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Minimizing dissatisfaction in colourful neighbourhoods

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Abstract

Colouring sparse graphs under various restrictions is a theoretical problem of significant practical relevance. Here we consider the problem of maximizing the number of different colours available at the nodes and their neighbourhoods, given a predetermined number of colours. In the analytical framework of a tree approximation, carried out at both zero and finite temperatures, solutions obtained by population dynamics give rise to estimates of the threshold connectivity for the incomplete to complete transition, which are consistent with those of existing algorithms. The nature of the transition as well as the validity of the tree approximation are investigated.

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1. Introduction

The spin glass theory of infinite-ranged models [1, 2] has inspired a generation of physicists to study many theoretically challenging and practically important problems in physics and information processing [3]. These problems share a common feature, in that the disordered interactions among their elements cause frustration and non-ergodic behaviour. The replica method [4] has been useful in explaining their macroscopic behaviour. At the same time, based on the microscopic descriptions of the models, the cavity method [5] resulted in many computationally efficient schemes. These approaches have laid the foundation for the study of many problems in complex optimization using statistical mechanics, such as graph partitioning [6], travelling salesman [7], K -satisfiability [8] and graph colouring [9].

Not only is the graph colouring problem [10] among the most basic NP-complete problems [11], but also it has direct relevance to a variety of applications in scheduling, distributed storage, content distribution and distributed computing.

In the original problem, one is given a graph and a number of colours, and the task is to find a colouring solution such that any two connected vertices are assigned different

colours. This is equivalent to the Potts glass with nearest neighbouring interactions in statistical physics. The problem has been studied by physicists using the cavity method [9, 12]. For a given number of colours, a phase transition takes place when the connectivity increases, changing from a colourable to an uncolourable phase. One of the statistical physics approaches was based on the replica symmetric (RS) ansatz. It gave an over-estimate of the threshold connectivity of this phase transition [13]. The one-step replica symmetry-breaking (1RSB) approach takes into account the possibility that the solution space can be fragmented [9, 12]. Besides giving an estimate of the threshold connectivity within the mathematical bounds, it correctly predicts the existence of a clustering phase below the threshold, in which the solution space spontaneously divides into an exponential number of clusters. This is called the hard colourable phase, in which local search algorithms are rendered ineffective, and is a feature shared by other constraint satisfaction problems [14, 15]. The sequence of phase transitions in the graph colouring problem, and their algorithmic implications, were further refined recently [16–19].

These advances in the spin glass theory stimulated the development of efficient algorithms. The cavity method gave rise to equations identical to those of the belief propagation (BP) algorithm for graphical models [20]. Inspired by the 1RSB solution, survey propagation (SP) algorithms were subsequently developed to cope with situations with fragmented solution space [21], and they work well even in the hard phase of the graph colouring problem [12].

In this paper, we study a variant of the graph colouring problem, namely, the colour diversity problem. In this problem, the aim is to maximize the number of colours within one link distance of any node. This is equivalent to the Potts glass with second nearest neighbouring interactions in statistical physics, and hence is more complex than the original graph colouring problem in terms of the increased number of frustrated links. Indeed, this variant of the colouring problem has been shown to be NP-complete [22].

This optimization problem is directly related to various application areas and in particular to the problem of distributed data storage where files are divided into a number of segments, which are then distributed over a graph representing the network. Nodes requesting a particular file collect the required number of file segments from neighbouring nodes to retrieve the original information. Distributed storage is used in many real-world applications such as OceanStore [23].

Compared with the original graph colouring problem, work done on the colour diversity problem mainly focused on algorithms [24, 25]. The belief propagation (BP) and Walksat algorithms for solving the problem have been presented in [24]. Both the algorithms revealed a transition from incomplete to complete colouring, and the possibility of a region of hard colouring immediately below the transition point. Approximate connectivity regimes for the solvable case have been found, given the number of colours [24]. However, since the algorithms are based on simplifying approximations (BP) and heuristics (Walksat), both algorithms provide only upper bounds to the true critical values.

The current study aims at providing a more principled approach to study the problem, a theoretical estimate of the transition point and more insights on the nature of the transition itself. The method employed is based on a tree approximation, which is equivalent to the RS ansatz of the replica method or the cavity method. It results in a set of recursive equations which can be solved analytically. The connectivity values for which the tree approximation is valid and the types of phases present at each value are also investigated at both zero and finite temperatures.

In section 2 we introduce the model, followed by section 3 that explains briefly the derivation and how the macroscopic behaviour can be studied. In section 4 we present the results obtained via population dynamics. Discussions on the behaviour at finite temperatures

are presented in section 5 followed by a concluding section. The appendices contain further mathematical details.

2. The model

2.1. The cost function

Consider a sparsely connected graph with connectivity c_i and colour q_i for node i . The connectivities c_i are drawn from a distribution $P(c_i)$ with mean $\langle c \rangle$. In this paper we consider the case of *linear connectivity*, that is, the nodes have connectivities $\lfloor \langle c \rangle \rfloor$ or $\lfloor \langle c \rangle \rfloor + 1$, with probabilities $1 - \langle c \rangle + \lfloor \langle c \rangle \rfloor$ and $\langle c \rangle - \lfloor \langle c \rangle \rfloor$, respectively. The colour q_i can take the values $1, \dots, Q$. The colour diversity problem is trivial for the case $\langle c \rangle > Q$, in which colour schemes with complete sets of colours available to all nodes can be found easily. Hence we will focus on the more interesting case $\langle c \rangle \leq Q$, in which a transition between complete and incomplete colouring exists, as shown in the previous work [24].

The set of colours available at the node and its local neighbourhood is

$$\mathcal{L}_i \equiv \{q_i\} \cup \{q_j | j \in N_i\},$$

where N_i is the set of nearest neighbours of node i . To find a colour scheme that maximizes the number of different colours in \mathcal{L}_i and averaged over all nodes i , we consider minimizing the energy (cost function) of the form

$$E = \sum_i \phi(\mathcal{L}_i). \quad (1)$$

Since the objective is equivalent to minimizing the number of identical colours in the set, an appropriate form of the function ϕ is

$$\phi(\mathcal{L}_i) = \sum_{q_j \in \mathcal{L}_i} \sum_{q_k \in \mathcal{L}_i} \delta(q_j, q_k), \quad (2)$$

where $\delta(a, b) = 1$ for $a = b$, and 0 otherwise. ϕ can be rewritten as

$$\phi(\mathcal{L}_i) = \sum_{q=1}^Q \left[\delta(q, q_i) + \sum_{j \in N_i} \delta(q, q_j) \right]^2. \quad (3)$$

The quadratic nature of ϕ confirms that it is an appropriate cost function for diversifying the colours in the neighbourhood of each node. Due to the convexity of its quadratic form, its minimum solution tends to equalize the numbers of all colours in the neighbourhood of a node. Thus, besides maximizing colour diversity, our choice of the cost function has an additional advantage for the distributed storage optimization task, which has motivated the current study, where an even distribution of segments (colours) in a neighbourhood is also a secondary objective, offering greater resilience.

The need for an even distribution of colours is especially important when the total number of colours is less than the connectivity of a node. Consider the contribution from the function ϕ centred on a node in such a case. Some colours can appear more than once. Then the exact form of the function ϕ determines the selection of these extra colours. In general, two types of selection can be made. In the first type, one may still use all colours, but they may be less evenly distributed than in the ground state. In the second type, one may use fewer colours. The former maximizes the number of available colours, but the latter does not. In this case, an inappropriate choice of the cost function will mix these two cases assigning the same energies, rendering it impossible to distinguish optimal and suboptimal colour choices.

On the other hand, equation (3) does not suffer from this shortcoming in the topology considered here. A geometric interpretation is able to illustrate this point. Let n_q be the number of times colour q appears in \mathcal{L}_i . Then the minimization of equation (3) reduces to the minimization of $\sum_{q=1}^Q n_q^2$ subject to the constraint that $\sum_{q=1}^Q n_q = |N_i| + 1$. Note that the constraint defines a hyperplane in the Q -dimensional space of n_q , and the problem is equivalent to finding the point with integer coordinates on the hyperplane such that its distance from the origin is minimized. The optimal solution is the point on the hyperplane closest to the normal, and no components should be zero when $Q \leq |N_i| + 1$. In fact, the optimal solution is $n_q = \text{int}[(|N_i| + 1)/Q]$ for $1 \leq q \leq \text{mod}(|N_i| + 1, Q)$, and $n_q = \text{int}[(|N_i| + 1)/Q] + 1$ otherwise (or its permutations).

We have also considered a worst case analysis of the change in the total cost due to colour changes in neighbouring nodes when the function ϕ , centred on a node i , is minimized. It shows that for networks with linear connectivities and $\langle c \rangle \leq Q$ the ground states consist of all satisfied nodes only, if they exist.

2.2. The statistical physics

We note that second nearest neighbour interactions are present in this cost function. This is different from that of the original graph colouring problem, where the cost function involves only nearest neighbour interactions. As we shall see, the messages in the resultant message-passing algorithm will be characterized by two components, instead of single components in the case of the original graph colouring problem [9, 13].

Analysis of the problem is done by writing the free energy of the system at a temperature T , given by

$$F = -T \ln Z, \tag{4}$$

where Z is the partition function given by

$$Z = \text{Tr}_{\{q_i\}} \exp \left[-\beta \sum_i \phi(\mathcal{L}_i) \right], \tag{5}$$

$\beta \equiv T^{-1}$ being the inverse temperature. In the zero temperature limit, the free energy approaches the minimum cost function. Several methods exist for deriving the free energy based on the replica and tree-based approximations. Here, the analysis adopts a tree-based approximation, which is valid for sparse graphs. When the connectivity of the graph is low, the probability of finding a loop of finite length on the graph is low, and the tree approximation well describes the local environment of a node. In the approximation, node i is connected to c_i branches in a tree structure, and the correlations among the branches of the tree are neglected. In each branch, nodes are arranged in generations. Node i is connected to an ancestor node of the previous generation, and another $c_i - 1$ descendant nodes of the next generation.

