability distribution of the neighboring spins $\sigma_{\partial i}$ in the system without σ_i. Bethe approximation amount to saying that

$$P_i(\sigma_{\partial i}) \overset{\text{Bethe}}{=} \prod_{j\in\partial i}\frac{e^{\beta h_j^{(i)}\sigma_j}}{2\cosh\beta h_j^{(i)}},\, . \tag{1.5}$$

Our approach consists in deriving a set of exact equations for the 'cavity' distributions $P_i(\,\cdot\,)$'s. When the form (1.5) is plugged in these equations, the Bethe equations (1.2) are derived. Corrections are computed by introducing correlations in $P_i(\sigma_{\partial i})$.

In Section 2 we shall explain the general method for computing corrections to BA. We then use it in Section 3 for computing the leading corrections to BA for two particular examples: the ferromagnet on cubic d-dimensional lattices and the spin glass on random graphs.

2 The general approach

In order to explain the general computation scheme, it is convenient to introduce some notation. We denote by $E^{(i)}(\sigma)$ a modified energy function in which the interactions between the spin i and its neighbors have been canceled. Analogously, $E^{(a)}(\sigma)$, with $a \in \mathcal{E}$, is the energy function modified by eliminating the interaction along the edge a. In formulae:

$$E^{(i)}(\sigma) = E(\sigma) + \sum_{j\in\partial i} J_{ij}\sigma_i\sigma_j\, , \qquad E^{(a)}(\sigma) = E(\sigma) + J_{i_a j_a}\sigma_{i_a}\sigma_{j_a}\, . \tag{2.1}$$

We denote by $\langle\,\cdot\,\rangle^{(i)}$ and $\langle\,\cdot\,\rangle^{(a)}$ the Boltzmann averages with respect to these modified energy functions. As in the introduction, $P_i(\sigma_{\partial i})$ the marginal distribution of the neighbors of i with respect to the system with energy $E^{(i)}(\sigma)$. Analogously, we define the distribution $P_a(\sigma_{i_a},\sigma_{j_a})$.

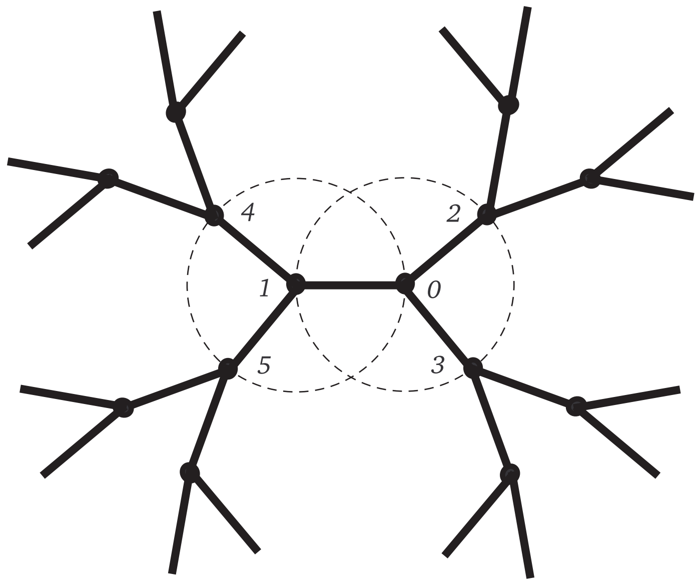

Figure 1: The magnetizations at site 0 and 1 in the absence of link J_{10} can be expressed in term of the correlations of the spins $0, 4, 5$ in the absence of spin 1 or of the correlations between spins $1, 2, 3$ in the absence of spin 0, the equality of the results yields the cavity equations.

In order to have a concrete representation for the distributions $P_i(\sigma_{\partial i})$, we shall use the correlation functions

$$\tilde{C}_{\mathcal{A}}^{(i)} \equiv \langle \prod_{j \in \mathcal{A}} \sigma_j \rangle^{(i)} = \sum_{\sigma_{\partial i}} P_i(\sigma_{\partial i}) \prod_{j \in \mathcal{A}} \sigma_j \,. \tag{2.2}$$

for any non-empty subset $\mathcal{A} \in \partial i$. In the special case $\mathcal{A} = \{j\}$ we shall also use the more conventional notation $M_j^{(i)} = \tilde{C}_j^{(i)}$. In Bethe approximation, the distribution $P_i(\sigma_{\partial i})$ is assumed to be factorized, cf. Eq. (1.5). In order to compute corrections, it is convenient to introduce the connected correlation functions $C_{\mathcal{A}}^{(i)}$. We have the usual relation

$$\tilde{C}_{\mathcal{A}}^{(i)} = \sum_{[\mathcal{A}_1 \ldots \mathcal{A}_n]} C_{\mathcal{A}_1}^{(i)} \cdots C_{\mathcal{A}_n}^{(i)} \,, \tag{2.3}$$

with $[\mathcal{A}_1, \ldots, \mathcal{A}_n]$ running over the partitions of $\mathcal{A}$. Finally $C^{(i)} \equiv \{C_{\mathcal{A}}^{(i)} : \mathcal{A} \subseteq \partial i\}$.

