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# Application of statistical mechanics to NP-complete problems in combinatorial optimisation

Yaotian Fu† and P W Anderson

Department of Physics, Princeton University, Princeton, NJ 08544, USA

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**Abstract.** Recently developed techniques of the statistical mechanics of random systems are applied to the graph partitioning problem. The averaged cost function is calculated and agrees well with numerical results. The problem bears close resemblance to that of spin glasses. We find a spin glass transition in the system, and the low temperature phase space has an ultrametric structure. This sheds light on the nature of hard computation problems.

## 1. Introduction

Recent developments in the theory of spin glasses have profound consequences in many branches of science. The application of the replica method [1] enables one to study random systems effectively. The idea of replica symmetry breaking and its interpretation [2] reveals the fascinating phase space structure of spin glasses. This method has far-reaching significance since it enables one to apply statistical mechanics to a system which, technically speaking, does not obey statistical mechanics at all because ergodicity is broken and, worse still, because no *a priori* knowledge about the pattern of this breaking down is available. In order to apply conventional equilibrium statistical mechanics to systems in which ergodicity is absent due to symmetry breaking, one has to know something about the order parameter of the system. A conjugate field is then applied and the partition function calculated. Equilibrium statistical mechanics becomes inadequate without such information. A hidden order parameter is always a headache. The power of the replica symmetry breaking formalism lies in that no such information is needed. The spin glass transition represents symmetry breaking on a higher level, one which has complexity and depth. As one of us anticipated many years ago [3], 'At some point we have to stop talking about decreasing symmetry and start calling it increasing complication'. In the studies of these problems the replica formalism has great promise to become a tool which can be routinely used in the same way that partition functions have been used, and perhaps beyond that.

One area in which this new development of statistical mechanics may have important applications is combinatorial optimisation. Several authors have already discussed the use of the spin glass analogy in this context [4]. In particular, the simulated annealing technique has been successfully applied to solve a number of hard optimisation problems. The performance of this and other techniques as heuristic algorithms has

†Address after September 1985: Department of Physics, 1110 West Green Street, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA.

been systematically evaluated. Here we wish to discuss the problem from a different angle. Instead of using the spin glass analogy as a practical aid in solving specific optimisation problems, we propose to study the general properties of such problems in the light of recent developments of statistical mechanics. This will include a discussion of the average solution of the problem when it is defined, the structure of solution space, the existence and the nature of phase transitions, and the effective use of local optimisation techniques.

Our work is motivated by the following consideration. Many computational problems, the so-called NP-complete problems [5], have proved difficult to solve. Despite great efforts no effective algorithm has been found for these problems, and there is good reason to believe that such algorithms do not exist. It is therefore highly desirable to seek alternatives. Practical strategies in attacking these problems go under three categories. The first consists of improved exhaustive searching. While it takes exponential time to go through all choices, it is sometimes possible to make decisions early in the process to terminate certain tree searches that are unlikely to be fruitful. This kind of branch and bound technique can benefit from the knowledge of the solution space structure. The second type of algorithm routinely used includes various kinds of heuristics which aim at producing almost optimised solutions at a faster rate. It will be very helpful if one can know something about the expected outcome of the cost function. The third group of techniques is quite unconventional. Anticipating future development of computer designing strategies these techniques may however become very useful. In particular, as observed by Hopfield and co-workers [6], two important features of computing in biological systems are parallelism and analog operation. Phase space structure information will facilitate the effective use of analog techniques and parallel computation becomes easier when local optimisation is possible. If we accept not only the best solution, but also the ones very close to it, a local optimisation may give us good results. In all these cases, analysing the problem using new techniques of statistical mechanics may provide us with valuable information.

Not every NP-complete problem can be analysed in this way. Some problems do not permit a discussion based on the most probable case. A randomly chosen satisfiability problem, for example, is almost always easy to solve, because a random sequence of symbols almost always does not make sense. Even in problems which are not intrinsically decision problems, such as the travelling salesman problem, an answer based on the most probable case, while not useless, is not very interesting, because by its very nature it does not provide a specific answer to a specific problem. Here we encounter one important difference between statistical mechanical problems and optimisation problems. In statistical mechanics we do not have complete information about the system, nor do we demand an answer complete to the minute detail. A prediction in terms of certain macroscopic variables will be quite appropriate. In optimisation problems we do know everything about the specific instance of the problem, and usually we are not content with a 'macroscopic' answer. An answer based on the most probable case, therefore, can only be regarded as a step towards a qualitative understanding of the problem. It may also be a useful aid in designing heuristic algorithms such as simulated annealing. In particular, the possible existence of phase transitions will affect the actual implementation and performance of such algorithms. Such transitions and the accompanying knowledge of the structure of solution space may also play an important role in complexity theory.