Consider the free energy $F_{ij}(a, b)$ of the tree terminated at node j with colour b , given its ancestor node i of colour a . In the tree approximation, one notes that this free energy can be written as $F_{ij}(a, b) = N_j F_{av} + F_{ij}^V(a, b)$, where N_j is the number of nodes in the tree terminated at node j , and $F_{ij}^V(a, b)$ is referred to as the *vertex free energy* [26, 27]. That is, the vertex free energy represents the contribution of the free energy extra to the average free energy due to the presence of the vertex. In the language of the cavity method, $F_{ij}^V(a, b)$ are equivalent to the *cavity fields*, since they describe the state of the system when node i is absent. The recursion relation of the vertex free energy of a node can be obtained by considering the contributions due to its descendant trees and the energy centred at itself. Using notations

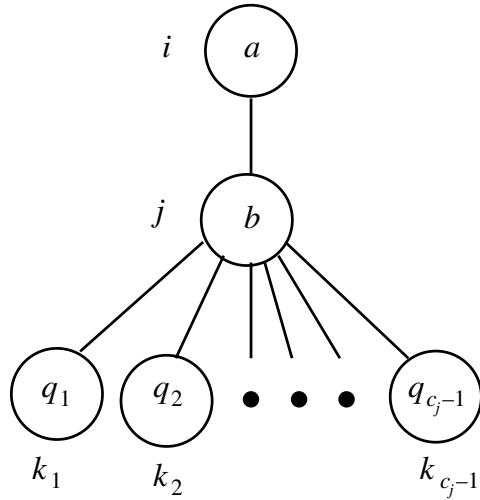


Figure 1. The notations used in computing the vertex free energy $F_{ij}^V(a, b)$.

described in figure 1, the vertex free energy obeys the recursion relation

$$F_{ij}^V(a, b) = -T \times \ln \text{Tr}_{\{q_k | k \in N_j \setminus \{i\}\}} \exp \left[-\beta \sum_{k \in N_j \setminus \{i\}} F_{jk}(b, q_k) - \beta \phi(b, \{a\} \cup \{q_k | k \in N_j \setminus \{i\}\}) \right] - F_{av}. \quad (6)$$

In this expression, the subtraction of F_{av} is due to the incorporation of node j with the descendant trees to form the tree terminated at node j . For brevity, we will use the alternative simplified notation

$$F_{ij}^V(a, b) = -T \ln \text{Tr}_{\mathbf{q}} \exp \left[-\beta \sum_{k=1}^{c_j-1} F_{jk}^V(b, q_k) - \beta \phi(a, b, \mathbf{q}) \right] - F_{av}, \quad (7)$$

where the vector \mathbf{q} refers to the colours of all descendants in figure 1.

To find the average free energy F_{av} , one considers the contribution to a node j due to all its c_j neighbours, that is,

$$F_{av} = -T \left\langle \ln \text{Tr}_{\{\mathcal{L}_i\}} \exp \left[-\beta \sum_{j \in N_i} F_{ij}^V(b, q_k) - \beta \phi(\mathcal{L}_i) \right] \right\rangle_{\text{node}}, \quad (8)$$

where the average $\langle \dots \rangle_{\text{node}}$ denotes sampling of nodes with connectivity c being drawn with probability $P(c)$. However, since the probability of finding a descendant node connecting to it is proportional to the number of links the descendant has, descendants are drawn with the excess probability $cP(c)/\langle c \rangle$.

Equations (7) and (8) can also be derived using the replica method as presented in appendix A. We remark that both the derivation and the results are very similar to those in the problem of resource allocation on sparse networks [26, 27], where the dynamical variables are the real-valued currents on the links of the networks. The parallelism between resource allocation and colour diversity is apparent when one notes that the currents in resource allocation can be expressed as the differences between current potentials defined on the nodes

of the networks. Hence the vertex free energies in both problems can be considered as functions of two variables.

Another useful relation can be obtained by substituting equation (7) into equation (8),

$$-T \left\langle \ln \text{Tr}_{a,b} \exp \left[-\beta F_{ij}^V(a, b) - \beta F_{ji}^V(b, a) \right] \right\rangle_{\text{link}} = 0, \quad (9)$$

where the average $\langle \dots \rangle_{\text{link}}$ denotes sampling of link vertices with connectivity c with the excess probability. This relation can be interpreted by considering the free energy of forming a link between vertices i and j . Since no extra nodes are added in this process, the extra free energy should average to zero.

The average of a function $\mathcal{A}(\mathcal{L}_i)$ is given by

$$\langle \mathcal{A} \rangle = \left\langle \frac{\text{Tr}_{\{\mathcal{L}_i\}} \exp \left[-\beta \sum_{j \in N_i} F_{ij}^V(q_i, q_j) - \beta \phi(\mathcal{L}_i) \right] \mathcal{A}(\mathcal{L}_i)}{\text{Tr}_{\{\mathcal{L}_i\}} \exp \left[-\beta \sum_{j \in N_i} F_{ij}^V(q_i, q_j) - \beta \phi(\mathcal{L}_i) \right]} \right\rangle_{\text{node}}. \quad (10)$$

Hence the average energy is given by

$$E_{\text{av}} \equiv \langle E \rangle = \langle \phi \rangle_{\text{node}}. \quad (11)$$

The Edwards–Anderson order parameter q_{EA} [28], whose nonzero value characterizes the Potts glass phase, is given by

$$q_{\text{EA}} = \frac{Q}{Q-1} \frac{1}{N} \sum_i \sum_q \left(\langle \delta(q, q_i) \rangle_{\text{node}} - \frac{1}{Q} \right)^2. \quad (12)$$

The performance measure of interest is the *incomplete fraction* f_{incom} , which is defined as the average fraction of nodes with an incomplete set of colours available at the node and its nearest neighbours,

$$f_{\text{incom}} = \left\langle \Theta \left[Q - \sum_{q=1}^Q \Theta \left(\delta(q, q_i) + \sum_{j \in N_i} \delta(q, q_j) \right) \right] \right\rangle_{\text{node}}, \quad (13)$$

where $\Theta(q) = 1$ for $q > 0$, and 0 otherwise. This performance measure is similar to the one used in [24], which we refer to as the *unsatisfied fraction* f_{unsat} , and is defined as the average fraction of colours unavailable at the node and its nearest neighbours (for the case that Q is not greater than the number of nearest neighbours plus 1),

$$f_{\text{unsat}} = \left\langle \left[1 - \frac{1}{Q} \sum_{q=1}^Q \Theta \left(\delta(q, q_i) + \sum_{j \in N_i} \delta(q, q_j) \right) \right] \right\rangle_{\text{node}}. \quad (14)$$

One might consider using equation (13) or (14) to define the cost function to be minimized, instead of equation (3). This is indeed possible and we expect that zero-energy ground states can be obtained when the condition of full colour diversity for each node is satisfiable. In the unsatisfiable case, no zero-energy ground states can be found, but one might still be interested in finding states that minimize the average number of colours unavailable to a node. In this case, f_{incom} might not be an appropriate choice, since it mixes up the energies of selecting more (but unevenly distributed) colours, and fewer colours. The second measure f_{unsat} favours those states with higher colour diversity, but for the same number of available colours, it does not distinguish states with different homogeneity of colour distribution. By comparison, the cost function in equation (3) has the additional advantage of favouring homogeneous colour distributions in the neighbourhood of the nodes.

3. Macroscopic properties

3.1. Population dynamics

Solutions to the recursive equation (6) are obtained by population dynamics [30]. We start with samples of N nodes, each with one of Q colours randomly assigned as the initial condition. At each time step of the population dynamics, all the N nodes are updated once in random order. At the instant we update node j , we select $c_j - 1$ nodes to be its descendants, where c_j is drawn from the distribution $P(c_j)$. Descendants with connectivities c_k are randomly selected with excess probabilities $c_k P(c_k)/\langle c \rangle$. The vertex free energy is then updated for all pairs (a, b) before another node is updated.

We have also computed the solutions using *layered* dynamics. At each time step of the layered dynamics, the new vertex free energies of all the N nodes are calculated, but are temporarily reserved until the end of the time step. Hence at the instant we renew node j , we select $c_j - 1$ nodes to be its descendants, whose vertex free energies were computed in the *previous* time step. Descendants with connectivities c_k are randomly selected with excess probabilities $c_k P(c_k)/\langle c \rangle$. After the new vertex free energies of all the N nodes have been computed, they are then updated synchronously and ready for the computation in the next time step.

We observe that a *modulation instability* is present in layered dynamics [29]. This means that after sufficient layers of computation, the colour distribution no longer remains uniform. Rather, each layer is dominated by a particular colour, and the dominant colour alternates from layer to layer. This modulation is expected to be suppressed in random graphs due to the presence of loops of incommensurate lengths. Furthermore, the average free energy computed by the layered dynamics has variances increasing rapidly with layers. Hence the layered dynamics is not adopted in our studies.

3.2. Average free energy at finite temperatures

To avoid growing fluctuations of the vertex free energies in the population dynamics, their constant components are subtracted off immediately after each update,

$$f_{ij}^V(a, b) \equiv F_{ij}^V(a, b) - G_{ij}, \quad (15)$$

where $G_{ij} \equiv \sum_{c,d} F_{ij}^V(c, d)/Q^2$ is a constant bias independent of colours a and b . The recursion relation of the vertex free energy then becomes

$$f_{ij}^V(a, b) = -T \ln \text{Tr}_{\mathbf{q}} \exp \left[-\beta \sum_{k=1}^{c_j-1} f_{jk}^V(b, q_k) - \beta \phi(a, b, \mathbf{q}) \right] + \text{constant}. \quad (16)$$

After every time step, we measure the average free energy. This is done by repeatedly creating a test node j and randomly selecting c_j nodes to connect with the test node. The average free energy is then given by

$$F_{\text{av}} = - \left\langle T \ln \text{Tr}_{\{\mathcal{L}_i\}} \exp \left[-\beta \sum_{j \in N_i} f_{ij}^V(q_i, q_j) - \beta \phi(\mathcal{L}_i) \right] \right\rangle_{\text{node}} + \langle c \rangle \langle G \rangle_{\text{link}}. \quad (17)$$

Note that G is averaged over links, since the descendants are drawn with excess probabilities. To calculate $\langle G \rangle_{\text{link}}$ we employ the consistency condition (9) for the average free energy of a link, which requires

$$- \langle T \ln \text{Tr}_{a,b} \exp [-\beta f_{ij}^V(a, b) - \beta f_{ji}^V(b, a)] \rangle_{\text{link}} + 2 \langle G \rangle_{\text{link}} = 0. \quad (18)$$

The node and link samplings are identical for graphs with uniform connectivity. This allows us to eliminate $\langle G \rangle$ in equations (17) and (18), and thus obtain F_{av} . To tackle the case of non-uniform connectivities, we need to generalize the consistency condition (18). This can be done by restricting our consideration to links with vertices of given connectivities A and B , and consider the free energy due to the link connecting the trees on both sides of such links

$$-\langle T \ln \text{Tr}_{a,b} \exp [-\beta F_{ij}^V(a, b) - \beta F_{ji}^V(b, a)] \rangle_{C_i=A, C_j=B} = 0. \quad (19)$$

The derivation is analogous to that of equation (18), resulting in

$$-\langle T \ln \text{Tr}_{a,b} \exp [-\beta f_{ij}^V(a, b) - \beta f_{ji}^V(b, a)] \rangle_{C_i=A, C_j=B} + \langle G \rangle_A + \langle G \rangle_B = 0, \quad (20)$$

which facilitates the elimination of the biases G in equation (17), resulting in an expression for the average free energy

$$F_{av} = -\left\langle T \ln \text{Tr}_{\{\mathcal{L}_i\}} \exp \left[-\beta \sum_{j \in N_i} f_{ij}^V(q_i, q_j) - \beta \phi(\mathcal{L}_i) \right] \right\rangle_{\text{node}} + \frac{\langle c \rangle}{2} \sum_{A,B} \frac{AP(A)BP(B)}{\langle c \rangle} \times \langle T \ln \text{Tr}_{a,b} \exp [-\beta f_{ij}^V(a, b) - \beta f_{ji}^V(b, a)] \rangle_{C_i=A, C_j=B}. \quad (21)$$

To evaluate F_{av} one first performs the node average in the first term of equation (21), keeping a record of the number of times each node k is sampled. Then one performs the average in the second term, randomly drawing the vertices i and j of the links from nodes k with exactly the same number of times they appear in the first term. Hence in this procedure, the descendants in both terms are drawn from the excess distribution. Furthermore, it ensures that the G_{ij} 's appearing in the first term are exactly cancelled by those appearing in the second term, thus eliminating a source of possible fluctuations.