Let us now derive the basic relation between the $P_i(\,\cdot\,)$'s to be exploited in the following. Consider two sites i and j which are joined by an edge in $\mathcal{G}$. We can construct the distribution $P_{(ij)}(\sigma_i, \sigma_j)$ in two ways:

$$P_{(ij)}(\sigma_i, \sigma_j) = \frac{1}{Z_j} \sum_{\sigma_{\partial j \setminus i}} P_j(\sigma_{\partial j}) \exp\Big\{\beta H_j \sigma_j + \beta \sum_{l \in \partial j \setminus i} J_{jl} \sigma_j \sigma_l\Big\} \,, \tag{2.4}$$

and the equivalent one (let us call $P'_{ij}(\sigma_i, \sigma_j)$ the corresponding expression) which is obtained by interchanging i and j. Here Z_j is a constant which ensures the correct normalization of $P_{(ij)}(\sigma_i,\sigma_j)$. We can now marginalize the right hand side of Eq. (2.4) with respect to σ_j (to σ_i) in order to compute the magnetizations on site i (site j) with respect to the system with energy function $E^{(ij)}(\sigma)$. The same calculation can be performed using the expression $P'_{(ij)}(\sigma_i,\sigma_j)$. Since the result of these two calculations must be the same, we obtain two equations of the form:

$$\mathbf{B}_j^{(i)}(C^{(i)}) = \mathbf{K}_i^{(j)}(C^{(j)})\,, \qquad \mathbf{K}_j^{(i)}(C^{(i)}) = \mathbf{B}_i^{(j)}(C^{(j)})\,. \tag{2.5}$$

The function $\mathbf{B}_j^{(i)}(\,\cdot\,)$ yields the magnetization at site j when the distribution $P_i(\sigma_{\partial i})$ is modified through the addition of the interactions J_{il}, $l \neq j$. Analogously, $\mathbf{K}_j^{(i)}(\,\cdot\,)$ yields the magnetization at site i for the same system. Elementary algebraic manipulations yields the explicit expressions:

$$\mathbf{B}_j^{(i)}(C) = \frac{\sum_{\mathcal{A}\,\mathrm{even}} t_{\mathcal{A}}\tilde{C}_{\mathcal{A}\cup j} + t(H_i)\sum_{\mathcal{A}\,\mathrm{odd}} t_{\mathcal{A}}\tilde{C}_{\mathcal{A}\cup j}}{\sum_{\mathcal{A}\,\mathrm{even}} t_{\mathcal{A}}\tilde{C}_{\mathcal{A}} + t(H_i)\sum_{\mathcal{A}\,\mathrm{odd}} t_{\mathcal{A}}\tilde{C}_{\mathcal{A}}}\,, \tag{2.6}$$

$$\mathbf{K}_j^{(i)}(C) = \frac{t(H_i)\sum_{\mathcal{A}\,\mathrm{even}} t_{\mathcal{A}}\tilde{C}_{\mathcal{A}} + \sum_{\mathcal{A}\,\mathrm{odd}} t_{\mathcal{A}}\tilde{C}_{\mathcal{A}}}{\sum_{\mathcal{A}\,\mathrm{even}} t_{\mathcal{A}}\tilde{C}_{\mathcal{A}} + t(H_i)\sum_{\mathcal{A}\,\mathrm{odd}} t_{\mathcal{A}}\tilde{C}_{\mathcal{A}}}\,, \tag{2.7}$$

where the sums over $\mathcal{A}$ run over all the subsets of neighbors of i, $\mathcal{A} \in \partial i$, which do not include j. Furthermore, we used the shorthands $t_{\mathcal{A}} \equiv \prod_{l\in\mathcal{A}} t_{il}$, $t_{il} \equiv \tanh(\beta J_{il})$ and $t(H_i) \equiv \tanh(\beta H_i)$. The above functions can be written in terms of the connected correlations $C_{\mathcal{A}}^{(i)}$ by using the relation (2.3).

Consider for instance the case depicted in Fig. 1 where $i = 0$ and $j = 1$ have both degree 3. We furthermore assume, for the sake of simplicity, $H_0 = H_1 = 0$. Then

$$\mathbf{B}_1^{(0)}(C^{(0)}) = M_1^{(0)} + t_{02}t_{03}\,\frac{C_{21}^{(0)}M_3^{(0)} + C_{31}^{(0)}M_2^{(0)} + C_{123}^{(0)}}{1 + t_{02}t_{03}M_2^{(0)}M_3^{(0)} + t_{02}t_{03}C_{23}^{(0)}}\,, \tag{2.8}$$

$$\mathbf{K}_1^{(0)}(C^{(0)}) = \frac{t_{02}M_2^{(0)} + t_{03}M_3^{(0)}}{1 + t_{02}t_{03}M_2^{(0)}M_3^{(0)} + t_{02}t_{03}C_{23}^{(0)}}\,. \tag{2.9}$$

The analogous expressions for $\mathbf{B}_0^{(1)}(C^{(1)})$ and $\mathbf{K}_0^{(1)}(C^{(1)})$ are obtained by interchanging $0 \leftrightarrow 1$ and $\{2,3\} \leftrightarrow \{4,5\}$. It is therefore easy to write explicitly the equation $\mathbf{B}_0^{(1)}(C^{(1)}) = \mathbf{K}_1^{(0)}(C^{(0)})$:

$$M_0^{(1)} + t_{14}t_{15}\,\frac{C_{40}^{(1)}M_5^{(1)} + C_{50}^{(1)}M_4^{(1)} + C_{045}^{(1)}}{1 + t_{14}t_{15}M_4^{(1)}M_5^{(1)} + t_{14}t_{15}C_{45}^{(1)}} = \frac{t_{02}M_2^{(0)} + t_{03}M_3^{(0)}}{1 + t_{02}t_{03}M_2^{(0)}M_3^{(0)} + t_{02}t_{03}C_{23}^{(0)}}\,.$$

There are $2|\mathcal{E}|$ equations of the form (2.5): one for each directed link in the graph. The number of unknowns is, on the other hand $\sum_i (2^{|\partial i|} - 1)$, with the sum running over the sites of the graph, and $|\partial i|$ being their connectivity. Therefore, these equations are not sufficient to determine the correlation functions $C^{(i)}$. If, on the other hand, we neglect multi-spin connected correlation functions and only retain the cavity magnetizations $M_j^{(i)}$ (as in Bethe approximation), we are left with $2|\mathcal{E}|$

variables to determine. In this case Eqs. (2.6) and (2.7) are considerably simplified:

$$\mathbf{B}_j^{(i)}(C^{(i)}) \stackrel{\text{Bethe}}{=} M_j^{(i)}\,, \tag{2.10}$$

$$\mathbf{K}_j^{(i)}(C^{(i)}) \stackrel{\text{Bethe}}{=} \tanh\left\{\beta H_i + \sum_{k\in\partial i\setminus j} \operatorname{atanh}\left[t_{ik}M_k^{(i)}\right]\right\}. \tag{2.11}$$

By setting $M_j^{(i)} = \tanh\beta h_j^{(i)}$, it is easy to see that the equations (2.5) are in this case the Bethe equations[2] (1.2). If, for instance, $\mathcal{G}$ is a tree, the connected cavity correlations $C_{\mathcal{A}}^{(i)}$ vanish if $|\mathcal{A}|\geq 2$. We thus proved recovered the well-known result that Bethe approximation is exact on tree graphs.

