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Application of Statistical Mechanics to Combinatorial Optimization Problems: The Chromatic Number Problem and q-Partitioning of a Graph

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Methods of statistical mechanics are applied to two important NP-complete combinatorial optimization problems. The first is the chromatic number problem, which seeks the minimal number of colors necessary to color a graph such that no two sites connected by an edge have the same color. The second is partitioning of a graph into q equal subgraphs so as to minimize intersubgraph connections. Both models are mapped into a frustrated Potts model, which is related to the q-state Potts spin glass. For the first problem, we obtain very good agreement with numerical simulations and theoretical bounds using the annealed approximation. The quenched model is also discussed. For the second problem we obtain analytic and numerical results by evaluating the ground-state energy of the $q=3$ and 4 Potts spin glass using Parisi's replica symmetry breaking. We also perform some numerical simulations to test the theoretical result and obtain very good agreement.

KEY WORDS: NP-complete optimization problems; spin glass; Potts model; graph coloring; graph partitioning.

1. INTRODUCTION

In recent years, there has been much interest in investigating various combinatorial optimization problems using the concepts and methods of statistical mechanics. Special attention has been concentrated on the so-called NP-complete optimization problems, which are very hard to deal with. Optimization problems such as the traveling salesman problem,[1-3]

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graph bipartitioning,[4] planar graph coloring,[5] and the bipartite matching problem[6] (a P-class problem) were analyzed using the ideas and techniques of disordered systems such as a spin glass.

In simple terms, NP-complete problems are difficult in the sense that it is extremely unlikely that an algorithm whose computing time goes as a polynomial function of the size of the problem can be found; "complete" means that for all those NP-complete problems, if a polynomial algorithm is found for any one of them, then polynomial algorithms exist for all the others.[7] But until now, despite the innumerable efforts by mathematicians and computer experts, no polynomial algorithm has been found for any of these NP-complete problems; so it is highly probable that such polynomial algorithms do not exist. Thus, from the practical point of view, the time needed to find a numerical solution to the NP-problems grows faster than any polynomial function of the size of the problem and for large systems, the direct approach very quickly becomes intractable.

Fortunately, statistical mechanics often deals with systems of large size (thermodynamic limit) and thus may provide a general understanding of the nature of the NP problem. The approach is to treat the NP problem as a random system with the random variables following a certain probability distribution and to extract the generic or average information and obtain the most probable results. Thus, one obtains results that do not depend on the particular realization of the problem, but are applicable to "almost all" realizations as the size of the problem becomes very large. In addition, this theoretical investigation might help to improve the heuristics of the algorithm in searching for the optimal solution.

Many of the combinatorial optimization problems have much in common with the spin-glass model.[1–4] The reason for this similarity is that in searching for the optimal solution in a combinatorial optimization problem, the algorithms can often get trapped in one of the many local minima and fail to reach the absolute minimal solution. A spin-glass model is also characterized by many local minima of its free energy.

In this paper, we will study the statistical mechanics of two NP-complete problems using the q-state Potts model as our tool. These problems are the chromatic number problem and the q-partitioning of a graph. The practical applications of these problems in the real world are discussed in the following sections.

2. THE CHROMATIC NUMBER PROBLEM

2.1. The Problem

The problem is specified as follows: Given a graph $G(V, E)$, where V is the set of vertices ($|V| = N$) and E is the set of edges, what is the minimum

number of colors (the chromatic number χ) needed to color the vertices such that no two vertices connected by an edge will have the same color? The planar version of this problem is related to the famous "four-color theorem," which states that for any planar map the chromatic number is at most four.[8] However, the general problem of determining the chromatic number was shown to be NP-complete.[9]

A well-known application of this problem is as follows: At the end of the semester, students should sit for examinations within a short period of time. It is desirable that each student sits daily for at most one examination and all students having the same examination take it at the same time, and the number of days needed to finish all examinations should be minimized. Let V be the set of examinations and Y be the set of students. For each examination v, let $S(v) \subset Y$ be the set of students who must take v. Construct the graph $G(V, E)$, where $(v, v') \in E$ if $S(v) \cap S(v') \neq \varnothing$ (i.e., v and v' cannot be held at the same time). Then a coloring of G corresponds to a possible assignment for the set of examinations. The number of colors is the number of days needed and the problem reduces to that of finding $\chi(G)$.