In this paper we will apply statistical mechanics to the graph partitioning problem. Apart from its theoretical interests the graph partitioning problem has been studied

for a number of practical purposes, ranging from IC chip wiring to memory structure management. This problem is chosen because of its close resemblance to the spin glass problem, and also because many aspects of its solution are known, either theoretically or experimentally. We hope, however, that similar techniques can be applied to other problems as well.

The rest of this paper is organised in the following way. In § 2 we introduce the graph partition problem and define a Hamiltonian formalism for it. We also derive certain aspects of the solution that can be obtained exactly. In § 3 we study the model Hamiltonian by two independent methods, heavily using the results from spin glass theory. An estimation of the cost function is obtained and compared with the numerical results of explicit optimisation. Section 4 contains a study of the phase space structure, again using ideas developed in spin glass theory as a guide. In § 5 we discuss some general problems encountered in applying statistical mechanics to optimisation problems.

## 2. The model

The graph partitioning problem is specified by a set of vertices  $V = \{v_1, v_2, \dots, v_N\}$  and a set of edges  $E = \{(v_i, v_j)\}$  with  $N$  even. In general some pairs of vertices are connected by edges while others are not. We are now asked to partition the  $N$  vertices into two sets  $V_1$  and  $V_2$  of equal size such that the number of edges joining  $V_1$  and  $V_2$  is minimised. This number is defined to be our cost function  $C$ .

The graph partition problem is an NP-complete problem [7]. The best algorithm known is due to Kernighan and Lin [8]. Here we study a modified version of the problem. We assume each pair of vertices are connected with probability  $p$  independent of whether other pairs are connected (model A in graph theory, see [9]). For large values of  $N$ ,  $\alpha = Np$  is the expectation value of the valence for each vertex. The random graph defined in this way was studied by Erdős and Rényi in their classic work on random networks [10]. One important result is that for large values of  $N$  and  $\alpha \geq 1$ , the largest cluster in the graph has  $G(\alpha)N$  vertices where

$$G(\alpha) = 1 - \frac{1}{\alpha} \sum_{n=1}^{\infty} \frac{n^{n-1}}{n!} (\alpha e^{-\alpha})^n. \tag{2.1}$$

One can verify that  $G(1) = 0$ . Hence  $\alpha = 1$  is the percolation threshold. Also  $G(\infty) = 1$ , showing that the graph becomes completely connected, in which case we expect the cost function to be equal to  $N^2/4$ , the number of edges joining two sets of size  $N/2$  each. Finally if the largest cluster has number of vertices  $\leq N/2$  the cost function per vertex number will be zero<sup>†</sup>. Notice that (this follows from the Lagrange expansion formula, see e.g. [11])

$$\sum_{n=1}^{\infty} \frac{n^{n-1}}{n!} x^n = y \Rightarrow x = y e^{-y}$$

we can solve  $G(\alpha_c) = \frac{1}{2}$  to get

$$\alpha_c = 2 \ln 2 = 1.3863 \dots \tag{2.2}$$

<sup>†</sup>Strictly speaking, the cost function is not necessarily zero, since the complement of the largest cluster does not consist of isolated vertices, and the partition may have to go through one of the small clusters in order to maintain the balance of the two subsets. However, the small clusters are expected to have sizes of the order of  $\log N$  only and in the large  $N$  limit  $C/N$  will be zero.

We will be interested in calculating the averaged cost function  $C(\alpha)$ .  $C(\alpha)/N = 0$  for  $\alpha \leq \alpha_c$ . For  $\alpha > \alpha_c$  we expect

$$C(\alpha) = (pN^2/4) - \Delta(\alpha) \tag{2.3}$$

where the first term is the expected value for a randomly chosen partition scheme which separates all vertices into two sets of  $N/2$  each and among the  $N^2/4$  edges that might be present only  $pN^2/4$  are there. The second term shows improvements due to the optimisation.