We want now to estimate the connected cavity correlations $C_{\mathcal{A}}^{(i)}$, for $|\mathcal{A}|\geq 2$, and then use Eq. (2.5) to improve the calculation of $M_j^{(i)}$. In synthesis, the correlations are estimated through the fluctuation-dissipation theorem:

$$\frac{1}{\beta^n}\frac{\partial^n M_{i_1}}{\partial H_{i_2}\cdots\partial H_{i_{n+1}}} = C_{i_1\cdots i_{n+1}}\,, \tag{2.12}$$

where $i_1\dots i_{n+1}$ are $n+1$ distinct index sites. Here M_i and $C_{i_1\cdots i_{n+1}}$ are magnetizations and correlations with respect to an arbitrary Hamiltonian of the form (1.1). In other terms, one can obtain equations for the correlations by taking appropriate derivatives of the exact equations (2.5) with respect to an external field.[3]

For, the sake of clarity, let us compute the leading-order correction to BA. We neglect all connected cavity correlation functions $C_{\mathcal{A}}^{(i)}$ with $|\mathcal{A}|\geq 3$. Moreover, we treat two point correlation functions to the linear order. To this order, the expressions (2.6) and (2.7) become

$$\mathbf{B}_j^{(i)}(C) = M_j^{(i)} + \sum_{l\in\partial i\setminus j}\Omega_{j,l}^{(i)}\,t_{il}C_{jl}^{(i)} + O(C^2)\,, \tag{2.13}$$

$$\mathbf{K}_j^{(i)}(C) = T_j^{(i)} + \sum_{(l_1,l_2)\in\partial i\setminus j}\Gamma_{j,l_1l_2}^{(i)}t_{il_1}t_{il_2}C_{l_1l_2}^{(i)} + O(C^2)\,, \tag{2.14}$$

where

$$\Omega_{j,l}^{(i)} = \frac{T_{jl}^{(i)}}{1+t_{il}M_l^{(i)}T_{jl}^{(i)}}\,, \tag{2.15}$$

$$\Gamma_{j,l_1l_2}^{(i)} = \frac{T_{jl_1l_2}^{(i)} - T_j^{(i)}}{1+t_{il_1}t_{il_2}M_{l_1}^{(i)}M_{l_2}^{(i)} + t_{il_1}M_{l_1}^{(i)}T_{jl_1l_2}^{(i)} + t_{il_2}M_{l_2}^{(i)}T_{jl_1l_2}^{(i)}}\,, \tag{2.16}$$

and

$$T_{l_1l_2\dots}^{(i)} = \tanh\left\{\beta H_i + \sum_{k\in\partial i\setminus l_1,l_2\dots}\operatorname{atanh}\left[t_{ik}M_k^{(i)}\right]\right\}. \tag{2.17}$$

[2]This derivation of BA is in fact mentioned as a side remark in Ref. [12].

[3]One can see that the differentiation procedure is well-defined through the following (numerically imprecise but conceptually simple) implementation. Compute the magnetization M_i, then change slightly the external field on site j, $H_j \to H_j + \delta H_j$, and evaluate the correlation function between sites i and j as $C_{ij} = \lim_{\delta H_j\to 0}(\delta M_i/\beta\delta H_j)$. Higher-order correlations are computed analogously by considering variations of the external fields at several points.

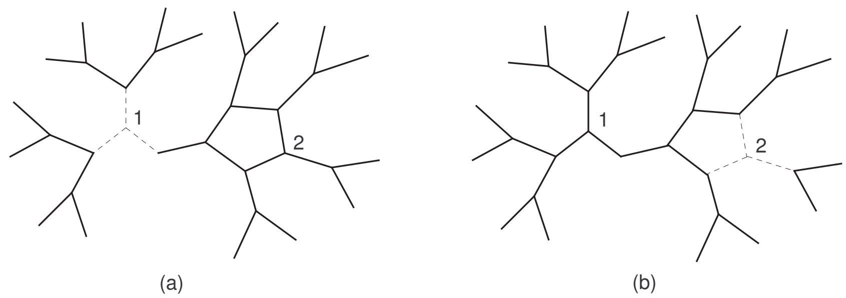

Figure 2: Graph $\mathcal{G}$ with a single loop. The first-order procedure described in the text is exact on such a model. This claim can be proved by considering two type cavities (a) and (b).

We can therefore proceed as follows. First solve the Bethe equations (1.2) for the original energy function (1.1). Then, for each site $i \in \mathcal{V}$, consider the energy function $E^{(i)}(\sigma)$ corresponding to the spin σ_i being removed. Compute the two point connected correlation functions in the reduced system $C^{(i)}_{j_1 j_2}$ using BA together with the fluctuation-dissipation relations (2.12). Finally write

$$M^{(i)}_j = \tanh(\beta h^{(i)}_j) + \Delta M^{(i)}_j + O(C^2)\,. \tag{2.18}$$

The first order corrections $\Delta M^{(i)}_j$ are computed by expanding the equations (2.5) up to first order in C. Using the expansion (2.13), (2.13), we get

$$\Delta M^{(i)}_j + \sum_{l\in\partial i\setminus j} t_{il}\Omega^{(i)}_{j,l} C^{(i)}_{jl} = \sum_{k\in\partial j\setminus i} Q^{(j)}_{i,k}\,\Delta M^{(j)}_k + \sum_{(l_1,l_2)\in\partial j\setminus i} \Gamma^{(j)}_{i,l_1 l_2} t_{jl_1} t_{jl_2} C^{(j)}_{l_1 l_2}\,. \tag{2.19}$$

where

$$Q^{(j)}_{i,k} = \frac{t_{jk}[1-(T^{(j)}_i)^2]}{1-(t_{jk}\tanh(\beta h^{(j)}_k))^2}\,\Delta M^{(j)}_k \tag{2.20}$$

Here the coefficients $\Omega^{(i)}_{j,l}$ and $\Gamma^{(j)}_{i,l_1 l_2}$ are computed through Eqs (2.15) and (2.16) by setting $M^{(l)}_k \to \tanh(\beta h^{(l)}_k)$. We thus obtained one equation of the form (2.19) for each directed edge in the lattice. These completely determine the $\Delta M^{(i)}_j$.