In this paper, we investigate the random version of the chromatic problem, i.e., the graph G is a random graph $G_{N,p}$, where N is the number of vertices and p is the probability that any two vertices are connected by an edge (model A in graph theory[10]). Two important results due to Erdos and Spencer[11] and Bollobas and Erdos[12] are on the bounds of χ for almost every $G_{N,p}$:

For $p = 2c/N$ and c large,

$$[1 + o(1)]\frac{c}{\ln c} < \chi < [1 + o(1)]\frac{2c}{\ln c} \tag{2.1}$$

where $o(1)$ is with respect to c.

For p fixed, independent of N,

$$\left(\frac{1}{2} - \varepsilon\right)\frac{N \ln[1/(1-p)]}{\ln N} < \chi < (1 + \varepsilon)\frac{N \ln[1/(1-p)]}{\ln N} \tag{2.2}$$

In the case of (2.2), the upper bound is obtained by the "greedy algorithm,"[13] which can color the graph satisfactorily, but the number of colors used may not be minimal. It is believed[12] that most likely the greedy algorithm uses twice as many colors as necessary and hence χ should be closer to the lower bound. Furthermore, it was conjectured[13] that χ goes to the lower bound as $N \to \infty$ in (2.1) and (2.2); however, there has been no proof of this. No known polynomial algorithm can approximate χ to within any constant factor.[14,15] Also, there has not been

much simulation work done for large N; after all, this is an NP problem. One result is,[16] for $G_{1000,\,0.5}$,

$$\chi \sim 85 \pm 12 \tag{2.3}$$

In the next section, we show how methods of statistical mechanics yield results that agree with (2.1)–(2.3).

2.2. Statistical Mechanical Treatment

It has been shown that the graph coloring problem is related to the Potts model[17,18] and we shall make use of this idea by considering the q-state antiferromagnetic Potts Hamiltonian

$$H = \sum_{i<j}^{N} J_{ij}\delta_{\sigma_i\sigma_j} \tag{2.4}$$

where σ_i, which can take q values (colors), is the spin at the ith vertex; $J_{ij} > 0$ is the coupling between the vertices i and j; and N is the number of vertices. We consider a random graph $G_{N,p}$; J_{ij} has the distribution

$$p(J_{ij}) = p\delta(J_{ij} - J) + (1-p)\,\delta(J_{ij}); \qquad J > 0 \tag{2.5}$$

$J_{ij} = 0$ means that there is no edge joining vertices i and j. Since

$$\lim_{\beta\to\infty} \exp(-\beta J_{ij}\delta_{\sigma_i\sigma_j}) = \begin{cases} 0 & \text{iff} \quad J_{ij} \neq 0 \text{ and } \sigma_i = \sigma_j \\ 1 & \text{iff} \quad J_{ij} = 0 \text{ or } \sigma_i \neq \sigma_j \end{cases} \tag{2.6}$$

it is evident that the zero-temperature partition function

$$\lim_{\beta\to\infty} Z_G = \lim_{\beta\to\infty} \operatorname{Tr} \exp\left(-\beta \sum_{i<j}^{N} J_{ij}\delta_{\sigma_i\sigma_j}\right) \equiv P_G(q, N) \tag{2.7}$$

gives the number of ways to color G with q colors such that no two vertices connected by a bond have the same color.

Since $P_G(q, N)$ is a nondecreasing function of q, χ is given by the minimal integer value of q such that $P_G(q, N)$ attains its least positive integer value. Notice that this model, (2.4) and (2.5), contains an important element, namely frustration, which gives rise to interesting features.

We then compute the average P_G with probability distribution given by (2.5), or in spin-glass terms, we calculate the "annealed average." Using (2.5), one has

$$\bar{Z}_G(q, N; \beta) = \operatorname*{Tr}_{\sigma} \prod_{i<j}^{N} [p \exp(-\beta J \delta_{\sigma_i \sigma_j}) + 1 - p]$$

$$= \operatorname*{Tr}_{\sigma} \exp\left\{\ln[1 - p(1 - e^{-\beta J})] \sum_{i<j}^{N} \delta_{\sigma_i \sigma_j}\right\} \tag{2.8}$$

Taking the limit $\beta \to \infty$, we obtain

$$\bar{P}_G(q, N) = \lim_{\beta \to \infty} \bar{Z}_G = \operatorname*{Tr}_{\sigma} \exp\left\{-\ln[1/(1-p)] \sum_{i<j}^{N} \delta_{\sigma_i \sigma_j}\right\} \tag{2.9}$$

i.e., the average number of ways to color $G_{N,p}$ using q colors can be written as the partition function of an infinite-range antiferromagnetic Potts model with coupling constant $\ln[1/(1-p)]$. Using the results of the infinite-range antiferromagnetic Potts model (see Appendix A), one gets from (A.3)

$$\operatorname*{Tr}_{\sigma} \exp\left(\frac{-K}{N} \sum_{i<j}^{N} \delta_{\sigma_i \sigma_j}\right) = q^N \exp \frac{-KN}{2q} \tag{2.10}$$