We also note that there can be a variety of choices of G_{ij} 's to be subtracted from the vertex free energies in equation (15). For example, one may choose G_{ij} to be $F_{ij}^V(1, 1)$ and arrive at the same result (21). In fact, this computationally simple choice is adopted in our computation.

3.3. Energy and entropy at finite temperatures

Expressions for the energy and entropy follow immediately using the identity $E = \partial(\beta F)/\partial\beta$ and the averaging of equation (10),

$$E_{av} = \left\langle \frac{\text{Tr}_{\{\mathcal{L}_i\}} \exp [-\beta \sum_{j \in N_i} F_{ij}^V(q_i, q_j) - \beta \phi(\mathcal{L}_i)] [\sum_{j \in N_i} E_{ij}^V(q_i, q_j) + \phi(\mathcal{L}_i)]}{\text{Tr}_{\{\mathcal{L}_i\}} \exp [-\beta \sum_{j \in N_i} F_{ij}^V(q_i, q_j) - \beta \phi(\mathcal{L}_i)]} \right\rangle_{\text{node}}, \quad (22)$$

where $E_{ij}^V(a, b)$ is the vertex energy with the recursion relation

$$E_{ij}^V(a, b) = \frac{\text{Tr}_{\mathbf{q}} \exp [-\beta \sum_{k=1}^{c_j-1} F_{jk}^V(b, q_k) - \beta \phi(a, b, \mathbf{q})] [\sum_{k=1}^{c_j-1} E_{jk}^V(b, q_k) + \phi(a, b, \mathbf{q})]}{\text{Tr}_{\mathbf{q}} \exp [-\beta \sum_{k=1}^{c_j-1} F_{jk}^V(b, q_k) - \beta \phi(a, b, \mathbf{q})]} - E_{av}, \quad (23)$$

and

$$S = \frac{E_{av} - F_{av}}{T}. \quad (24)$$

Compared with the previous equation (11) for the average energy, equation (22) includes the vertex energies of the descendants. These vertex energies transmit the energy deviations from the average energy, from the descendants to the ancestors. Hence equation (22) can be

regarded as a global estimate of the average energy, and equation (11) is a local estimate. Theoretically, one expects that both estimates should yield the same result. Numerically, however, we found that this is only valid in the paramagnetic phase. In the Potts glass phase, the discrepancy between the two estimates can be very significant. This shows that in the paramagnetic phase memories about the initial conditions are lost easily. In contrast, in the Potts glass phase, memories about the initial conditions can propagate for a long time through the vertex energies.

To avoid propagating fluctuations in the computation of the average energy, we subtract $E_{ij}^V(1, 1)$ from all components $E_{ij}^V(a, b)$ immediately after each update, and find E_{av} using

$$E_{av} = \left\langle \frac{\text{Tr}_{\{\mathcal{L}_i\}} \exp \left[-\beta \sum_{j \in N_i} f_{ij}^V(q_i, q_j) - \beta \phi(\mathcal{L}_i) \right] \left[\sum_{j \in N_i} E_{ij}^V(q_i, q_j) + \phi(\mathcal{L}_i) \right]}{\text{Tr}_{\{\mathcal{L}_i\}} \exp \left[-\beta \sum_{j \in N_i} f_{ij}^V(q_i, q_j) - \beta \phi(\mathcal{L}_i) \right]} \right\rangle_{\text{node}} - \frac{\langle c \rangle}{2} \sum_{A,B} \frac{AP(A)BP(B)}{\langle c \rangle} \times \left\langle \frac{\text{Tr}_{a,b} \exp \left[-\beta f_{ij}^V(a, b) - \beta f_{ji}^V(b, a) \right] \left[E_{ij}^V(a, b) + E_{ji}^V(b, a) \right]}{\text{Tr}_{a,b} \exp \left[-\beta f_{ij}^V(a, b) - \beta f_{ji}^V(b, a) \right]} \right\rangle_{c_i=A, c_j=B}. \quad (25)$$

3.4. Free energy, energy and entropy at zero temperature

The derivation at zero temperature should be carried out with extra care due to possible degeneracy in the solutions. In the zero temperature limit, equation (7) reduces to

$$F_{ij}^V(a, b) = \min_{\mathbf{q}} \left[\sum_{k=1}^{c_j-1} F_{jk}^V(b, q_k) + \phi(a, b, \mathbf{q}) \right] - F_{av}. \quad (26)$$

The expression of the entropy at zero temperature can be computed directly from the *vertex entropies*. Differentiating equation (7) with respect to T , and taking the zero temperature limit, one obtains

$$S_{ij}^V(a, b) = \ln \left[\sum_{\{\mathbf{q}^*\}} \exp \left(\sum_{k=1}^{c_j-1} S_{jk}^V(b, q_k^*) \right) \right] - S_{av}, \quad (27)$$

where $\{\mathbf{q}^*\}$ is the set of colours minimizing the free energy $\sum_{k=1}^{c_j} F_{jk}^V(b, q_k) + \phi(a, b, \mathbf{q})$ at node j . Similarly, differentiating equation (8) with respect to T and taking the zero temperature limit, one obtains

$$S_{av} = \left\langle \ln \left[\sum_{\{\mathcal{L}_i^*\}} \exp \left(\sum_{j \in N_i} S_{ij}^V(q_i^*, q_j^*) \right) \right] \right\rangle_{\text{node}} - \frac{\langle c \rangle}{2} \sum_{A,B} \frac{AP(A)BP(B)}{\langle c \rangle} \times \left\langle \ln \left[\sum_{\{a^*, b^*\}} \exp \left(S_{ij}^V(a^*, b^*) + S_{ji}^V(b^*, a^*) \right) \right] \right\rangle_{c_i=A, c_j=B}, \quad (28)$$

where $\{\mathcal{L}_i^*\}$ are the set of colours minimizing the free energy $\sum_{j \in N_i} F_{ij}^V(q_i, q_j) + \phi(\mathcal{L}_i)$ at node i , and $\{a^*, b^*\}$ are the set of the pair of colours minimizing the free energy $F_{ij}^V(a, b) + F_{ji}^V(b, a)$ at link ij .

The performance measures are now weighted by the entropies, and equation (10) is replaced by the expression

$$\langle \mathcal{A} \rangle = \left\langle \frac{\text{Tr}_{\{\mathcal{L}_i^*\}} \exp \left[\sum_{j \in N_i} S_{ij}(q_i^*, q_j^*) \right] \mathcal{A}(\mathcal{L}_i^*)}{\text{Tr}_{\{\mathcal{L}_i^*\}} \exp \left[\sum_{j \in N_i} S_{ij}(q_i^*, q_j^*) \right]} \right\rangle_{\text{node}}. \quad (29)$$

3.5. The paramagnetic state at finite temperatures

In the paramagnetic state, the vertex free energies are symmetric with respect to the permutation of colours at each node. Hence there are only two distinct values of the vertex free energy for each node, corresponding to the cases that the colours of the node and its ancestor are the same or different. Hence, we can derive the recursion relation for the single variable $z_{ij} \equiv \exp[-\beta(F_{ij}^V(a, a) - F_{ij}^V(a, b))]$, where $a \neq b$. This is a significant simplification of the original recursion relation for $F_{ij}^V(a, b)$, which involves Q^2 components.

Specifically, we consider graphs with linear connectivity $3 \leq \langle c \rangle \leq 4$. We first consider the vertex free energy of a node j with $c_j = 3$, whose descendants are labelled 1 and 2. The recursion relations are given by

$$\begin{aligned} F_{ij}^V(a, a) &= -T \ln \text{Tr}_{q_1, q_2} \exp[-\beta F_{j1}^V(a, q_1) - \beta F_{j2}^V(a, q_2) - \beta \phi(a, a, q_1, q_2)] - F_{\text{av}}, \\ F_{ij}^V(a, b) &= -T \ln \text{Tr}_{q_1, q_2} \exp[-\beta F_{j1}^V(a, q_1) - \beta F_{j2}^V(b, q_2) - \beta \phi(a, b, q_1, q_2)] - F_{\text{av}}. \end{aligned} \quad (30)$$

By explicitly tabulating the different colour configurations and introducing the notations $z \equiv \exp(-\beta)$ and $Q_n \equiv Q - n$, one can rewrite equation (30) as

$$\begin{aligned} F_{ij}^V(a, a) &= -T \ln [z^{16} z_{j1} z_{j2} + Q_1 z^{10} (z_{j1} + z_{j2}) + Q_1 z^8 + Q_1 Q_2 z^6] + \sum_k F_{jk}^V(a, b) - F_{\text{av}}, \\ F_{ij}^V(a, b) &= -T \ln [z^{10} z_{j1} z_{j2} + (z^8 + Q_2 z^6)(z_{j1} + z_{j2}) + z^{10} + 3Q_2 z^6 + Q_2 Q_3 z^4] \\ &\quad + \sum_k F_{jk}^V(a, b) - F_{\text{av}}. \end{aligned} \quad (31)$$

These give rise to the recursion relation for z_{ij} ,

$$z_{ij} = z^2 \left(\frac{Q_1 Q_2 + Q_1 z^2 + Q_1 z^4 (z_{j1} + z_{j2}) + z^{10} z_{j1} z_{j2}}{Q_2 Q_3 + 3Q_2 z^2 + z^6 + (Q_2 z^2 + z^4)(z_{j1} + z_{j2}) + z^6 z_{j1} z_{j2}} \right). \quad (32)$$

Similarly, for node j with $c_j = 4$,

$$z_{ij} = z^2 \left(\frac{Z_N}{Z_D} \right), \quad (33)$$

where

$$\begin{aligned} Z_N &= Q_1 Q_2 Q_3 + 3Q_1 Q_2 z^2 + Q_1 z^6 + (Q_1 Q_2 z^4 + Q_1 z^6)(z_{j1} + z_{j2} + z_{j3}) \\ &\quad + Q_1 z^{10} (z_{j1} z_{j2} + z_{j2} z_{j3} + z_{j1} z_{j3}) + z^{18} z_{j1} z_{j2} z_{j3}, \\ Z_D &= Q_2 Q_3 Q_4 + 6Q_2 Q_3 z^2 + 3Q_2 z^4 + 4Q_2 z^6 + z^{12} \\ &\quad + (Q_2 Q_3 z^2 + 3Q_2 z^4 + z^8)(z_{j1} + z_{j2} + z_{j3}) \\ &\quad + (Q_2 z^6 + z^8)(z_{j1} z_{j2} + z_{j2} z_{j3} + z_{j1} z_{j3}) + z^{12} z_{j1} z_{j2} z_{j3}. \end{aligned} \quad (34)$$

Expressions of the average free energy and average energy can be found in appendix B.