It is important to stress that the above procedure is not uniquely defined. One could consider equivalent calculations which differ from the above by higher order corrections. Here are two examples:

1. One could compute the connected cavity correlations without removing the spin i from the system but rather using the relation

$$C^{(i)}_{jl} = (1-\tanh^2\beta h^{(i)}_j)\,\beta\frac{\partial h^{(i)}_j}{\partial H_l}\,, \tag{2.21}$$

which in turns follows from $M^{(i)}_j = \tanh\beta h^{(i)}_j$. Equations for $\frac{\partial h^{(i)}_j}{\partial H_l}$ are easily obtained by differentiating Eq. (1.2).

2. Instead of expanding the equations (2.5) to the first order in $C^{(i)}_{jl}$ and $\Delta M^{(i)}_j$, one could proceed as follows. Set to zero all the correlation functions $C^{(i)}_{\mathcal{A}}$, $|\mathcal{A}| \geq 3$, replace $C^{(i)}_{jl}$ by their Bethe approximation, and solve for $M^{(i)}_j$.

In particular, the last implementation is exact whenever the graph $\mathcal{G}$ contains (at most) a unique loop (thus improving over BA). Since the equations (2.5) are exact, in order to prove this claim it is enough to show that the procedure defined above computes correctly the correlation functions $C^{(i)}_{\mathcal{A}}$, $|\mathcal{A}| \geq 2$. If $|\mathcal{A}| \geq 3$ and $\mathcal{G}$ has a single loop, then $C^{(i)}_{\mathcal{A}} = 0$, and the algorithm does not make any error in neglecting these correlations. Consider now the computation of $C^{(i)}_{l_1 l_2}$ and distinguish two cases. In the first case, the graph obtained by removing the vertex i is a tree (as e.g. for site 1 in Fig. 2). Therefore BA is exact for the energy function $E^{(i)}(\sigma)$ and correctly computes the correlations $C^{(i)}_{l_1 l_2}$. In the second case upon removing site i, the resulting graph, let us call it $\mathcal{G}\backslash i$, still contains a loop (as for site 2 in Fig. 2). Notice that $\mathcal{G}\backslash i$ is disconnected, and each of the neighbors of i belongs to a distinct connected component. Therefore $C^{(i)}_{j_1 j_2} = 0$ for any two neighbors j_1, j_2 of i. While BA is not exact for $\mathcal{G}\backslash i$, it is easy to see that it correctly gives yields vanishing correlations among sites belonging to different connected components.

At this point it should be clear how to improve the above first-order scheme. After removing the spin i, one can compute the correlations $C^{(i)}_{\mathcal{A}}$ within the first order scheme rather than Bethe approximation (and retain three points correlation as well) and then recompute the magnetizations $M^{(i)}_j$ using Eq. (2.5).

The general procedure can be explained as a recursive pseudocode. The code makes use of a routine `Correlation(` $\mathcal{G}$, $E(\cdot)$, $\{C^{(i)}\}$ `)` which takes as input a graph $\mathcal{G}$, an Hamiltonian $E(\cdot)$ of the form (1.1), an estimation of the n-points cavity correlations $\{C^{(i)}\}$ for any $i \in \mathcal{G}$. The output consists of a new estimation of all n-points correlation functions. This is obtained (let's repeat ourselves) by a joint solution of Eqs. (2.5) and (2.12). A particular case of the routine `Correlation(` $\cdot$ `)` is obtained when all the multi-point cavity correlations $\{C^{(i)}\}$ are set to 0. This corresponds of course to BA. For the sake of clarity, we shall denote the corresponding routine `Bethe(` $\mathcal{G}$, $E(\cdot)$ `)` instead of `Correlation(` $\mathcal{G}$, $E(\cdot)$, `0 )`.

The recursive routine, `Loop()`, takes as input a graph $\mathcal{G}$, an Hamiltonian of the form (1.1), and the order of approximation ℓ to be achieved. The output consists of an estimation of all n-points connected correlation functions in the system.

```
Loop( G, E(·), ℓ )
If (ℓ == 1) Output Bethe( G, E(·) )
Else
    For (i ∈ V) C^(i) := Loop( G\i, E^(i)(·), ℓ − 1 )
    Output Correlation(  G, E(·), {C^(i)} )
End
```

Let us stress that this algorithm deals with particular samples of the model, without need for an average over disorder realizations. Its complexity is (for graphs with bounded connectivity) $O(N^\ell)$, i.e. polynomial for any fixed ℓ. This makes its application to inference/optimization problems a viable research direction. The algorithm implements the strategy 2 above (actual elimination of a site): arguing as above, it can be proved that by induction that `Loop( ·, ·, ℓ )` is exact on graphs with cyclic number not larger than ℓ.

3 Applications

In this Section we apply the method developed so far to two simple problems: the spin glass on random graphs with general connectivity distributions, and the ferromagnetic Ising model on the cubic d-dimensional lattice. In both examples we will keep ourselves to the high temperature, no external field phase. The precise nature of the corrections computed within our approach is different for these two applications. In the first case, they correspond to higher orders in the loop expansion. While there is no formal parameter to order the loop expansion for the Ising model on cubic lattices, we are able to recover the well known Ginzburg criterion and the associated one-loop integral. In the second one, successive terms in our expansion correspond to higher powers in $1/N$ (N being the number of spins).