We distinguish now the two cases $p = 2c/N$ and p independent of N. In the first case

$$\ln \frac{1}{1-p} = \frac{2c}{N} + O\left(\frac{1}{N^2}\right) \tag{2.11}$$

In this case $K = 2c$ and

$$\bar{P}_G(q, N) = (qe^{-c/q})^N \tag{2.12}$$

Thus, the value of q that makes this quantity equal to 1 is given by

$$q^* e^{-c/q^*} = 1 \qquad \text{i.e.,} \qquad q^* \ln q^* = c \tag{2.13}$$

or

$$q^* = \frac{c}{\ln c}\left\{1 + \frac{\ln \ln c}{\ln c} + O\left[\left(\frac{\ln \ln c}{\ln c}\right)^2\right]\right\} \tag{2.14}$$

Note that in this case the "free energy" $\overline{\ln P_G}$ is extensive ($\propto N$). The χ is given by $[q^*]$, where $[\ ]$ denotes the next higher integer.

In the case that p is independent of N,

$$K = N \ln \frac{1}{1-p}$$

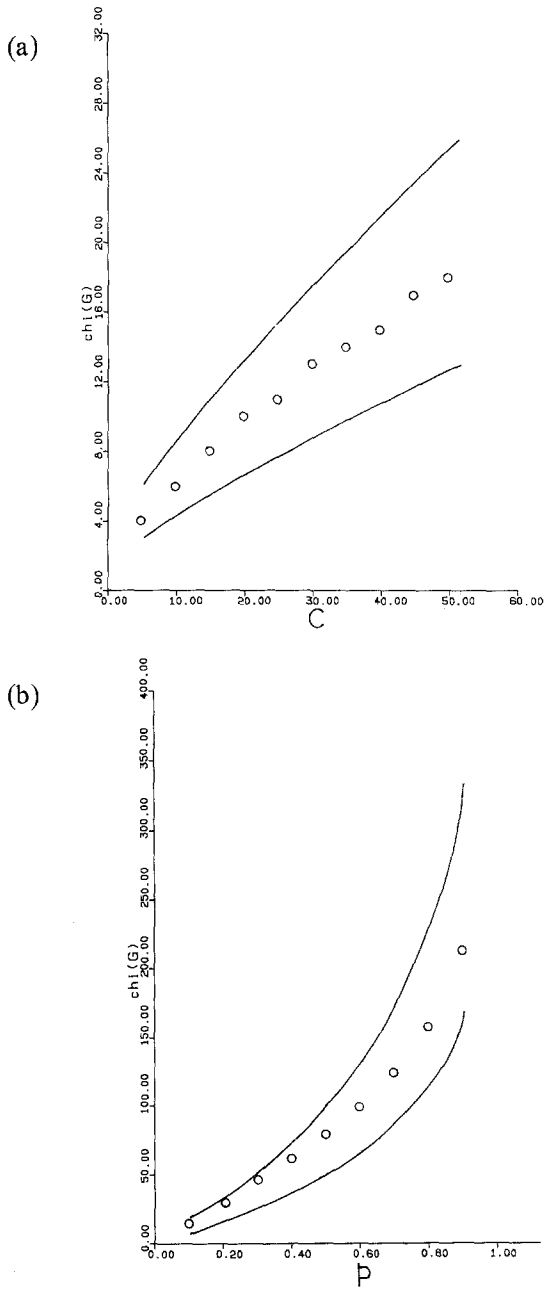

Fig. 1. (a) Solution of (2.13): χ versus c. (—) The upper and lower bounds from (2.1). (b) Solution of (2.16): χ versus p for $N = 1000$. (—) The upper and lower bounds from (2.2).

and we find from Eq. (A.3) that

$$\bar{P}_G(q, N) = [q(1-p)^{N/2q}]^N \tag{2.15}$$

and hence

$$q^*(1-p)^{N/2q^*} = 1 \tag{2.16}$$

which implies

$$q^* = \frac{N \ln[1/(1-p)]}{2 \ln N}(1+\gamma) \tag{2.17}$$

where

$$\gamma = \frac{\ln \ln N}{\ln N} - \frac{\ln\{\ln[1/(1-p)]/2\}}{\ln N} + O\left[\left(\frac{\ln \ln N}{\ln N}\right)^2\right] \tag{2.18}$$

and χ is equal to $[q^*]$.