3.6. The paramagnetic state at zero temperature

In the zero temperature limit for $Q \leq 4$, equations (32) and (33) reduce to

$$\begin{aligned} z_{ij} &= \left(\frac{Q_1}{Q_3} \right) z^2 \rightarrow 0 & \text{for } c_j = 3, \\ z_{ij} &= \frac{Q_1}{6 + z_{j1} + z_{j2} + z_{j3}} & \text{for } c_j = 4. \end{aligned} \quad (35)$$

For $c_j = 4$, the range of values of z_{ij} is $2Q_1/(Q_1 + 12) \leq z_{ij} \leq Q_1/6$. Hence the distribution of the vertex partition function is given for $c_j = 4$ by

$$P(z) = \sum_{k=0}^3 \binom{3}{k} f_3^{3-k} f_4^k \prod_{r=1}^k \left[\int_{2Q_1/(Q_1+12)}^{Q_1/6} dz_r P(z_r) \right] \delta \left(z - \frac{Q_1}{6 + \sum_{r=1}^k z_r} \right), \quad (36)$$

where $f_3 \equiv 3(4 - \langle c \rangle)/\langle c \rangle$ and $f_4 \equiv 4(\langle c \rangle - 3)/\langle c \rangle$ are the excess probabilities, and are distinctive from the connectivity probabilities $p_3 \equiv 4 - \langle c \rangle$ and $p_4 \equiv \langle c \rangle - 3$ in subsequent expressions.

For the average free energy, equation (B.2) becomes

$$\begin{aligned} F_{\text{av}}|_{c=3} &= 4 - T \ln(Q Q_1 Q_2 Q_3), \\ F_{\text{av}}|_{c=4} &= 7 - T \sum_{k=0}^4 \binom{4}{k} f_3^{4-k} f_4^k \prod_{r=1}^k \left[\int_{2Q_1/(Q_1+12)}^{Q_1/6} dz_r P(z_r) \right] \ln \left[Q Q_1 Q_2 Q_3 \left(6 + \sum_{r=1}^k z_r \right) \right], \\ F_{\text{link}}|_{C_1 C_2} &= -(1 - \delta_{C_1,4} \delta_{C_2,4}) T (1 - f_4^2) \ln Q Q_1 - \delta_{C_1,4} \delta_{C_2,4} T f_4^2 \int_{2Q_1/(Q_1+12)}^{Q_1/6} dz_1 P(z_1) \\ &\quad \times \int_{2Q_1/(Q_1+12)}^{Q_1/6} dz_2 P(z_2) \ln [Q(Q_1 + z_1 z_2)]. \end{aligned} \quad (37)$$

Hence in the zero temperature limit,

$$F_{\text{av}} = 3\langle c \rangle - 5. \quad (38)$$

This value of the average free energy interpolates between 4 and 7 at $\langle c \rangle = 3$ and 4, respectively. This means that in the paramagnetic phase, there is a freedom in assigning the colours of the nodes so that all local energies are minimized. For a node with three neighbours and $Q = 4$, the state of local energy minimum has one of each colour among itself and its neighbours. Hence the energy is 4. Similarly, for a node with four neighbours and $Q = 4$, the state of local energy minimum has, among itself and its neighbours, two nodes of the same colour and three nodes of mutually different colours. Hence the energy is 7. The result of $3\langle c \rangle - 5$ is the average of 4 and 7, weighted by the fraction of nodes with three and four neighbours, respectively. This is the lowest possible energy of the system.

The average entropy of the paramagnetic state is given by

$$\begin{aligned} S_{\text{av}} &= \ln(Q Q_1 Q_2 Q_3) + p_4 f_3 \ln Q_1 - \frac{\langle c \rangle}{2} [\ln(Q Q_1) - f_4^2 \ln Q_1] \\ &\quad - p_4 \int_{2Q_1/(Q_1+12)}^{Q_1/6} dz P(z) \ln z - \left(\frac{\langle c \rangle}{2} f_4 - p_4 \right) f_4 \int_{2Q_1/(Q_1+12)}^{Q_1/6} dz_1 P(z_1) \\ &\quad \times \int_{2Q_1/(Q_1+12)}^{Q_1/6} dz_2 P(z_2) \ln [Q(Q_1 + z_1 z_2)]. \end{aligned} \quad (39)$$

Consider the case $Q = 4$. When $\langle c \rangle = 3$, $S_{\text{av}} = -\ln 3/2$. For general values of Q , we have $S_{\text{av}} = \ln(Q_2 Q_3 / \sqrt{Q Q_1})$. Hence the entropy becomes negative for $Q = 4$, although the entropy remains positive for $Q > 4$.

On the other hand, when $\langle c \rangle = 4$, the vertex partition function becomes node independent, implying $z = \sqrt{2} - 1$, and $S_{\text{av}} = \ln[(15 + 12\sqrt{2})/28] = 0.13$. Hence at an intermediate value of $\langle c \rangle$, the entropy changes sign. Thus, there is a range of negative entropy for $\langle c \rangle$ below 4 where the RS ansatz is unstable.

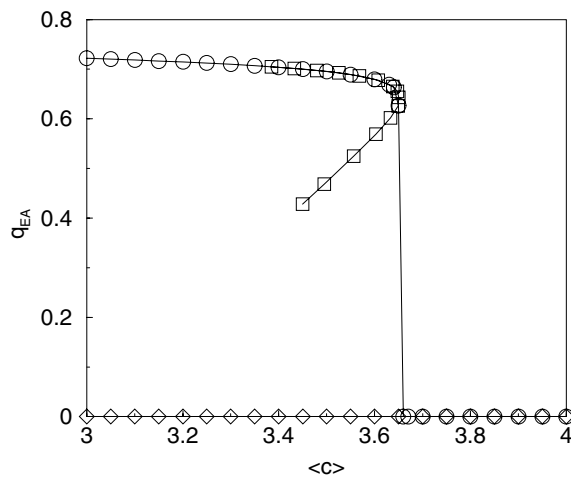


Figure 2. The dependence of the Edwards–Anderson order parameter q_{EA} on the average connectivity $\langle c \rangle$, obtained from the population dynamics at fixed $\langle c \rangle$ (\circ), at fixed f_{incom} (\square) and for the paramagnetic state (\diamond). Parameters: $N = 10\,000$, $Q = 4$ and 30 samples.

4. Numerical results

Numerical solutions to the equations are obtained using population dynamics in the manner explained in subsection 3.1. Results are obtained for $Q = 4$ and ensembles of graphs with linear connectivity $3 \leq \langle c \rangle \leq 4$, mixing nodes with connectivities 3 and 4 in varying proportions. After every time step, we measure the following measures: the local estimate of the average energy, the incomplete fraction and the Edwards–Anderson order parameter. This is done by creating a test node i and randomly selecting c_i nodes to connect with the test node. The node contributions to the average free energy, the global estimate of the average energy and (for zero temperature) the entropy are also computed. The computed measures are repeated for $N = 10\,000$ nodes for each sample. The set of descendant nodes of these N test nodes is recorded. Then, pairs of nodes are randomly drawn from this set to form links, and the link contributions to the average free energy, the global estimate of the average energy and (for zero temperature) the entropy are computed.

4.1. Paramagnetic and Potts glass phases

Figure 2 shows the Edwards–Anderson order parameter as a function of $\langle c \rangle$. It can be seen that the value of q_{EA} is 0 in the paramagnetic phase, which spans the region $\langle c \rangle \geq \langle c \rangle_{\text{sp}} = 3.65$. In this phase, all nodes have free choices of colours. The Potts glass phase spans the region $\langle c \rangle < \langle c \rangle_{\text{sp}}$, where q_{EA} remains at a value around 0.7, and its transition to the paramagnetic phase is of the first order.

Figure 3 shows incomplete fraction obtained from the steady state solution of the population dynamics at fixed $\langle c \rangle$ values. It remains nonzero in the Potts glass phase, and vanishes discontinuously above $\langle c \rangle_{\text{sp}}$ in the paramagnetic phase. To find the stable as well as the unstable solutions of the population dynamics, which correspond to multiple solutions at fixed $\langle c \rangle$, we may run the population dynamics at fixed nonzero f_{incom} . This can be done by monitoring f_{incom} conditionally averaged on the nodes with $c_j = \lfloor \langle c \rangle \rfloor$

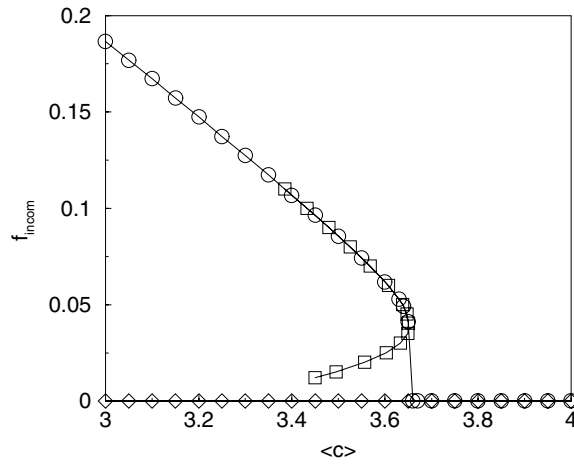


Figure 3. The dependence of the incomplete fraction f_{incom} on the average connectivity $\langle c \rangle$. Symbols and parameters: as in figure 2.