3.1 Ising model on the cubic lattice

We take $\mathcal{G}$ to be the d–dimensional cubic lattice, i.e. $\mathbb{Z}^d$ with edges joining neighboring vertices. Vertices of the lattices will be denoted in this Section by $x, y, z, \dots \in \mathbb{Z}^d$, while unit vectors by $\mu, \nu, \dots \in \{(1,0,\dots),(0,1,\dots),\dots\}$. We consider the usual Ising ferromagnet, i.e. $J_{xy} = 1$ and $H_x = H$.

Because of translational invariance, the Bethe equations admit an uniform solution $h_y^{(x)} = h$, with h solving

$$h = H + \frac{(2d-1)}{\beta}\,\text{atanh}[\tanh\beta\tanh\beta h]\,. \tag{3.1}$$

Analogously, the cavity magnetizations do not depend on the site: $M_j^{(i)} = M^{\text{cav}}$, and we have $M^{\text{cav}} = \tanh\beta h + \Delta M^{\text{cav}} + O(C^2)$. In order to write the results in a compact form, it is convenient to introduce the field

$$h_p \equiv H + \frac{p}{\beta}\,\text{atanh}[\tanh\beta\tanh\beta h]\,. \tag{3.2}$$

We shall furthermore use the shorthand $t \equiv \tanh\beta$. After some tedious but straightforward calculations, Eq. (2.19) yields

$$\Delta M^{\text{cav}} = -\frac{A}{B}\sum_{(\mu,\nu)} C^{(0)}_{\mu,\nu}\,, \tag{3.3}$$

where

$$A = \frac{1}{d}\,\frac{t\,\tanh\beta h_{2d-2}}{(1+t\tanh\beta h\tanh\beta h_{2d-2})(1-\tanh^2\beta h)} + \frac{d-1}{d}\,\frac{2t^3\tanh\beta h}{1-t^2\tanh^2\beta h}\,, \tag{3.4}$$

$$B = \frac{1}{1-\tanh^2\beta h} - (2d-1)\,\frac{t}{1-t^2\tanh^2\beta h}\,. \tag{3.5}$$

Using these expressions, we can compute the (non-cavity) magnetization $M = \langle \sigma_x \rangle$

$$M = M_0 + M_1 \sum_{(\mu,\nu)} C^{(0)}_{\mu,\nu} + O(C^2)\,, \tag{3.6}$$

$$M_0 = \tanh \beta h_{2d}\,, \tag{3.7}$$

$$M_1 = t^2 \frac{\tanh \beta h_{2d-2} - \tanh \beta h_{2d}}{1 + t^2 \tanh^2 \beta h + 2t \tanh \beta h \tanh \beta h_{2d-2}} - 2dt\, \frac{1 - \tanh^2 \beta h_{2d}}{1 - t^2 \tanh^2 \beta h} \frac{A}{B}\,. \tag{3.8}$$

By taking the $H \to 0$ limit, we can compute the zero field susceptibility defined by $M = \chi H + O(H^2)$. This admits the expansion $\chi = \chi_0 + \chi_1 \sum_{(\mu,\nu)} C^{(0)}_{\mu,\nu} + O(C^2)$, where

$$\chi_0 = \beta\, \frac{1+t}{1-(2d-1)t}\,, \qquad \chi_1 = -2\,\beta\, \frac{t^2(1-t^2)}{[1-(2d-1)t]^2}\,. \tag{3.9}$$

We are left with the task of computing the parameter $\overline{C} \equiv \sum_{(\mu,\nu)} C^{(0)}_{\mu,\nu}$. We will follow the strategy 1 described in the previous Section. By differentiating the Bethe equations, we get

$$\frac{\partial h_x^{(x+\mu)}}{\partial H_z} = \delta_{x,z} + t\, \frac{1 - \tanh^2 \beta h}{1 - t^2 \tanh^2 \beta h} \sum_{\nu(\neq \mu)} \frac{\partial h^{(x)}_{x+\nu}}{\partial H_z}\,. \tag{3.10}$$

Using the fluctuation-dissipation relation (2.21) and translation invariance, we get the following equation for the cavity correlations

$$C^{(0)}_{z,-\mu} = q \delta_{z,-\mu} + r \sum_{\nu(\neq\mu)} C^{(0)}_{z+\mu,\nu}\,, \tag{3.11}$$

$$q \equiv 1 - \tanh^2 \beta h\,, \qquad r \equiv \frac{t}{1 - t^2 \tanh^2 \beta h}\,. \tag{3.12}$$

These equations are easily solved by introducing the Fourier transform

$$C^{(0)}_\mu(p) = \sum_x e^{ipx} C^{(0)}_{x,\mu}\,, \qquad C^{(0)}_{x,\mu} = \int \frac{\mathrm{d}^d p}{(2\pi)^d}\, C_\mu(p)\, e^{-ipx}\,, \tag{3.13}$$

where the integral over p runs over the Brillouin zone $[-\pi,\pi]^d$. We obtain

$$C_\mu(p) = \frac{q(e^{ip\mu} - r)}{1 - 2dr + (2d-1)r^2 + r\hat{p}^2}\,, \tag{3.14}$$

where $\hat{p}^2 \equiv 2d - \sum_\mu e^{ip\mu}$. Therefore the correlation parameter entering in the corrections to BA is

$$\overline{C} = -\frac{q}{2r^2} + \frac{(1-r^2)q}{2r^2} \int \frac{\mathrm{d}^d p}{(2\pi)^d}\, \frac{1}{1 - 2dr + (2d-1)r^2 + r\hat{p}^2}\,. \tag{3.15}$$