We see that the value (2.14) is consistent with the bounds given by (2.1) and actually coincides with the lower bound. If one is to trust the annealed approximation, it also yields the $o(1)$ term in (2.1) as spelled out in Eq. (2.14). Similarly, Eq. (2.17) lies between the bounds given in (2.2) and the leading corrections to the lower bound are given in Eq. (2.18). Ignoring terms of $O(1)$ with respect to N, the result coincides with the lower bound as given in Eq. (2.2), as has been conjectured.[12,13] Numerical solutions of Eqs. (2.13) and (2.16) that take into account the corrections to the leading N results are displayed in Fig. 1. For $G_{1000,0.5}$, Eq. (2.2) yields $50 < \chi < 100$, whereas our numerical result gives $\chi = 80$. As mentioned before, numerical simulations[16] yield $\chi = 85 \pm 12$.

2.3. Discussion

Unlike the graph partitioning, matching, and traveling salesman problems, in which the cost function is directly related to the energy or Hamiltonian of the corresponding spin system, in the chromatic number problem, the variable of interest, χ, is not directly related to the energy. The relevant quantity is the zero-temperature partition function or $P_G(q)$, which is the number of ways to color G. In a simulation, one would first find χ_G for each G generated by calculating the lowest integer $[q^*]$ for which $P_G(q) \geqslant 1$, and then take the average $\chi = \bar{\chi}_G$. But there is no guarantee for the self-averageness of χ! Loosely speaking, extensive quantities are self-averaging. By a simple argument similar to Brout,[19] for $p = 2c/N$ (a

short-range system), $\ln P_G$ is self-averaging. In fact, our calculation shows that, for finite q, in order to keep $\ln P_G$ extensive, one has to choose

$$N \ln[1/(1-p)] = \text{const}, \qquad \text{i.e.,} \qquad p = \text{const}/N + O(1/N^2) \quad (2.19)$$

However, the short-ranged spin glass is still intractable, which makes $\overline{\ln P_G}$ impossible to calculate. And the "annealed" result (2.17) seems the best one can get at this time. In Appendix B, we show the version of the short-range spin glass corresponding to the chromatic number problem.

For the case $p = \text{const}$, independent of N, things get more complicated. First, we know that $\chi \sim N/\ln N$, which is not extensive, hence χ may not be self-averaging. Second, since now $\overline{\ln P_G}$ depends on q, which goes as $N/\ln N$, this strange dependence on N makes $\overline{\ln P_G}$ also not extensive. Even before taking the zero-temperature limit and retaining both J and β in the calculation, we did not find a way to scale J or β with N to make $\overline{\ln P_G}$ extensive.

3. q-PARTITIONING OF GRAPH

3.1. The Problem and Statistical Model

This problem is also specified by a graph $G(V, E)$, where $|V| = N$ is an integral multiple of q. One is then asked to divide the N vertices into q groups of equal size, say $V = \bigcup_{i=1}^{q} V_i$, such that the total number of intergroup edges is minimized. This problem and its generalizations are frequently encountered in the real world; a few examples are listed below:

In assigning chips to circuit boards in computer design, one likes to group electrical modules into packages so as to minimize the connections between packages.[20] In placing a collection of intercommunicating routines onto a paged storage device, one wishes to put routines that reference each other on the same page in order to minimize page faults during execution.[21] In the business world, workers in a multistory office building who frequently interact with each other should be placed on the same floor in order to minimize the effort of traveling up and down.

The q-partitioning of a graph is an NP-complete problem and some studies had been done by MacGregor[22] and Bui *et al.*[23] The special case of graph bipartitioning was investigated in terms of statistical mechanics by Fu and Anderson.[4] In this paper, we generalize the case to q-partitioning of a graph and obtain results for 3- and 4-partitioning of random graphs.