A number of authors have tried to estimate  $C$ . Bui [12], in particular, has reviewed and improved many of these results. All previous results are in the form of upper and lower bounds. Some of them will be compared with our result in § 3. Here we wish to point out that in this paper an actual optimisation is attempted, that is, we try to look for the cost function of the optimised configuration rather than that of an arbitrary configuration used in ‘typical case’ or ‘worst case’ studies which have led to various bounds.

Using the spin glass analogy we can define a Hamiltonian for the system. With each vertex  $v_i$  we associate an Ising spin  $S_i$ .  $S_i = +1$  when  $v_i$  belongs to the set  $V_1$  and  $S_i = -1$  if  $v_i$  is in  $V_2$ . Since the two sets have the same size the total spin must be zero

$$\sum_{i=1}^N S_i = 0. \tag{2.4}$$

Each spin configuration then corresponds to a partition scheme. For each pair of vertices  $(v_i, v_j)$  we define a coupling constant  $J_{ij}$ .  $J_{ij} = J$  if  $(v_i, v_j) \in E$  and  $J_{ij} = 0$  otherwise. Hence  $J_{ij} = J$  with independent probability  $p = \alpha/N$  and zero otherwise. The Hamiltonian

$$H = -\sum_{i < j} J_{ij} S_i S_j \tag{2.5}$$

is then equal to

$$\begin{aligned} H &= -\frac{1}{2} \left( \sum_{i \in V_1, j \in V_1} + \sum_{i \in V_2, j \in V_2} + \sum_{i \in V_1, j \in V_2} + \sum_{i \in V_2, j \in V_1} \right) J_{ij} + \left( \sum_{i \in V_1, j \in V_2} + \sum_{i \in V_2, j \in V_1} \right) J_{ij} \\ &= -\frac{J}{2} [2N(N-1)p/2] + 2CJ \end{aligned}$$

or

$$C = \frac{H}{2J} + \frac{N(N-1)p}{4}. \tag{2.6}$$

Therefore to solve the graph partitioning problem is to minimise the Hamiltonian (2.5) under the constraint (2.4). Physically, this is a dilute infinite range ferromagnetic Ising system with a strong antiferromagnetic constraint (2.4). The conflict between these two types of interactions leads to frustration and gives rise to all the interesting properties of this problem.

### 3. The cost function

In order to calculate the averaged optimised cost function  $C$ , we will first calculate the averaged free energy  $F$  of the system. The zero temperature free energy should give us  $C$ .

We will first study  $C$  for very large  $\alpha \sim N$  so that  $p \sim O(1)$  (model 1). This corresponds to highly connected systems. Systems with small  $\alpha \sim O(1)$  (model 2) need special treatment and will be discussed elsewhere. In the following we use  $C(p)$  and  $C(\alpha)$  to denote the cost functions of these two functions of these two models respectively. Clearly the two models are distinct only in the infinite  $N$  limit. To compare with experimental results on finite samples we will take the ratio of the experimental value to the theoretical estimation and extrapolate it to large  $N$ . We will evaluate the quality of solutions on the basis of such extrapolations.

3.1. Model 1:  $p$  independent of  $N$

We use the replica method to compute  $F$ :

$$-\beta F = \lim_{n \rightarrow 0} \frac{1}{n} (\mathcal{Z}^n - 1) = \lim_{n \rightarrow 0} \left[ \text{Tr}' \exp \left( -\beta \sum_{\alpha=1}^n H_{\alpha} \right) - 1 \right] \tag{3.1}$$

where  $\beta$  is the inverse temperature,  $\alpha$  is a replica index which runs from 1 to  $n$ , and  $\text{Tr}'$  denotes the trace over all spin configurations which satisfy the constraints

$$\sum_{i=1}^N S_i^{\alpha} = 0 \quad \alpha = 1, 2, \dots, n. \tag{3.2}$$

$F$  is a self-averaging quantity and in a large  $N$  limit it will not depend on the specific choice of  $J_{ij}$ . Averaging over the randomness in  $J_{ij}$  we obtain