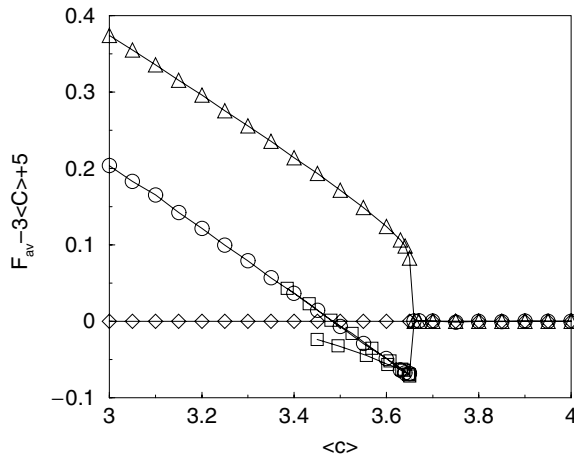


Figure 4. The dependence of the average free energy on the average connectivity, after subtracting the baseline $3\langle c \rangle - 5$ of the paramagnetic free energy. Symbols: (Δ): local estimate of the average energy, other symbols as in figure 2. Parameters: as in figure 2.

and $c_j = \lfloor \langle c \rangle \rfloor + 1$ at each step, and adjusting the value of $\langle c \rangle$ to approach its targeted value, which is related to the targeted value of f_{incom} estimated at each time step by $f_{\text{incom}} = (\langle c \rangle - \lfloor \langle c \rangle \rfloor) f_{\text{incom}}|_{c=\lfloor \langle c \rangle \rfloor + 1} + (1 - \langle c \rangle + \lfloor \langle c \rangle \rfloor) f_{\text{incom}}|_{c=\lfloor \langle c \rangle \rfloor}$. The population dynamics at fixed f_{incom} yields both stable and unstable solutions of the Potts glass state below $\langle c \rangle_{\text{sp}}$, confirming that the transition to the paramagnetic phase is discontinuous, and that $\langle c \rangle_{\text{sp}}$ corresponds to the spinodal point. The Edwards–Anderson order parameter for both stable and unstable Potts glass states are also shown in figure 2, bearing features similar to those in figure 3.

Figure 4 shows the average free energy. The paramagnetic free energy of $3\langle c \rangle - 5$ provides a baseline for comparing the energy and free energy of the different phases. Below the spinodal point $\langle c \rangle_{\text{sp}}$, the paramagnetic state continues to exist. It is not accessible by the population

dynamics, but one can find the paramagnetic free energy by first finding a paramagnetic state at $\langle c \rangle \geq \langle c \rangle_{\text{sp}}$, and then gradually reducing the connectivity to the desired value. The resultant paramagnetic free energy is identical to that found directly in subsection 3.5.

As shown in figure 4, the Potts glass free energy becomes lower than the paramagnetic free energy near the spinodal point $\langle c \rangle_{\text{sp}}$. A first-order transition appears to take place at $\langle c \rangle_{\text{c,zic}} = 3.48$, where the free energies of the two states cross each other. The subscript zic refers to the zero initial condition used here, as distinguished from the random initial condition (subscript ric) to be discussed in the following subsection. However, since the Potts glass energy equals the free energy at zero temperature, this implies that the average energy is below the lowest possible energy of $3\langle c \rangle - 5$ in the range $3.48 < \langle c \rangle < 3.65$! Similar observations of contradictory results have been observed in the RS ansatz of the original graph colouring problem [13, 9] and the 3-SAT problem [31]. This indicates that the RS ansatz in the present analysis is insufficient, and has to be improved by including further steps of replica symmetry-breaking. Furthermore, the solution of the population dynamics is insensitive to this transition point in the large N limit. Instead, it yields the Potts glass state above this transition point right up to the spinodal point $\langle c \rangle_{\text{sp}}$. (For smaller values of N , say, $N = 1000$, the discontinuous transition takes place below the spinodal point.) Thus, the transition at $\langle c \rangle_{\text{sp}}$ looks like a zeroth-order one, with a discontinuous jump of the average free energy from the Potts glass phase below $\langle c \rangle_{\text{sp}}$ to the paramagnetic phase above $\langle c \rangle_{\text{sp}}$.

As mentioned in subsection 3.3, the local and global estimates of the average energy are different and are given by equations (11) and (25), respectively. The global estimate yields results identical to the average free energy, showing that memories about initial conditions in both variables have been compensated. However, we observe that the global average energy is numerically unstable in the Potts glass phase. For $N = 1000$, it diverges from the average free energy after about 100 steps in the population dynamics.

As shown in figure 4, the local estimate of the average energy is indistinguishable from the global estimate in the paramagnetic phase. However, the local estimate is significantly higher than the global estimate in the Potts glass phase. Unlike the global estimate which contradicts the lowest possible energy, the local estimate remains above it.

Next, we consider the entropy. The entropy of the paramagnetic state obtained from the theoretical prediction of equation (39) agrees well with the results of population dynamics. As shown in figure 5, the entropy of the paramagnetic state becomes negative for $\langle c \rangle < \langle c \rangle_s = 3.82$, while the entropy of the Potts glass state is negative throughout. At the spinodal point $\langle c \rangle_{\text{sp}}$, the entropy exhibits a small discontinuous jump. Clearly, results for $\langle c \rangle < \langle c \rangle_{\text{sp}}$ should be investigated using a replica symmetry-breaking ansatz to identify the exact transition point, which is beyond the scope of this paper.

4.2. Initial conditions

One puzzle of our results is that the Edwards–Anderson order parameter remains at a level around 0.7 in the entire Potts glass phase. This implies that a considerable fraction of nodes have free choices of colours even in the Potts glass phase. This is illustrated by the distribution of colour moments $\langle \delta(q_i, q) \rangle$ in figure 6(a), which consists of a continuous background with peaks at simple rational numbers ($1/5, 1/4, 1/3, 2/5$, etc). In fact, the existence of free spins at zero temperature has been considered an indication of broken replica symmetry [9].

However, this is apparently inconsistent with extrapolations from finite temperatures, which will be discussed in the following section. As will be seen, q_{EA} approaches 1 in the limit of low but finite temperature, implying that all nodes lose the freedom of choosing more than one colour.

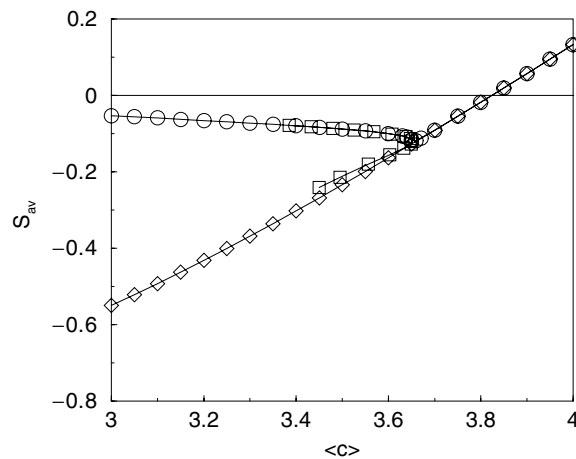


Figure 5. The dependence of the entropy S_{av} on the average connectivity. Symbols and parameters: as in figure 2.

To resolve this inconsistency, we consider the effects of introducing a small randomness in the initial condition, that is, a small random bias is added to the initial values of the vertex free energies, which take integer values otherwise. Such randomness were known to cause significant changes in the optimal solution in the graph bipartitioning problem, where the field distribution is initialized to a rectangular distribution [32].

Figure 6(b) shows that when a very small randomness is introduced in the initial condition, the final values of the Edwards–Anderson order parameter q_{EA} remain around 1 in both the paramagnetic and Potts glass phase. This means that effectively all spins are frozen due to the randomness in the initial condition. The distribution of colour moments consists of two delta function peaks, located at $\langle \delta(q_i, q) \rangle = 0$ and 1, respectively. This is consistent with the extrapolation of finite temperature results. The difference between zero temperature and low but finite temperature distributions was also observed in the RS approximation of the original graph colouring problem [9, 13].

Randomness in the initial condition causes a significant change in the transition point between the Potts glass and paramagnetic states. Figure 6(c) shows that the average free energy of the Potts glass state crosses that of the paramagnetic state at $\langle c \rangle_{c, zic} = 3.48$ and $\langle c \rangle_{c, ric} = 3.65$ for the zero and random initial conditions, respectively. As far as we can tell from our numerical precision, $\langle c \rangle_{c, ric} = 3.65$ is effectively the same as the spinodal point $\langle c \rangle_{sp} = 3.65$. As will be seen in the following section, the transition point $\langle c \rangle_{c, ric}$ is consistent with the phase transition line at finite temperatures.

The effects of randomness in the initial condition on the performance are shown in figure 6(d). For the random initial condition, the incomplete fraction in the Potts glass phase vanishes effectively continuously to 0 at $\langle c \rangle_{sp}$. This is in contrast with the incomplete fraction for the zero initial condition, which is much higher, and vanishes discontinuously at the spinodal point.

The entropy is effectively zero in both the Potts glass phase and the paramagnetic phase in the case of random initial conditions. This is different from the case of zero initial conditions shown in figure 5, in which the entropy is negative in the entire Potts glass phase and part of the paramagnetic phase.

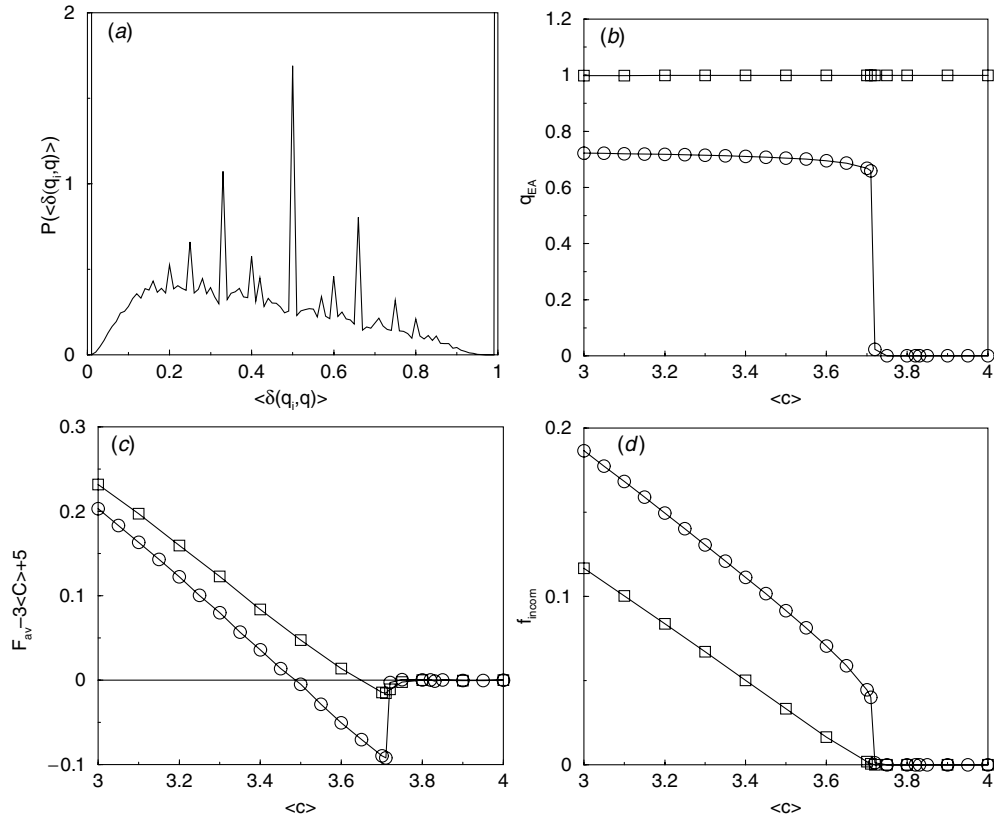


Figure 6. Results for system size $N = 10000$, $Q = 4$ and 30 samples, obtained from the steady state solution of the population dynamics using zero and random initial conditions (labelled (\circ) and (\square) , respectively). (a) The colour moments distribution obtained from the zero initial condition at $\langle c \rangle = 3$. (b) The Edwards–Anderson order parameter q_{EA} . (c) The average free energy after subtracting the baseline $3\langle c \rangle - 5$ of the paramagnetic free energy. (d) The incomplete fraction.