A simple application of the above calculation consists in computing the critical temperature. We can do this by solving the equation $\chi^{-1} = 0$, which to this order implies

$$1 - (2d-1)\tanh^2 \beta_{\rm c} + 2 \tanh^2 \beta_{\rm c} (1 - \tanh \beta_{\rm c}) \overline{C} = 0\,, \tag{3.16}$$

d	$\beta_{\rm c}^{\rm num}$	$\beta_{\rm c}^{\rm new}$	$\beta_{\rm c}^{1/d}$
3	0.221654(6) [13]	0.237708	0.207407
4	$0.1497^{\dagger}$ [14]	0.151650	0.145833
5	0.11388(3) [15]	0.114356	0.112592
6	$*$	0.092446	0.091750

Table 1: Critical temperature for the Ising model on d–dimensional cubic lattices as determined by numerical simulations, the new expansion presented in this paper, and second order $1/d$ expansion. The numerical result for $d = 4$ is quoted in Ref. [14] without statistical errors. A more accurate estimate $\beta_{\rm c} = 0.14966(3)$ was obtained from high temperature expansion in Ref. [16].

By solving this equation to the first order in $\overline{C}$, we get

$$\tanh \beta_{\rm c} = \frac{1}{2d-1} - \frac{2d-2}{(2d-1)^3}[(2d-1) - 2d(2d-2)I_d]\,, \tag{3.17}$$

$$I_d \equiv \int \frac{{\rm d}^d p}{(2\pi)^d}\,\frac{1}{\hat{p}^2} = \int_0^\infty [e^{-2t} I_0(2t)]^d\,, \tag{3.18}$$

where $I_0(\,\cdot\,)$ is the Bessel function. The integral I_d is convergent for $d > 2$. A numerical calculation of I_d yields the values of $\beta_{\rm c}$ reported in Table 1. This is compared with numerical simulations and with the second order $1/d$ expansion

$$\beta_{\rm c}^{1/d} = \frac{1}{2d-1}\left[1 + \frac{1}{3d^2} + O(d^{-3})\right]. \tag{3.19}$$

We can also derive the critical behavior of the susceptibility. From Eq. (3.9) we get $\beta\chi^{-1} = K\,(\beta_{\rm c} - \beta) + O((\beta_{\rm c} - \beta)^2)$ where

$$K = 2d - \left\{\frac{2d}{2d-1} - \frac{4d(2d-2)(2d^2-d+1)}{(2d-1)^2}\,I_d + \frac{4d^2(2d-2)^2}{(2d-1)^2}\,J_d\right\}, \tag{3.20}$$

$$J_d \equiv \int \frac{{\rm d}^d p}{(2\pi)^d}\,\frac{1}{(\hat{p}^2)^2} = \int_0^\infty t\,[e^{-2t} I_0(2t)]^d\,. \tag{3.21}$$

The integral J_d is infrared divergent for $d \le 4$. We have therefore rederived the well known upper-critical dimension $d_{\rm up} = 4$.

3.2 Spin glass on random graphs

We consider here the case in which $\mathcal{G}$ is an Erdös-Renyi random graph with N vertices and average connectivity γ. Such a graph is constructed by drawing an edge between any couple (i,j) of distinct vertices independently with probability γ/N. Spins joined by an edge interact via a coupling J_{ij} which are i.i.d. symmetric random variables with probability density function $p(J) = p(-J)$. This is also known as the Viana-Bray model and was first studied in Ref. [17]. In the following $\mathbb{E}$ will denote expectation with respect to the couplings and/or the graph realization. Finally we shall focus on the case of vanishing external field $H_i = 0$.

The interest of such a simple model is that it can be easily treated by the replica method, thus providing an useful check of our approach.[4] Before applying the strategy outlined in the previous Section, let us briefly recall the replica results. Averaging over disorder, one gets the following representation for the moments of the partition function [20]

$$\mathbb{E}\, Z^n = \int \exp\{-NS[c]\}\, \mathcal{D}c\,, \tag{3.22}$$

where $c(\vec{\sigma}) = c(\sigma^1,\dots,\sigma^n)$, $\sigma^a \in \{\pm 1\}$ is the replica order parameter. The integral is then evaluated using the saddle point method, the paramagnetic saddle point being $c(\vec{\sigma}) = 1/2^n$. The free energy density $\beta f_N(\beta) = -(1/N)\mathbb{E}\,\log Z_N$ is then obtained by taking the $n \to 0$ limit:

$$\beta f_N(\beta) = -\log 2 - \frac{\gamma}{2}\mathbb{E}\,\log\cosh\beta J + \frac{1}{N}\,\beta f^{(1)} + O(N^{-2})\,, \tag{3.23}$$

$$\begin{aligned}\beta f^{(1)} &= -\frac{1}{2}\,\gamma^2\,\mathbb{E}\log\cosh\beta J + \frac{1}{4}\gamma^2\,\mathbb{E}\log\cosh\beta(J_1+J_2)\\ &\quad -\frac{1}{2}\sum_{k=1}^{\infty}\frac{\gamma^k}{k}\,\mathbb{E}\log\big\{1+\prod_{i=1}^{k}\tanh\beta J_i\big\}.\end{aligned} \tag{3.24}$$

Here expectations are taken with respect to the $J_1, J_2, \dots$ which are i.i.d. with distribution $p(J)$. The $O(1/N)$ term is the contribution of Gaussian fluctuations around this saddle point. As expected, it diverges upon approaching the spin glass critical temperature β_c (defined by $\gamma\,\mathbb{E}\,\tanh^2\beta_c J = 1$). More precisely we have

$$f^{(1)}(\beta) = -\frac{1}{4}\log(\beta_c - \beta) + O(1)\,. \tag{3.25}$$

We shall now rederive the above results by using the approach outlined in the previous Section. A serious shortcoming of this approach is that it does not provide an explicit expression for the free energy. One can circumvent this problem by considering the internal energy density $u_N(\beta) = \mathbb{E}\,E(\sigma)/N$. Since all the edges of the graph are equivalent,

$$u_N(\beta) = -\frac{N-1}{2N}\,\gamma\,\mathbb{E}\left\{J_{ij}\langle\sigma_i\sigma_j\rangle\,|\,(i,j)\in\mathcal{G}\right\}\,. \tag{3.26}$$