Random graphs $G_{N,p}$ of the type discussed in the previous section are again considered. We define a spin system corresponding to the graph by

associating a q-state Potts spin σ_i with the ith vertex and considering the Hamiltonian

$$H=\frac{-2}{q}\sum_{i<j}^{N} J_{ij}(q\delta_{\sigma_i\sigma_j}-1) \tag{3.1}$$

where $J_{ij}=J$ if the corresponding edge of G exists and zero otherwise. Thus, for random graphs that obey the distribution (2.5), this is essentially a dilute, infinite-range ferromagnetic Potts system with the constraint

$$\sum_{i,j}^{N}\left(\delta_{\sigma_i\sigma_j}-\frac{1}{q}\right)=0 \tag{3.2}$$

If we choose the possible values of σ_i to the various qth roots of unity, then the constraint (3.2) is equivalent to the $q-1$ constraints

$$\sum_{i=1}^{N}\sigma_i^r=0 \qquad \text{for} \quad r=1, 2,..., q-1 \tag{3.2'}$$

When the graph G is partitioned into q equal subgraphs, all the spins that take the same value belong to the same subgraph. Thus, (3.2) and (3.2') just follow from the requirement that the q subgraphs are equal and mutually exclusive. From (3.1) we can write H as

$$\begin{aligned} H=&-(q-1)\left(\sum_{i,j\in V_1}+\cdots+\sum_{i,j\in V_q}\right)J_{ij}\Big/q \\ &+\left(\sum_{\substack{i\in V_1\\ j\in V_2}}+\cdots+\sum_{\substack{i\in V_1\\ j\in V_q}}+\cdots+\sum_{\substack{i\in V_q\\ j\in V_1}}+\cdots+\sum_{\substack{i\in V_q\\ j\in V_{q-1}}}\right)J_{ij}\Big/q \\ =&\frac{-p(q-1)JN(N-1)}{q}+2CJ \end{aligned} \tag{3.3}$$

where C is the cost function to be minimized. It measures the total number of bonds (edges) that connect sites belonging to different subgraphs. From (3.3) it follows that

$$C=\frac{H}{2J}+\frac{N(N-1)\,p(q-1)}{2q} \tag{3.4}$$

Note that the antiferromagnetic constraint (3.2) causes spin frustration and leads to the difficulty of an NP problem. To calculate the average optimized cost function, one needs to compute the average free energy at zero temperature, as shown in the following section.

3.2. RESULTS AND DISCUSSION

Starting with the Hamiltonian (3.1) and the constraint (3.2), we derive in Appendix C an expression for the cost function C given Eq. (3.4) in the form

$$C = \frac{N^2 p(q-1)}{2q} + \lim_{\beta \to \infty} \frac{F}{2J} \tag{3.5}$$

with

$$-\beta F = N(q-1)\, K^2 p(1-p) + \lim_{n \to \infty} \frac{1}{n} \left\{ \operatorname{Tr}_{\sigma} \exp \left[\frac{2K^2 p(1-p)}{N} \sum_{\alpha < \gamma}^{n} \sum_{r,r=1}^{q-1} \left| \sum_{i=1}^{N} (\sigma_i^{\alpha})^r (\sigma_i^{\gamma})^{r'} \right|^2 \right] - 1 \right\} \tag{3.6}$$

where $K = \beta J N^{1/2}/q$. Here J is taken to be of $O(1/N^{1/2})$, and thus $K \sim O(1)$ with respect to N.

Equation (3.6) is of the form of the free energy of a Potts spin glass, and can be simplified along lines similar to that of the Ising spin glass as was first done by Sherrington and Kirpatrick[24] and further improved in the ordered phase by Parisi.[25] Some aspects of the Potts spin glass of the infinite-range type were investigated by Elderfield and Sherrington[26] and by Gross *et al.*[27] These authors found that the order of the finite-temperature phase transition changes for $q > 4$ as opposed to $q < 4$. But the ground-state energy for the case of $q = 3$ and $q = 4$ that is required for the 3- and 4-fold graph partitioning has not been done. Here we will report on a derivation of the ground-state energy with a first-stage replica-symmetry breaking (RSB), using similar steps to those used by Parisi[25] in the case of $q = 2$.

Performing a Gaussian transformation to decouple the quartic spin term in the exponent of Eq. (3.6) by introducing the Edwards–Anderson order parameter $Q_{\alpha\gamma}$, one obtains

$$\beta F/N = -(q-1)\, K^2 p(1-p) + \operatorname{Max}\{f(Q)\} \tag{3.7}$$

with

$$f(Q) = \lim_{n \to 0} \frac{1}{n} \left\{ \frac{q-1}{8K^2 p(1-p)} \sum_{\alpha < \gamma}^{n} Q_{\alpha\gamma}^2 - \ln \operatorname{Tr}_{\sigma} \exp \left[\sum_{\alpha < \gamma}^{n} Q_{\alpha\gamma} \sum_{r=1}^{q-1} (\sigma^{\alpha} \sigma^{\gamma})^r \right] \right\} \tag{3.8}$$