4.3. Evolution of damages

To illustrate the difference between the paramagnetic and Potts glass phases, we consider the evolution of damages for different average connectivities $\langle c \rangle$. The damaged configuration, with colours $\{q'_i\}$, is initialized identically to $\{q_i\}$, except that the colours of the descendants of one randomly chosen node j have been inverted, that is, $q_k = Q - q'_k$, where k are the descendants of node j . We define the *distance measure* between $\{q_i\}$ and $\{q'_i\}$ as the distance between the colour moments

$$d = \frac{1}{N} \sum_i \sum_{q=1}^Q (\langle \delta(q_i, q) \rangle - \langle \delta(q'_i, q) \rangle)^2. \quad (40)$$

We monitor the population dynamics of the colour configuration $\{q_i\}$ and its *damaged* configuration $\{q'_i\}$. They evolve with the same sequence of updates and choice of descendants. As shown in figure 7, the distance is nonzero in the Potts glass phase, but vanishes in the paramagnetic phase. This shows that multiple solutions of the saddle point equation exist in the Potts glass phase, but the solution is unique in the paramagnetic phase. The spread of damage is consistent with the instability of the replica symmetric solution in the Potts glass phase.

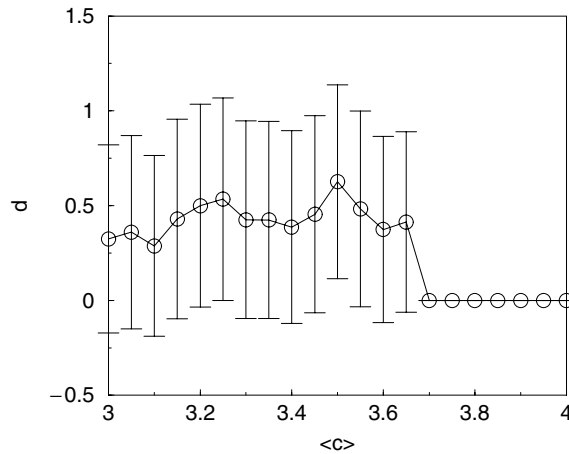


Figure 7. The dependence of the distance measure d on the average connectivity $\langle c \rangle$ using population dynamics with 10 000 nodes, $Q = 4$ and 30 samples.

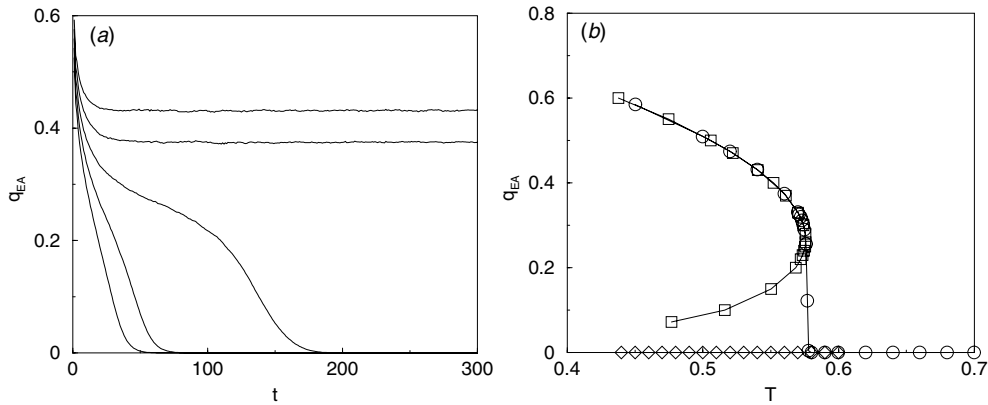


Figure 8. (a) The evolution of the Edwards–Anderson order parameter q_{EA} in the population dynamics at $\langle c \rangle = 3$ and $T = 0.54, 0.56, 0.58, 0.60, 0.62$ (top to bottom). (b) The dependence of q_{EA} at the steady state on temperature T . Symbols: thermodynamic state (\circ), Potts glass state (\square), paramagnetic state (\diamond). Parameters: $N = 10\,000$, $Q = 4$ and 30 samples.

5. Finite temperature behaviour

5.1. The example of $\langle c \rangle = 3$

Further insights about the thermodynamic behaviour can be obtained by considering the finite temperature behaviour. First, let us study the example of $\langle c \rangle = 3$. Figure 8(a) shows that q_{EA} of the thermodynamic state vanishes at temperatures above 0.575. To verify that this phase transition is discontinuous, we look for solutions of the population dynamics with variable T for given values of q_{EA} , which yield the Potts glass state. As shown in figure 8(b), the Potts glass phase with positive q_{EA} does not vanish continuously into the paramagnetic phase. Rather, its stable and unstable branches merge at the temperature 0.575, which is therefore identified to be the spinodal temperature.

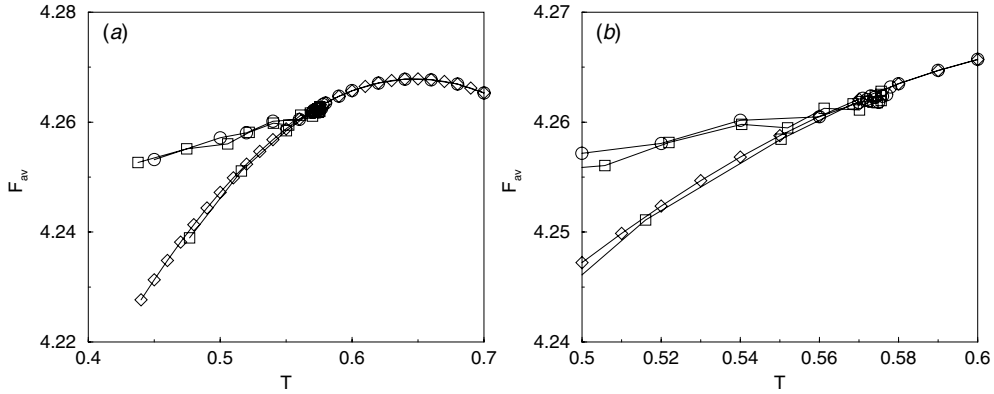


Figure 9. The dependence of the average free energy F_{av} on temperature at $\langle c \rangle = 3$. Symbols and parameters: as in figure 8(b).

Figure 9(a) shows the free energies of the paramagnetic state and the results of the population dynamics. The free energy at the paramagnetic state reaches a maximum at $T = 0.65$. Below this temperature, the entropy becomes negative. The population dynamics is in good agreement with the paramagnetic state down to the spinodal temperature, below which the population dynamics deviates from the paramagnetic state.

Figure 9(b) shows the free energies in the neighbourhood of the spinodal temperature, including the stable and unstable branches of the Potts glass state. The free energies of the Potts glass and paramagnetic states become equal at $T = 0.56$. While this can be interpreted as the thermodynamic transition temperature, we observe that it is not relevant to the population dynamics, in which the jump of q_{EA} , as shown in figures 8(a) and (b), takes place at the spinodal temperature instead. This behaviour is consistent with the irrelevance of the first-order transition point $\langle c \rangle_{c,zic} = 3.48$ at zero temperature, as described in subsection 4.1.

The behaviour of the entropy is shown in figure 10(a). The entropy of the paramagnetic state becomes negative below $T = 0.65$. The stable and unstable branches of the Potts glass state are shown in figure 10(b), and the population dynamics yields results jumping discontinuously from the stable branch of the Potts glass state to the paramagnetic state at the spinodal temperature.

Regions of negative entropy are often found in spin glasses. They usually signal that the RS ansatz is unstable. However, in the original Sherrington–Kirkpatrick model, the region of negative entropy is restricted to the low-temperature regime deep inside the spin glass phase [1, 2]. In contrast, the region of negative entropy at $\langle c \rangle = 3$ spans the entire Potts glass phase and even covers part of the paramagnetic phase. This indicates that frustration effects in the present model are unusually strong.

We propose that this increased frustration effect is a consequence of the second nearest neighbouring interactions present in the colour diversity problem, and does not exist in most models investigated so far. To verify this, we consider the model

$$E = \sum_i \left[4 + 2 \sum_{j \in N_i} \delta(q_i, q_j) + 2\lambda \sum_{j \neq k \in N_i} \delta(q_j, q_k) \right]. \quad (41)$$

The cases $\lambda = 0$ and 1 correspond to the graph colouring and colour diversity problems, respectively. We will consider the range $0 \leq \lambda \leq 1$. In the paramagnetic phase, expressions

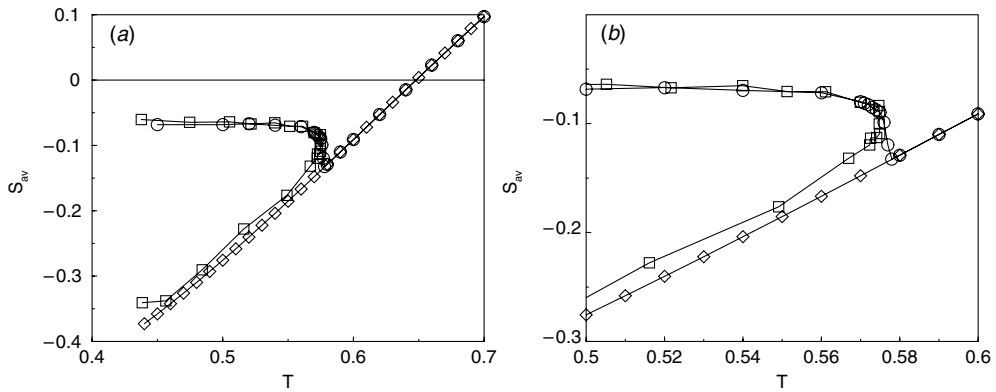


Figure 10. The dependence of the average entropy S_{av} on temperature at $\langle c \rangle = 3$. Symbols and parameters: as in figure 8(b), except that $N = 1000$ and 100 samples for the Potts glass state.