Here $\mathbb{E}\{\,\cdot\,|\,(i,j)\in G\}$ denotes expectation conditional to the edge (i,j) belonging to the graph $\mathcal{G}$. Consider now a particular graph $\mathcal{G}$ in which the link (i,j) is present. It is simple to show that

$$\langle\sigma_i\sigma_j\rangle = t_{ij} + (1-t_{ij}^2)\,\frac{C_{ij}^{(ij)}}{1+t_{ij}C_{ij}^{(ij)}}\,, \tag{3.27}$$

where $C_{ij}^{(ij)}$ denotes the correlation $\langle\sigma_i\sigma_j\rangle$ after link (i,j) has been removed (notice that local magnetizations $\langle\sigma_i\rangle$ vanish by symmetry), and $t_{ij} = \tanh\beta J_{ij}$. Notice that

[4] Some of the properties of the high temperature phase can be furthermore derived rigorously, see [18]. For ideas on $1/N$ corrections in the low temperature phase see [19].

sampling $\mathcal{G}$ under the condition $(i,j) \in \mathcal{G}$, and then removing (i,j) is equivalent (fro the Erdös-Renyi ensemble) to sampling $\mathcal{G}$ under the condition $(i,j) \notin \mathcal{G}$. Substituting in Eq. (3.26), we get

$$u_N(\beta) = -\frac{N-1}{2N}\,\gamma\,\mathbb{E}\{Jt_J\} - \frac{N-1}{2N}\,\gamma\,\mathbb{E}\left\{ J(1-t_J^2)\frac{C_{ij}}{1+t_J\,C_{ij}} \,\middle|\, (i,j)\notin\mathcal{G}\right\}\,, \quad (3.28)$$

where we used the shorthand $t_J = \tanh\beta J$. The second term vanishes as $N \to \infty$, since it behaves as the correlation between two uniformly random sites in the system. We will therefore estimate it to the leading non-trivial order. Moreover, we can expand $(1 + t_J\,C_{ij})^{-1}$ in an absolutely convergent series to get

$$\begin{aligned} u_N(\beta) = &-\frac{\gamma}{2}\,\mathbb{E}\{Jt_J\} + \frac{1}{N}\frac{\gamma}{2}\,\mathbb{E}\{Jt_J\} - \\ &-\frac{\gamma}{2}\sum_{k=0}^{\infty}(-1)^k\,\mathbb{E}\{J(1-t_J^2)t_J^k\}\,\mathbb{E}\{C_{ij}^{k+1}|\,(i,j)\notin\mathcal{G}\} + O(N^{-2})\,, \end{aligned} \quad (3.29)$$

where we factorized the expectation thanks to the fact that $\mathcal{G}$ does not contain (i,j) and therefore C_{ij} is independent of J.

We are left with the task of computing the moments of C_{ij}. According to our general strategy, we use the identity $C_{ij} = \frac{1}{\beta}\left.\frac{\partial M_i}{\partial H_j}\right|_{H=0}$. It is well known [11] that, for the Erdös-Renyi random graph, $M_l \overset{\mathrm{d}}{=} \tanh\beta h_i^{(j)}$ up to corrections vanishing as $N \to \infty$ (here $\overset{\mathrm{d}}{=}$ denoted equality in distribution). Furthermore, by differentiating Bethe equations (1.2) we get

$$\frac{\partial h_i^{(m)}}{\partial H_j} = \delta_{ij} + \sum_{l\in\partial i\setminus m}\tanh\beta J_{il}\,\frac{\partial h_l^{(i)}}{\partial H_j}\,. \quad (3.30)$$

By averaging over the graph and couplings and recalling that the degree of a site is, for large N, a Poisson random variable of mean γ, we obtain (here we use the shorthand ∂_j for partial derivative with respect to H_j):

$$\mathbb{E}\left\{\left(\partial_j h_i^{(m)}\right)^k\right\} \;=\; \frac{1}{N} + \gamma\,\mathbb{E}\{t_J^k\}\,\mathbb{E}\left\{\left(\partial_j h_l^{(i)}\right)^k\right\} + O(N^{-2})\,. \quad (3.31)$$

Moreover if we condition on i, j being distinct and not connected by an edge, the term δ_{ij} in Eq. (3.30) is surely missing for at least two iterations, leading to

$$\mathbb{E}\left\{\left(\partial_j h_i^{(m)}\right)^k \,\middle|\, i\neq j,\,(i,j)\notin\mathcal{G}\right\} \;=\; (\gamma\,\mathbb{E}\{t_J^k\})^2\,\mathbb{E}\left\{\left(\partial_j h_l^{(i)}\right)^k\right\} + O(N^{-2})\,. \quad (3.32)$$

By solving these equations and identifying $\mathbb{E}\{C_{ij}^{k+1}|\,(i,j)\notin\mathcal{G}\}$ with the left hand side of the last equation, we finally get

$$\mathbb{E}\{C_{ij}^k|\,(i,j)\notin\mathcal{G}\} = \frac{1}{N}\,\frac{(\gamma\,\mathbb{E}\{t_J^k\})^2}{1-\gamma\,\mathbb{E}\{t_J^k\}} + O(N^{-2})\,, \quad (3.33)$$

for k even (for k odd the expectation vanishes by symmetry. We can now plug this into Eq. (3.29) to get the final result

$$u_N(\beta) \;=\; -\frac{\gamma}{2}\,\mathbb{E}\{Jt_J\} + \frac{1}{N}\,u^{(1)}(\beta) + O(N^{-2})\,, \quad (3.34)$$

$$u^{(1)}(\beta) \;=\; \frac{\gamma}{2}\,\mathbb{E}\{Jt_J\} + \frac{\gamma}{2}\sum_{k\text{ odd}}\mathbb{E}\{J(1-t_J^2)t_J^k\}\,\frac{(\gamma\,\mathbb{E}\{t_J^{k+1}\})^2}{1-\gamma\,\mathbb{E}\{t_J^{k+1}\}}\,. \quad (3.35)$$

One can then compute the free energy density by integrating over the temperature with boundary condition $\beta f_N(\beta) \to -\log 2$ as $\beta \to 0$. It is easy to check that the resulting expression coincides with the replica result (3.23), (3.24).