$$[\mathcal{Z}^n]_{\text{av}} = (1-p)^{N(N-1)/2} \left[ \text{Tr}' \prod_{i < j} \left( 1 + p_0 \exp \beta J \sum_{\alpha=1}^n S_i^{\alpha} S_j^{\alpha} \right) \right] \tag{3.3}$$

where we have introduced  $p_0 = p/(1-p)$ . The square bracket in (3.3) can be written as

$$\begin{aligned} & \text{Tr}' \exp \sum_{i < j} \ln \left( 1 + p_0 \exp \beta J \sum_{\alpha=1}^n S_i^{\alpha} S_j^{\alpha} \right) \\ &= \text{Tr}' \exp \left( \frac{N(N-1)}{2} \ln(1+p_0) \right) \exp \left( -N \sum_{l=1}^{\infty} \frac{(J\beta)^l}{2} C_l n^l \right) \\ & \quad \times \exp \left[ \sum_{l=2}^{\infty} \frac{(J\beta)^l}{2} C_l \sum_{[\alpha_l]} \left( \sum_i S_i^{\alpha_1} \dots S_i^{\alpha_l} \right)^2 \right] \end{aligned} \tag{3.4}$$

where we have expanded the logarithm and the exponential functions in Taylor series, changed the order of summation and rearranged the terms to separate the zeroth-, first- and higher-order terms in the expansion of the exponential. We have also used the constraints (3.2) to set the terms

$$C_1 \left( \sum_i S_i^{\alpha} \right)^2 \tag{3.5}$$

to zero. In (3.4)

$$C_l = \frac{1}{l!} \sum_{m=1}^{\infty} \frac{(-1)^{m-1}}{m} p_0^m m^l \propto p \tag{3.6}$$

and are of order one for  $p \sim O(1)$ . In particular,

$$C_1 = p_0 / (p_0 + 1) = p \qquad C_2 = \frac{1}{2} p_0 (p_0 + 1)^2 = \frac{1}{2} p (1 - p).$$

Hence

$$C(p) = \frac{1}{4} N^2 p + (2J)^{-1} F_1(\beta \rightarrow \infty)$$

and

$$-\beta F_1 = \lim_{n \rightarrow 0} \frac{1}{n} \left[ \text{Tr}' \exp \sum_{l=2}^{\infty} (\beta J)^l \frac{N^2}{2} C_l \sum_{[\alpha_l]} \left( \frac{1}{N} \sum_i S_i^{\alpha_1} \dots S_i^{\alpha_l} \right)^2 - 1 \right]. \tag{3.7}$$

While in this problem  $J$  is for bookkeeping purposes only and can take any value, only  $J = J_0 N^{-1/2}$  gives us a sensible thermodynamic limit. Keeping the lowest term in  $1/N$  (the  $l=2$  term), we see this is formally identical to the expression for the free energy of the Sherrington-Kirkpatrick spin glass. The only difference is that here the trace is taken over a subset of spin configurations as determined by the constraints (3.2). These constraints can be replaced by a convenient global soft constraint term

$$\frac{1}{2} J_1 \left( \sum_i S_i \right)^2 \qquad J_1 > 0 \tag{3.8}$$

in the Hamiltonian. The model can now be solved using standard techniques. Introducing Lagrange multipliers to decouple the quadratic terms we find that the constraint is irrelevant at  $T = 0$ , and the equivalence with the sk spin glass becomes exact in this limit, as shown in appendix 1. Alternatively we can argue that, since the ground states of the sk spin glass do not have finite magnetisation per spin, lifting the constraint at this stage will not affect  $C/N$  for large  $N$ . The largest contribution to the free energy due to ferromagnetic fluctuations has already been eliminated as in (3.5). Using the known value of the zero temperature energy of the sk spin glass  $U_0$  [2] we have

$$C(p) = \frac{1}{4} N^2 p + \frac{1}{2} U_0 N^{3/2} [p(1-p)]^{1/2} = \frac{1}{4} N^2 p - 0.38 N^{3/2} [p(1-p)]^{1/2}. \tag{3.9}$$

Let us compare this with the known results. The narrowest bounds of  $C$  as given in Bui [12] are the following:

$$\frac{1}{4} N^2 p - 0.17 N^{3/2} [p(1-p)]^{1/2} > C > \frac{1}{4} N^2 p - 0.42 N^{3/2} [p(1-p)]^{1/2}. \tag{3.10}$$

Our result is certainly consistent with this. Bui has also performed optimisation on random graphs generated on a computer. Figure 1 is taken from his work. We see the agreement is very good. Even for  $p = 0.01$  and  $N = 500$  the agreement is satisfactory [13] (experiments give  $C = 207$  while (3.9) gives  $C = 203$ ).