To take the limit $n \to 0$, one has to break the replica symmetry of the

matrix $Q_{\alpha\gamma}$ in order to obtain the correct answer. With first-stage RSB approximation, the matrix $Q_{\alpha\gamma}$ is divided into blocks characterised by the parameter m in the following way: The replica index α is grouped into n/m clusters, where $n \geqslant m \geqslant 1$, with

$$Q_{\alpha\alpha} = 0$$
$$Q_{\alpha\gamma}(\alpha \neq \gamma) = \begin{cases} Q_0 & \text{if } \alpha, \gamma \in \text{same cluster} \\ Q_1 & \text{otherwise} \end{cases} \tag{3.9}$$

In taking the limit $n \to 0$, m may take nonintegral values $1 \geqslant m \geqslant 0$. In other words, the well-known order parameter function $Q(x)$ is a single step function with the breaking point $x = m$. The replica-symmetric case can be obtained by setting $Q_0 = Q_1$. Following a similar procedure as in the Ising case, we obtain for the q-state Potts model

$$\begin{aligned} f(Q) = & -(q-1)\, q^2 \bar{K}^2 \{q^2[(1-m)\, Q_0^2 + m Q_1^2]/16 - Q_0/2\} \\ & - \frac{1}{m} \int D(x, y) \ln \Bigg[\int D(u, v) \\ & \times \Bigg(\operatorname*{Tr}_{\sigma} \exp \Bigg\{ q\bar{K} \Bigg[Q_1^{1/2} \sum_{r=1}^{q-1} (x_r \operatorname{Re} \sigma^r + y_r \operatorname{Im} \sigma^r) \\ & + (Q_0 - Q_1)^{1/2} \sum_{r=1}^{q-1} (u_r \operatorname{Re} \sigma^r + v_r \operatorname{Im} \sigma^r) \Bigg] \Bigg\} \Bigg)^m \Bigg] \end{aligned} \tag{3.10}$$

where $\bar{K} = [p(1-p)]^{1/2} K$ and

$$\int D(x, y) \equiv \int_{-\infty}^{\infty} \prod_{r=1}^{q-1} \left(\frac{dx_r\, dy_r}{2\pi} \exp - \frac{x_r^2 + y_r^2}{2} \right)$$

Then F is maximized using a standard routine and the zero-temperature energy is obtained. From (3.5) the cost function is then

$$C = \frac{N^2 p(q-1)}{2q} + \frac{u_q N^{3/2} [p(1-p)]^{1/2}}{2} \tag{3.11}$$

where u_q is independent of p and N. Values of u_q for $q = 2, 3, 4$ with no and first-stage replica symmetry breaking are shown in Table I. The value of u_∞ is obtained from Gross *et al.*,[27] who discuss the limit $q \to \infty$.

From a simple consideration, the expected number of intercluster edges without minimization would be

$$\frac{N}{q}(q-1)\, Np \frac{1}{2} = \frac{N^2 p(q-1)}{2q} \tag{3.12}$$

Table I. Values of u_q^0, No Replica Symmetry Breaking, and u_q^1, First-Stage Replica Symmetry Breaking[a]

q	$-u_q^0$	$-u_q^1$
2	0.80	0.76
3	1.00	0.98
4	1.10	1.08
∞	$2(\ln q/q)^{1/2}$	

[a] The value of $q \to \infty$ is from Gross *et al.*[27]

Thus, the second term in (3.11) is the improvement due to optimization.

To compare our result for $q = 3$, we simulate random graphs and find the near-optimal cost function (after all, this is an NP problem; no polynomial algorithm can guarantee an absolute optimal solution) with the computer. The algorithm we use first divides the graph arbitrarily into three parts. It then checks if interchanging two sites belonging to two different subgraphs lowers the number of intersubgraph edges. If it does, the two sites are interchanged and the procedure continues until no further improvement can be achieved. The results are shown in Table II. The agreement is better for larger N, as expected, since (3.11) holds in the large-N limit. Also, MacGregor's[22] result on random graph analysis indicated that for $q \gg 2$ almost all edges are intercluster edges (i.e., $C \to N^2p/2$) and there is no improvement due to optimization. This agrees with our result from (3.11) and Table I for $q \to \infty$.

Table II. Values of C_1/C_2 for $q = 3$[a]

	C_1/C_2		
p	$N = 30$	$N = 48$	$N = 99$
0.2	1.51	1.14	1.07
0.5	1.12	1.08	1.06
0.8	1.49	1.15	1.02

[a] C_1 is the average cost function from simulation of several random graphs, ten graphs for $N = 30$, five for $N = 48$, and one for $N = 99$. The values of C_2 are from (3.11) with u_q^1 in Table I.