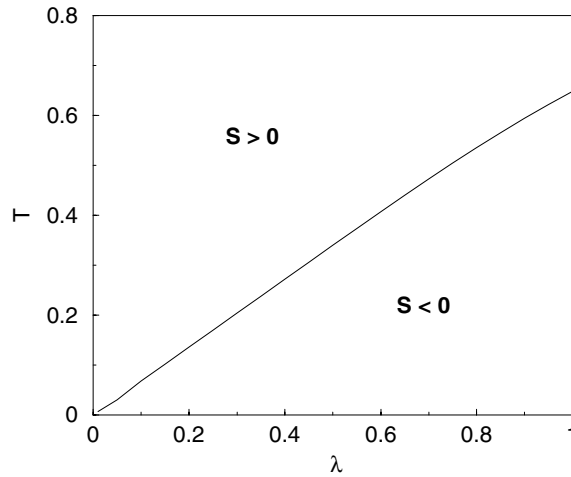


Figure 11. Regions of positive and negative entropies of the paramagnetic state for $\langle c \rangle = 3$ and $Q = 4$.

for the entropy can be derived analogously to appendix B. As shown in figure 11, the region of negative entropy of the paramagnetic state shrinks when the second nearest neighbouring interaction is reduced. Thus, in the absence of the second nearest neighbouring interaction, the region of paramagnetic phase with negative entropy is preempted by the Potts glass phase.

5.2. General values of $\langle c \rangle$

For general values of $\langle c \rangle$ we will consider three transition lines in the space of $\langle c \rangle$ and T : the zero entropy line in the paramagnetic phase, the spinodal line of the glassy state, and the paramagnetic–glass transition line. The transition lines are plotted in figure 12. When extrapolated to $T = 0$, the zero entropy, spinodal and free-energy crossing lines pass through the points $\langle c \rangle = 3.82, 3.65$ and 3.65 , respectively, in full agreement with the results obtained for the zero temperature case.

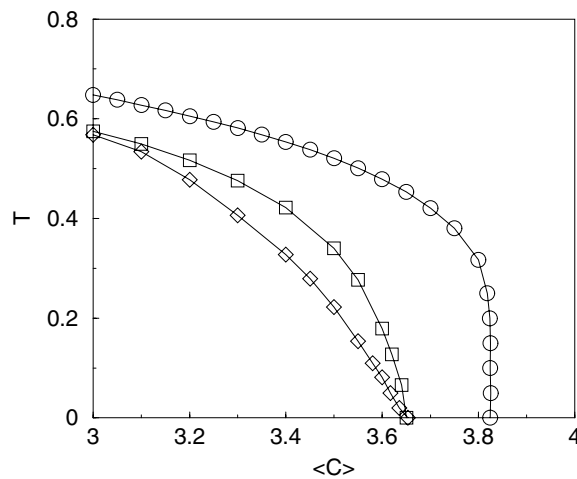


Figure 12. The zero entropy line (\circ), spinodal line (\square) and the paramagnetic–glass transition line (\diamond) in the space of the average connectivity $\langle c \rangle$ and temperature T for $Q = 4$.

In summary, the system has a paramagnetic phase at high temperature or high connectivity. Inferring from the studies of the graph colouring problem [9, 12], we expect that a phase transition to replica symmetry-breaking states takes place at the high temperature (and high connectivity) side of the zero entropy line, even when the system is still in the paramagnetic state. However, the location of this transition cannot be found in the present framework of replica symmetry.

Nevertheless, the replica symmetric solution has provided us insights on the full solution, suggesting the following picture. One expects the existence of the spinodal line, where the Potts glass state with a nonzero Edwards–Anderson order parameter exists in its low temperature (and low connectivity) side. The Potts glass state exists as a metastable state in the vicinity of the spinodal line. Then, at the low temperature (and low connectivity) side of the paramagnetic–glass transition line, the Potts glass state becomes thermodynamically stable.

6. Conclusion

We have studied the macroscopic behaviour in the colour diversity problem, a variant of the graph colouring problem of significant practical relevance, especially in the area of distributed storage and content distribution. To cope with the presence of second nearest neighbouring interactions, the analysis makes use of vertex free energies of two arguments, which enable us to study the behaviour in the RS analysis, and lays the foundation for future analyses incorporating replica symmetry-breaking effects. The analysis is successfully applied to graphs with mixed connectivities.

For $Q = 4$ and graphs with linear connectivity $3 \leq \langle c \rangle \leq 4$, the RS analysis identifies three transition lines according to: (i) when the entropy becomes negative (ending at $\langle c \rangle_s = 3.82$ when $T = 0$), signalling the breakdown of the RS ansatz, (ii) when q_{EA} becomes a multiple-valued function of T —the spinodal point (ending at $\langle c \rangle_{sp} = 3.65$ when $T = 0$) and (iii) the free-energy crossing point between the paramagnetic and Potts glass state (ending at $\langle c \rangle_c = 3.65$ when T approaches 0). The regime of negative entropy is so extensive that it covers

the entire Potts glass phase as well as part of the paramagnetic phase, and can be attributed to the increased frustration due to the presence of second nearest neighbouring interactions.

The picture that emerges is that the system is in a paramagnetic state at high temperature or high connectivity; the RS ansatz breaks down prior to the temperature that identifies the zero entropy transition point. The Potts glass state exists first as a metastable state but becomes dominant at a lower temperature (connectivity). Evidence from the population dynamics shows that the discontinuous transition takes place at the spinodal point rather than the crossing point. However, the RS analysis results in the average energy falling below the lowest possible energy for $3.48 < \langle c \rangle < 3.65$, and a region of negative entropy.

Since the entropy remains positive at the colourable–uncolourable transition [9, 12], we conjecture that if replica symmetry-breaking is taken into account, the Potts glass–paramagnetic transition should take place at the higher temperature (and high connectivity) side of the zero entropy line. For the optimization of the colour diversity, one should consider $T = 0$, implying that the incomplete–complete transition should take place at $\langle c \rangle$ beyond $\langle c \rangle_s = 3.82$. This estimate of the transition point seems to be supported by simulation results using the Walksat and BP algorithms [24].

In summary, we have demonstrated the value of different analytical approaches and the use of population dynamics in elucidating the system behaviour of the colour diversity problem on a sparse graph. They provide insights on the estimates of the transition points, the existence of metastable states and the nature of phase transitions.

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Appendix A. Replica approach to colour diversity

Consider the minimization of the energy (cost function) on a graph of connectivity c :

$$E = \sum_i \sum_{j_1 \neq \dots \neq j_c} a_{ij_1} \dots a_{ij_c} \phi(q_i, q_{j_1}, \dots, q_{j_c}), \quad (\text{A.1})$$

where ϕ is symmetric with respect to the permutation of the neighbours, $q_i \in \{1, \dots, Q\}$, and $a_{ij} = 1$ if nodes i and j are connected on the graph, and 0 otherwise. Since there are Q^{c+1} values of the function ϕ , one can write

$$\phi(q_i, q_{j_1}, \dots, q_{j_c}) = \sum_{m_0, \dots, m_c=1}^Q \phi_{m_0 \dots m_c} q_i^{m_0} \dots q_{j_c}^{m_c}. \quad (\text{A.2})$$

The partition function is

$$Z = \text{Tr}_{\mathbf{q}} \exp \left[-\beta \sum_i \sum_{j_1 \neq \dots \neq j_c} a_{ij_1} \dots a_{ij_c} \sum_{\mathbf{m}} \phi_{m_0 \dots m_c} q_i^{m_0} \dots q_{j_c}^{m_c} \right]. \quad (\text{A.3})$$

The replicated partition function, averaged over all graph configurations with connectivity c , is given by

$$\langle Z^n \rangle = \frac{1}{\mathcal{N}} \sum_{a_{ij}=0,1} \prod_i \delta \left(\sum_j a_{ij} - c \right) \times \text{Tr}_{\mathbf{q}} \exp \left[-\beta \sum_i \sum_{j_1 \neq \dots \neq j_c} a_{ij_1} \dots a_{ij_c} \sum_{\mathbf{m}, \alpha} \phi_{\mathbf{m}}(q_i^\alpha)^{m_0} \dots (q_{j_c}^\alpha)^{m_c} \right], \quad (\text{A.4})$$

where \mathcal{N} is the total number of graph representations with connectivity c .

It is convenient to express the exponential argument as an unrestricted sum over the nodes j_1, \dots, j_c ,

$$-\frac{\beta}{c!} \sum_i \left(\sum_{j_1 \dots j_c} -B_2 \sum_{j_1=j_2} \sum_{j_3 \dots j_c} -\dots + (-)^{c-1} B_c \sum_{j_1=\dots=j_c} \right) a_{ij_1} \dots a_{ij_c} \sum_{\mathbf{m}, \alpha} \phi_{\mathbf{m}}(q_i^\alpha)^{m_0} \dots (q_{j_c}^\alpha)^{m_c}, \quad (\text{A.5})$$

where B_2, \dots, B_c are integers accounting for the over-counting in rewriting the summations in terms of equal indices. Their precise values are not required in our final result. This allows us to factorize the expression into

$$-\frac{\beta}{c!} \sum_{\mathbf{m}, \alpha} \phi_{\mathbf{m}} \sum_i (q_i^\alpha)^{m_0} \left\{ \left[\sum_{j_1} a_{ij_1} (q_{j_1}^\alpha)^{m_1} \right] \dots \left[\sum_{j_c} a_{ij_c} (q_{j_c}^\alpha)^{m_c} \right] - B_2 \left[\sum_{j_1} a_{ij_1} (q_{j_1}^\alpha)^{m_1+m_2} \right] \left[\sum_{j_c} a_{ij_c} (q_{j_c}^\alpha)^{m_3} \right] \dots \left[\sum_{j_c} a_{ij_c} (q_{j_c}^\alpha)^{m_c} \right] + \dots + (-)^{c-1} B_c \left[\sum_{j_1} a_{ij_1} (q_{j_1}^\alpha)^{m_1+\dots+m_c} \right] \right\}. \quad (\text{A.6})$$

Following steps similar to those in [27], one gets

$$\langle Z^n \rangle = \exp N \left\{ \frac{c}{2} - c \sum_{\mathbf{r}, \mathbf{s}} \hat{Q}_{\mathbf{r}, \mathbf{s}} Q_{\mathbf{r}, \mathbf{s}} + \ln \text{Tr}_{\mathbf{q}} \prod_{m, \alpha} \left(\int \frac{d\hat{h}_m^\alpha dh_m^\alpha}{2\pi} \exp \left[\sum_{m, \alpha} (i\hat{h}_m^\alpha h_m^\alpha) \right] \right) \times \left[\sum_{r_m^\alpha, s_m^\alpha} \hat{Q}_{\mathbf{r}, \mathbf{s}} \prod_{m, \alpha} (-i\hat{h}_m^\alpha)^{r_m^\alpha} (q^\alpha)^{m s_m^\alpha} + \frac{1}{2} \sum_{r_m^\alpha, s_m^\alpha} \prod_{m, \alpha} \frac{(-i\hat{h}_m^\alpha)^{s_m^\alpha}}{r_m^\alpha! s_m^\alpha!} (q^\alpha)^{m r_m^\alpha} \right]^c \times \exp \left\{ -\frac{\beta}{c!} \sum_{\mathbf{m}, \alpha} \phi_{\mathbf{m}}(q^\alpha)^{m_0} [h_{m_1}^\alpha \dots h_{m_c}^\alpha - B_2 h_{m_1+m_2}^\alpha h_{m_3}^\alpha \dots h_{m_c}^\alpha + \dots + (-)^{c-1} B_c h_{m_1+\dots+m_c}^\alpha] \right\} \right\}, \quad (\text{A.7})$$

where $Q_{\mathbf{r}, \mathbf{s}}$ and $\hat{Q}_{\mathbf{r}, \mathbf{s}}$ are given by the saddle point equations of equation (A.7).