We have repeated the experiment for systems with  $N \leq 200$ . For each combination of  $N$  and  $p$  we randomly generate 10 graphs. The Kernighan-Lin algorithm is applied to each one of them. Usually the best result can be found in 20-40 passes. The longest run takes about 20 min CPU time on a VAX 11/750. The results for the 10 graphs are averaged to give  $C(p)$ . As can be seen from table 1, for  $p \geq 0.1$  our estimation is good to within about 10%. There are, however, increasingly large deviations from (3.9) for small  $p$ . In particular, (3.9) becomes zero at  $\alpha = 2.31 \dots$  which is very far from the threshold (2.2). We also observe large fluctuations from sample to sample for small  $p$ .

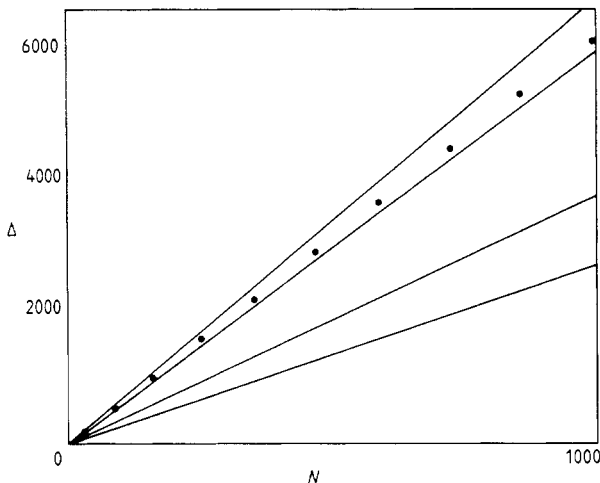


Figure 1.  $\Delta = N^2p/4 - C$  is the improvement due to optimisation, plotted against  $N^{3/2}$ .  $p = \frac{1}{2}$ . From bottom: the upper bound, results of the block algorithm, results of Kernighan-Lin algorithm, and the lower bound (from Bui [12]). The upper and lower bounds are given in equation (3.10). Closed circles: predictions of (3.9).

Table 1.  $C_1/C_2$ .  $C_1$ : average result of 10 different graphs (Kernighan-Lin algorithm).  $C_2$ :  $N^2p/4 - 0.38N^{3/2}[p(1-p)]^{1/2}$ .

p	N			
	50	100	150	200
0.05	5.5	1.5	1.19	1.13
0.1	1.24	1.12	1.11	1.10
0.25	1.03	1.04	1.05	1.02
0.5	1.07	1.03	1.03	1.02

We can estimate  $C$  in a different way. Define the density of states

$$\rho(E) = \text{Tr}' \delta(E - H) \tag{3.11}$$

and the averaged density of states

$$\rho_{\text{av}}(E) = [\text{Tr}' \delta(E - H)]_{\text{av}}. \tag{3.12}$$

The ground state energy can be estimated by solving

$$\int_{-\infty}^{E_0} \rho_{\text{av}}(E) dE = 1. \tag{3.13}$$

Notice that in principle one should calculate  $E_0$  using the density of states (3.11) and then do the average. Here we use the mathematically more tractable (3.13) in the hope that the density of states near  $E_0$  is not too low, in which case (3.13) should not be a bad approximation. In the language of spin glass theory we are taking the annealed average. In general this will produce a lower free energy as we can see from the Peierls inequality:

$$\langle e^{-\beta F} \rangle \geq e^{-\beta \langle F \rangle}. \tag{3.14}$$



It is straightforward to calculate

$$\rho_{av}(E) = N_0 \int_{-\infty}^{+\infty} \frac{dx}{2\pi} e^{ixE} \exp\left(\frac{N^2}{2} A - \frac{N}{2} B\right) (1-p)^{N(N-1)/2} \tag{3.15}$$