One surprising feature of the above calculation is the behavior of correlations. One would naively assume that the correlation between two random spins is concentrated around a typical value of order $N^{-\delta}$, with $\delta > 0$, leading to $\mathbb{E}\{C_{ij}^k\} \sim N^{-k\delta}$, in contradiction with the correct result, Eq. (3.33). It is therefore interesting to study the distribution of C_{ij}. For the sake of simplicity we shall admit the cases $i = j$ and $(i, j) \in \mathcal{G}$ which where excluded in the above calculation. In the $N \to \infty$ limit, the correlations satisfy the same distributional equation as the response functions, cf. Eq (3.30):

$$C \stackrel{\mathrm{d}}{=} \sum_{i=1}^{k} (\tanh \beta J_i)\, C_i\,. \tag{3.36}$$

Here k is a Poisson random variable of mean γ and J_i are i.i.d. with distribution $P(J)$. Notice that this equation can only fix the distribution of C, to be denoted by $\rho(C)$, up to a scaling factor. In fact, if C is a random variable satisfying the above equation, also $a\,C$ does. We shall therefore write $\rho(C) = (1/C_0)\rho_*(C/C_0)$, where the solution $\rho_*(C)$ is fixed arbitrarily and $C_0 = C_0(N)$ is the typical scale of correlations in a system of size N. The scale C_0 will be determined by a matching procedure.

Consider the characteristic function $\phi(s) \equiv \int \exp(isC)\, \mathrm{d}\rho_*(C)$. This satisfies the equation

$$\phi(s) = \exp\{-\gamma[1 - \mathbb{E}\, \phi(ts)]\}\,, \tag{3.37}$$

where expectation is taken with respect to $t = \tanh \beta J$. From this is easy to derive the small s behavior $\phi(s) \simeq 1 - \phi_0 |s|^\alpha$ where we can fix the freedom in the scale of C by setting $\phi_0 = 1$. The exponent α is determined by

$$\gamma\, \mathbb{E}\{|\tanh \beta J|^\alpha\} = 1\,. \tag{3.38}$$

Therefore α grows monotonously with β and takes the value $\alpha = 2$ at $\beta = \beta_{\mathrm{c}}$. The large C behavior of the correlations distribution is $\rho_*(C) \simeq (\frac{1}{\pi}\Gamma(1+\alpha)\sin(\frac{\pi\alpha}{2}))|C|^{-1-\alpha}$. The physical reason of this power law tail is easily understood. Consider the neighborhood of a site i. Asymptotically, this will be a random tree with Poisson degree distribution (a Galton-Watson tree). For a site j at distance r from i, we have $C_{ij} = \tanh \beta J_1 \cdots \tanh \beta J_r$, where $J_1, \dots, J_r$ are the couplings on the path joining i to j. If we only consider these sites and sum over all finite r as $N \to \infty$, we get

$$\rho_{\mathrm{neigh}}(C) = \frac{1}{N} \sum_{r=0}^{\infty} \gamma^r\, \mathbb{E}\; \delta\left(C - \prod_{i=1}^{r} \tanh \beta J_i\right)\,. \tag{3.39}$$

The small C asymptotics of this distribution is $\rho^{\mathrm{neigh}}(C) \simeq \rho_0^{\mathrm{neigh}}\, |C|^{-1-\alpha}$. By computing ρ_0^{neigh} and matching this behavior with the large C behavior of $\rho(C) = (1/C_0)\rho_*(C/C_0)$, we determine

$$C_0(N) = \left\{\frac{\pi}{\Gamma(1+\alpha)\sin\frac{\pi\alpha}{2}}\, \frac{1}{(-\gamma\mathbb{E}\,|t_J|^\alpha \log|t_J|)}\right\}^{1/\alpha} N^{-1/\alpha}\,, \tag{3.40}$$

where $t_J = \tanh \beta J$. As the temperature decreases from ∞ to the critical temperature, α increases from 0 to 2 and therefore the typical correlation scale increases from $N^{-\infty}$ to $N^{-1/2}$. However, correlations are never concentrated around a particular value but have a power-law behavior at all temperature. Integer moments are therefore governed by the largest correlations in the system (in particular they are ruled by $\rho^{\rm neigh}(C)$) and are always of order N^{-1}. Finally notice that, because of the power-law behavior, there is no definite loop length responsible for corrections to BA.

Let us conclude with a comment. One could have been skeptical about the success of the present approach in computing $1/N$ effects in for spin models on random graphs. In fact, an average fraction $1/N$ of spins of such systems lies in a neighborhood of finite-size loops (e.g. triangles). For such spins the violation of BA is non-perturbative and our approach could have seemed a priori hopeless. However, the exactness of our method for uni-cyclic graph allows to overcome this problem. On the other hand, it was crucial not to neglect terms of order $\mathbb{E}\{C_{ij}^{k+1}\}$, $k > 0$ in Eq. (3.29), i.e. to follow the procedure 2 described in Section 2.

The same kind of argument suggest that the systematic expansion described in Section 2 corresponds in fact to the $1/N$ expansion for random graphs. The next correction is due to couples of joined closed loops, an event occurring in average near a fraction $1/N^2$ of the sites.

Acknowledgments

While this paper was being completed, we discovered that Giorgio Parisi and František Slanina had been working at a similar loop expansion using a completely different approach [21]. We are grateful to them for letting us know about their results.

This work was supported by EVERGROW, i.p. No. 1935 in the complex systems initiative of the Future and Emerging Technologies directorate of the IST Priority, EU Sixth Framework.

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