Consider the generating function

$$P_s(\mathbf{z}) = \sum_{\mathbf{r}} Q_{\mathbf{r}, \mathbf{s}} \prod_{m, \alpha} \frac{(z_\alpha)^{m r_m^\alpha}}{r_m^\alpha!}. \quad (\text{A.8})$$

In the replica symmetric ansatz, we consider functions of the form

$$P_s(\mathbf{z}) = \left\langle \prod_{\alpha} (\text{Tr}_{\mu} R(z_{\alpha}, \mu^{\alpha} | \mathbf{T}) (\mu^{\alpha})^{\sum_m m_s^{\alpha}}) \right\rangle. \quad (\text{A.9})$$

Substituting the saddle point equation for $Q_{r,s}$ into equation (A.8), one finds $P_s(\mathbf{z}) = N_P/D_P$ where

$$N_P = \left\langle \prod_{\alpha} \left\{ \text{Tr}_q \prod_{k=1}^{c-1} [\text{Tr}_{\mu_k} R(q^{\alpha}, \mu_k^{\alpha} | \mathbf{T}_k)] \prod_m (q^{\alpha})^{m_s^{\alpha}} \right. \right. \\ \times \exp \left[-\frac{\beta}{c!} \sum_{\mathbf{m}, \alpha} \phi_{\mathbf{m}}(q^{\alpha})^{m_0} (h_{m_1}^{\alpha} \cdots h_{m_c}^{\alpha} - B_2 h_{m_1+m_2}^{\alpha} h_{m_3}^{\alpha} \cdots h_{m_c}^{\alpha} \right. \\ \left. \left. + \cdots + (-)^{c-1} B_c h_{m_1+\cdots+m_c}^{\alpha} \right) \Big|_{h_m^{\alpha} = (z_{\alpha})^m + \sum_{k=1}^{c-1} (\mu_k^{\alpha})^m} \right] \Big\} \Bigg\rangle, \quad (\text{A.10})$$

and D_P is a constant having the same expression as that of N_P , except that k runs from 1 to c and z^{α} are set to 0.

The expression in the exponential argument of N_P can be further simplified. Rewriting ϕ as unrestricted sums over the neighbours analogously to equation (A.6),

$$\phi(q^{\alpha}, \mu_1^{\alpha}, \dots, \mu_c^{\alpha}) = \frac{1}{c!} \sum_{\mathbf{m}} \phi_{\mathbf{m}}(q^{\alpha})^{m_0} \left\{ \left[\sum_{k=1}^c (\mu_k^{\alpha})^{m_1} \right] \cdots \left[\sum_{k=1}^c (\mu_k^{\alpha})^{m_c} \right] \right. \\ \left. - B_2 \left[\sum_{k=1}^c (\mu_k^{\alpha})^{m_1+m_2} \right] \left[\sum_{k=1}^c (\mu_k^{\alpha})^{m_3} \right] \cdots \left[\sum_{k=1}^c (\mu_k^{\alpha})^{m_c} \right] \right. \\ \left. + \cdots + (-)^{c-1} B_c \left[\sum_{k=1}^c (\mu_k^{\alpha})^{m_1+\cdots+m_c} \right] \right\}. \quad (\text{A.11})$$

Identifying each term in the square bracket as $h_1^{\alpha}, \dots, h_Q^{\alpha}$, we recognize the exponential argument as $-\beta \sum_{\alpha} \phi(q^{\alpha}, z^{\alpha}, \mu_1^{\alpha}, \dots, \mu_{c-1}^{\alpha})$. We can now identify a recursion relation for the function R which does not involve replica indices,

$$R(z, q | \mathbf{T}) = \frac{1}{D_R} \prod_{k=1}^{c-1} [\text{Tr}_{\mu_k} R(q, \mu_k | \mathbf{T}_k)] \exp[-\beta \phi(q, z, \mu_1, \dots, \mu_{c-1})]. \quad (\text{A.12})$$

The denominator is given, in the limit n approaching 0,

$$D_R = \exp \left\langle \ln \left\{ \text{Tr}_{q, \mu_k} \prod_{k=1}^c [R(q, \mu_k | \mathbf{T}_k)] \exp[-\beta \phi(q, \mu_1, \dots, \mu_c)] \right\} \right\rangle. \quad (\text{A.13})$$

Letting the vertex free energy be defined by $F^V(z, q | \mathbf{T}) = -T \ln R(z, q | \mathbf{T})$, we arrive at the recursion relation (7) and the average free energy (8).

Appendix B. Free energy and energy in the paramagnetic state

The average free energy is given by

$$F_{\text{av}} = P(C_j = 3) F_{\text{av}}|_{C=3} + P(C_j = 4) F_{\text{av}}|_{C=4} - \frac{\langle c \rangle}{2} \sum_{C_i C_j} \frac{C_i P(C_i)}{\langle c \rangle} \frac{C_j P(C_j)}{\langle c \rangle} F_{\text{link}}|_{C_i C_j}, \quad (\text{B.1})$$

where

$$\begin{aligned}
F_{\text{av}}|_{C=3} &= 4 - \langle T \ln Q \{ Q_1 Q_2 Q_3 + 3Q_1 Q_2 z^2 + Q_1 z^6 + [Q_1 Q_2 z^2 + Q_1 z^4](z_{j1} + z_{j2} + z_{j3}) \\
&\quad + Q_1 z^6(z_{j1} z_{j2} + z_{j2} z_{j3} + z_{j1} z_{j3}) + z^{12} z_{j1} z_{j2} z_{j3} \} \rangle, \\
F_{\text{av}}|_{C=4} &= 5 - \langle T \ln Q \{ Q_1 Q_2 Q_3 Q_4 + 6Q_1 Q_2 Q_3 z^2 + 3Q_1 Q_2 z^4 + 4Q_1 Q_2 z^6 + Q_1 z^{12} \\
&\quad + [Q_1 Q_2 Q_3 z^2 + 3Q_1 Q_2 z^4 + Q_1 z^8](z_{j1} + z_{j2} + z_{j3} + z_{j4}) \\
&\quad + [Q_1 Q_2 z^6 + Q_1 z^8](z_{j1} z_{j2} + z_{j1} z_{j3} + z_{j1} z_{j4} + z_{j2} z_{j3} + z_{j2} z_{j4} + z_{j3} z_{j4}) \\
&\quad + Q_1 z^{12}(z_{j1} z_{j2} z_{j3} + z_{j1} z_{j2} z_{j4} + z_{j1} z_{j3} z_{j4} + z_{j2} z_{j3} z_{j4}) + z^{20} z_{j1} z_{j2} z_{j3} z_{j4} \} \rangle, \\
F_{\text{link}}|_{C_i C_j} &= \langle -T \ln Q [Q - 1 + z_{ij} z_{ji}] \rangle_{C_i C_j}. \tag{B.2}
\end{aligned}$$

The average energy is given by

$$E_{\text{av}} = P(C_j = 3) E_{\text{av}}|_{C=3} + P(C_j = 4) E_{\text{av}}|_{C=4}, \tag{B.3}$$

the components of which take the form

$$E_{\text{av}}^{(3)}|_{C=3} = \left\langle \frac{E_N^{(3)}}{E_D^{(3)}} \right\rangle \quad \text{and} \quad E_{\text{av}}^{(4)}|_{C=4} = \left\langle \frac{E_N^{(4)}}{E_D^{(4)}} \right\rangle, \tag{B.4}$$

where

$$\begin{aligned}
E_D^{(3)} &= Q_1 Q_2 Q_3 + 3Q_1 Q_2 z^2 + Q_1 z^6 + [Q_1 Q_2 z^2 + Q_1 z^4](z_{j1} + z_{j2} + z_{j3}) \\
&\quad + Q_1 z^6(z_{j1} z_{j2} + z_{j2} z_{j3} + z_{j1} z_{j3}) + z^{12} z_{j1} z_{j2} z_{j3}, \\
E_N^{(3)} &= 4Q_1 Q_2 Q_3 + 18Q_1 Q_2 z^2 + 10Q_1 z^6 + [6Q_1 Q_2 z^2 + 8Q_1 z^4](z_{j1} + z_{j2} + z_{j3}) \\
&\quad + 10Q_1 z^6(z_{j1} z_{j2} + z_{j2} z_{j3} + z_{j1} z_{j3}) + 16z^{12} z_{j1} z_{j2} z_{j3}, \\
E_D^{(4)} &= Q_1 Q_2 Q_3 Q_4 + 6Q_1 Q_2 Q_3 z^2 + Q_1 Q_2 z^4 + 4Q_1 Q_2 z^6 + Q_1 z^{12} \\
&\quad + [Q_1 Q_2 Q_3 z^2 + 3Q_1 Q_2 z^4 + Q_1 z^8](z_{j1} + z_{j2} + z_{j3} + z_{j4}) \\
&\quad + [Q_1 Q_2 z^6 + Q_1 z^8](z_{j1} z_{j2} + z_{j1} z_{j3} + z_{j1} z_{j4} + z_{j2} z_{j3} + z_{j2} z_{j4} + z_{j3} z_{j4}) \\
&\quad + Q_1 z^{12}(z_{j1} z_{j2} z_{j3} + z_{j1} z_{j2} z_{j4} + z_{j1} z_{j3} z_{j4} + z_{j2} z_{j3} z_{j4}) + z^{20} z_{j1} z_{j2} z_{j3} z_{j4}, \\
E_N^{(4)} &= 5Q_1 Q_2 Q_3 Q_4 + 42Q_1 Q_2 Q_3 z^2 + 27Q_1 Q_2 z^4 + 44Q_1 Q_2 z^6 + 17Q_1 z^{12} \\
&\quad + [7Q_1 Q_2 Q_3 z^2 + 27Q_1 Q_2 z^4 + 13Q_1 z^8](z_{j1} + z_{j2} + z_{j3} + z_{j4}) \\
&\quad + [11Q_1 Q_2 z^6 + 13Q_1 z^8](z_{j1} z_{j2} + z_{j1} z_{j3} + z_{j1} z_{j4} + z_{j2} z_{j3} + z_{j2} z_{j4} + z_{j3} z_{j4}) \\
&\quad + 17Q_1 z^{12}(z_{j1} z_{j2} z_{j3} + z_{j1} z_{j2} z_{j4} + z_{j1} z_{j3} z_{j4} + z_{j2} z_{j3} z_{j4}) + 25z^{20} z_{j1} z_{j2} z_{j3} z_{j4}.
\end{aligned}$$

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