where

$$A = \ln(1 + p_0^2 + 2p_0 \cos x)^{1/2}$$

$$B = A + i \tan^{-1} \left( \frac{p_0 \sin x}{1 + p_0 \cos x} \right)$$

and

$$N_0 = N! / [(N/2)!]^2.$$

The equation for  $E_0$

$$1 = N_0 \int_{-\infty}^{E_0} dE \int_{-\infty}^{+\infty} \frac{dx}{2\pi} e^{ixE} \exp\left[\frac{(N^2 - N)}{4} \ln[1 + p(1-p)(-1 + \cos x)] - i \tan^{-1} \left( \frac{p_0 \sin x}{1 + p_0 \cos x} \right)\right] \tag{3.16}$$

can be solved using saddle point expansion. Substituting into (2.6) we find the cost function

$$C(p) \geq \frac{1}{4} N^2 p - \frac{1}{2} (\ln 2)^{1/2} N^{3/2} [p(1-p)]^{1/2} = \frac{1}{4} N^2 p - 0.42 N^{3/2} [p(1-p)]^{1/2}. \tag{3.17}$$

Since this result is not restricted to model 1,

$$C(\alpha) \geq (\frac{1}{4} \alpha - 0.42 \alpha^{1/2}) N. \tag{3.18}$$

This is precisely Bui's lower bound.

### 3.2. Model 2: $p = \alpha / N$ , $\alpha = \text{constant}$

Many practical random graphs belong to this category. The treatment of the previous model has to be modified for such graphs, for two independent reasons. A graph with finite valence  $\alpha$  is equivalent to a spin system with finite interaction range (the antiferromagnetic interaction responsible for maintaining the balance of the two subsets still has infinite interaction range). Therefore the mean-field theory solution may not be applicable. In addition, one can no longer choose  $J = J_0 N^{-1/2}$  to simplify (3.7). Instead one should choose  $J$  independent of  $N$ , so that the free energy is extensive, and keep all the terms in (3.7). One can see this in a different way. If we use the antiferromagnetic term (3.8) to represent the constraints (3.2), the Hamiltonian is

$$H = \sum_{i < j} (J_1 - J_{ij}) S_i S_j = \sum_{i < j} K_{ij} S_i S_j \tag{3.19}$$

where  $K_{ij}$  takes two values  $J_1$  and  $J_1 - J$  with probability  $1 - p$  and  $p$  respectively. If  $p$  is independent of  $N$  and remains finite when  $N \rightarrow \infty$ , one can approximate the distribution of  $K_{ij}$  by a Gaussian distribution centred at  $J_1$ . This is precisely what we did in keeping the  $l = 2$  term in (3.7) while ignoring the rest. As a result, the asymmetry in the distribution of  $K_{ij}$  is no longer visible. Indeed the free energy (and the optimised cost function thus obtained) depends on  $p$  only through the combination  $p(1 - p)$ . This approximation clearly breaks down for small  $p$ . So far, the spin glass problem for finite-range interactions has proved remarkably intractable in all cases, and ours is no exception.

#### 4. Phase space structure and phase transitions

In addition to providing estimations for the most probable outcome of the cost function, the spin glass analogy is useful in analysing the solution space structure. In this section we will discuss this aspect of the problem.

The phase transition in the pure Ising model is associated with the existence of two disconnected minima of the free energy at low temperature. These two minima are related by a global symmetry. To go from one minimum to another one has to flip all  $N$  spins in the system. On the other hand, the low temperature phase of a spin glass has many local free energy minima, not related to each other by any symmetry, and the transition between two local minima usually involves flipping many fewer than  $N$  spins. It is precisely this property that makes the spin glass analogy relevant in optimisation. If there are too many local minima, sitting very close to each other, the transition between neighbouring minima would involve  $O(1)$  spins, there will be no rigidity of the low temperature phases and hence no phase transition (e.g. the infinite-range antiferromagnetic model), and the optimisation will be easy. Computationally non-trivial cases arise when local minima are numerous but not excessively numerous, the distances between them large but not of the order of  $N$ . These are features shared by the SK spin glass, and we expect the existence of a spin-glass-like transition in these systems to reflect the difficulty involved in optimisation.