4. CONCLUSION

In this paper, we have studied the chromatic number problem and the problem of q-partitioning of a graph. Both are NP-complete optimization problems, which can be formulated in statistical mechanical terms by a dilute Potts model with the essential feature of frustration.

The "annealed" results (2.14) and (2.17) of the chromatic number problem agree surprisingly well with all the known bounds, the experimental datum, and even with the conjecture. However, difficulties arise in the "quenched" case, first in the intractability of the short-range ($p \sim 1/N$) spin-glass system and the inextensivity of $\overline{\ln P_G}$ in the long-range ($p = \text{const}$) situation.

For the problem of q-partitioning of a graph, we generalized the 2-partitioning problem and obtained analytically the expression for the cost function for general q. Explicit results are obtained for $q = 3$ and 4, and the $q = 3$ result is checked against our numerical simulation; the agreement seems very good.

APPENDIX A

For $\beta H = (K/N) \sum_{i<j}^{N} \delta_{\sigma_i \sigma_j}$ with $K > 0$, one gets[17]

$$\frac{\beta F(x_i)}{N} = \sum_{i=1}^{q} \left(x_i \ln x_i + \frac{K x_i^2}{2} \right) \qquad \text{with} \quad \sum_{i=1}^{q} x_i = 1 \tag{A.1}$$

where x_i is the fraction of spins in the ith state. $x_i = 1/q$ for all i is a disordered solution and is the ground-state solution, since the system is fully frustrated. Thus

$$\beta F = -N \ln q + \frac{KN}{2q} = -\ln Z \tag{A.2}$$

and

$$Z = q^N e^{-KN/2q} \tag{A.3}$$

APPENDIX B

In this Appendix, we show how the calculation of $\overline{\ln P_G}$ for the graph coloring problem maps into a Potts spin-glass model. This method is a generalizaton of the method used by Fu and Anderson[4] for a bond dilute Ising model. Starting from the Hamiltonian (2.4),

$$H = \sum_{i<j}^{N} J_{ij} \delta_{\sigma_i \sigma_j} \tag{B.1}$$

the quenched average of $\ln \operatorname{Tr} e^{-\beta H}$ over the probability distribution (2.5)

$$p(J_{ij}) = p\delta(J_{ij} - J) + (1-p)\,\delta(J_{ij}) \tag{B.2}$$

is performed using the replica trick:

$$\begin{aligned}
\overline{Z^n} &= \operatorname*{Tr}_{\sigma} \prod_{i<j}^{N} \int dJ_{ij}\, p(J_{ij}) \exp\left(-\beta \sum_{\alpha=1}^{n} J_{ij} \delta_{\sigma_i^\alpha \sigma_j^\alpha} \right) \\
&= \operatorname*{Tr}_{\sigma} \prod_{i<j}^{N} \left[p \exp\left(-\beta J \sum_{\alpha=1}^{n} \delta_{\sigma_i^\alpha \sigma_j^\alpha} \right) + (1-p) \right] \\
&= (1-p)^{N(N-1)/2} \operatorname*{Tr}_{\sigma} \exp \sum_{i<j}^{N} \ln \left[1 + p_0 \exp\left(-\beta J \sum_{\alpha=1}^{n} \delta_{\sigma_i^\alpha \sigma_j^\alpha} \right) \right]
\end{aligned} \tag{B.3}$$

where $p_0 = p/(1-p)$. After expanding the logarithm in a power series and some algebra, we find

$$\overline{Z^n} = \operatorname*{Tr}_{\sigma} \exp\left[\frac{-N}{2} \sum_{k=1}^{\infty} (-\beta J)^k c_k n^k \right] \exp\left[\sum_{k=1}^{\infty} \frac{(-\beta J)^k}{2} c_k \sum_{i,j}^{N} \left(\sum_{\alpha=1}^{n} \delta_{\sigma_i^\alpha \sigma_j^\alpha} \right)^k \right] \tag{B.4}$$

where

$$c_k = \sum_{l=1}^{\infty} \frac{(-)^{l+1}}{l} p_0^l \frac{l^k}{k!} \tag{B.5}$$

In the limit $n \to 0$, only the term with $k = 1$ in the first exponential of (B.4) has to be retained. In the second exponential, the term with $k = 1$ induces an antiferromagnetic interaction between the spins; the term with $k = 2$ is the same as for the ordinary Potts spin glass. When $p = 2c/N$ we have $c_k \sim 1/N$ and hence one has to take $\beta J \sim O(1)$ with respect to N in order to obtain an extensive "free energy." Hence, in this short-range problem, all values of k contribute. Such a model is still intractable at this time.

On the other hand, for $p \sim O(1)$, one has $c_k \sim O(1)$. If q were also of $O(1)$ with respect to N, one could choose $J \sim O(1/\sqrt{N})$ and only the $k = 2$ term would have contributed. Unfortunately, in the chromatic number problem under consideration, $q \sim O(N/\ln N)$, and so far we have not found an appropriate way to scale J in order to obtain a correct solvable thermodynamic limit out of (B.4).

APPENDIX C

We start with the Hamiltonian (3.1) and choose a representation where the spins σ_i take their values from the set of q-roots of unity:

$$\sigma_i \in \{\exp(2\pi i n/q) \mid n = 0, 1, \ldots, q-1\} \tag{C.1}$$

We then go through similar steps to those outlined in Appendix B and obtain instead of Eq. (B.4) the result

$$\overline{Z^n} = \operatorname*{Tr}_{\sigma}{}' \exp\left[\frac{-N}{2}\sum_{k=1}^{\infty}(\beta J)^k c_k n^k\right] \times \exp\left\{\sum_{k=1}^{\infty}\frac{1}{2}\left(\frac{2\beta J}{q}\right)^k c_k \sum_{i,j}^{N}\left[\sum_{\alpha=1}^{n}(q\delta_{\sigma_i^\alpha \sigma_j^\alpha}-1)\right]^k\right\} \tag{C.2}$$

and the free energy is given by

$$-\beta F = \lim_{n\to 0}\frac{\overline{Z^n}-1}{n} \tag{C.3}$$

The prime on the trace reminds us that the summation over the spins is subjected to (3.2) or (3.2′). From (3.2) it follows that

$$\overline{Z^n} = \operatorname*{Tr}_{\sigma}{}' \exp\left[\frac{-N}{2}\sum_{k=1}^{\infty}(\beta J)^k c_k n^k\right] \times \exp\left\{\sum_{k=2}^{\infty}\frac{1}{2}\left(\frac{2\beta J}{q}\right)^k c_k \sum_{i,j}^{N}\left[\sum_{\alpha=1}^{n}(q\delta_{\sigma_i^\alpha \sigma_j^\alpha}-1)\right]^k\right\} \tag{C.4}$$

As $\beta \to \infty$, the free energy F becomes the energy of the system. Hence, from Eq. (3.4) and (C.3), we find

$$C = \frac{N^2 p(q-1)}{2q} + \lim_{\beta\to\infty}\frac{F}{2J} \tag{C.5}$$

with

$$-\beta F = \lim_{n\to 0}\frac{1}{n}\left(\operatorname*{Tr}{}' \exp\left\{\sum_{k=2}^{\infty}\frac{1}{2}\left(\frac{2\beta J}{q}\right)^k c_k \sum_{i,j}^{N}\left[\sum_{\alpha=1}^{n}\sum_{r=1}^{q-1}(\sigma_i^\alpha \sigma_j^{\alpha *})^r\right]^k\right\} - 1\right) \tag{C.6}$$

where we have used the representation

$$q\delta_{\sigma_i\sigma_j} = 1 + \sum_{r=1}^{q-1}(\sigma_i \sigma_j^*)^r \tag{(C.7)}$$

In order to obtain a sensible thermodynamic limit, it is necessary to scale J to be order $1/\sqrt{N}$ [since $c_k \sim O(1)$ with respect to N]. In that case only the term with $k=2$ needs to be kept and we find, with $c_2 = p(1-p)/2$,

$$-\beta F = N(q-1)\,K^2 p(1-p) + \lim_{n\to 0}\frac{1}{n}\left\{\mathrm{Tr}'\exp\left[\frac{2NK^2p(1-p)}{N}\sum_{\alpha<\gamma}^{n}\sum_{r,r=1}^{q-1}\left|\sum_{i=1}^{N}(\sigma_i^{\alpha})^r(\sigma_i^{\gamma})^{r'}\right|^2\right]-1\right\} \tag{C.8}$$

where $K = \beta J N^{1/2}/q$. It can be shown that the constraints (3.2) are irrelevant at $T=0$ (by arguing along lines similar to Fu and Anderson[4]), and one can evaluate the trace over the spins in (3.8) disregarding the constraint. Equation (C.8) is the form of the free energy of the infinite-range Potts spin glass.

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