From the viewpoint of heuristics designing the information of phase space structure is also important (for a good discussion of heuristic algorithms, see [14]). The so-called  $\lambda$ -opt solution is an iterative local optimal solution within a distance  $\lambda$  from a given starting point. The starting points are randomly generated and the optimal solutions in their neighbourhood are compared to give the result of optimisation. If, however, one knows something about the distances between local optimal solutions, we can imagine generating the new random starting point by keeping an appropriate distance from the previous one and thus having a good chance to be in the neighbourhood of a different optimal solution. The common features of these solutions, such as the clustering of certain spins, could be used as guidelines in generating new starting points. In such a way we quickly scan the solution space while always trying to adapt the good features of different local optimal solutions. These kinds of intelligent algorithms will be expected to substantially speed up the computation process.

The spin glass theory provides a convenient formalism for this kind of discussion. In this section we will demonstrate the existence of a phase transition in model 1. Throughout the section we work in the neighbourhood of the critical point. The approximation used is not valid for ground state energy calculations.

Keeping the  $l = 2$  term in (3.7), we have

$$\begin{aligned}
 [Z^n]_{av} &= \text{Tr}' \exp \left[ \frac{\beta^2 v^2}{2N} \sum_{a < b} \left( \sum_i S_i^a S_i^b \right)^2 \right] \\
 &= \int \prod_{a < b} dQ_{ab} \left( \frac{N}{2\pi\beta^2 v^2} \right)^{1/2} \exp \left( -\frac{N}{2\beta^2 v^2} \sum_{a < b} Q_{ab}^2 \right) \text{Tr}' \exp \left( \sum_{a < b} \sum_i Q_{ab} S_i^a S_i^b \right)
 \end{aligned}
 \tag{4.1}$$

where  $v^2 = J_0^2 p(1-p)$ , and the restricted trace equals

$$\int_0^{2\pi} \prod_{a=1}^n \frac{dx_a}{2\pi} \left[ \text{Tr} \exp \left( ix_a S^a + \sum_{a < b} Q_{ab} S^a S^b \right) \right]^N \equiv \exp nNf(Q).
 \tag{4.2}$$

In the high temperature phase the replica symmetry is expected to be unbroken; the

integral is dominated by the saddle point

$$Q_{ab} = q \tag{4.3}$$

and (4.2) then equals

$$2^{nN} e^{-nNq/2} \int_0^{2\pi} \frac{dx_a}{2\pi} \left( \int Dz \prod_{a=1}^n \cosh(ix_a + \sqrt{q} z) \right)^N \tag{4.4}$$

where

$$\int Dz = \int_{-\infty}^{\infty} \frac{dz}{\sqrt{2\pi}} e^{-z^2/2}. \tag{4.5}$$

The large bracket in (4.4) is

$$\begin{aligned} & \int Dz \prod_{a=1}^n (\cos x_a \cosh \sqrt{q} z + i \sin x_a \sinh \sqrt{q} z) \\ &= \prod_{a=1}^n \cos x_a \left( \int Dz \cosh^n \sqrt{q} z + \sum_{s=1}^n (-1)^s T_s \int Dz \cosh^n \sqrt{q} z \tanh^{2s} \sqrt{q} z \right) \end{aligned} \tag{4.6}$$

$$T_s = \sum_{b_1 \neq b_2 \neq \dots \neq b_{2s}} \tan x_{b_1} \tan x_{b_2} \dots \tan x_{b_{2s}}. \tag{4.7}$$

The *s*th term in (4.6) is of the order of  $q^s$ . Near the critical point  $q$  is small. We will need  $f(q)$  up to the  $q^3$  term only. Writing

$$A = \int Dz \cosh^n \sqrt{q} z = 1 + n \int Dz \ln \cosh \sqrt{q} z \tag{4.8}$$

and

$$q^s B_s = (-1)^s \int Dz \cosh^n \sqrt{q} z \tanh^{2s} \sqrt{q} z \tag{4.9}$$

the integral in (4.4) is approximately

$$\left( \int \frac{dx_a}{2\pi} \cos^N x_a \right)^n A^N + \int \frac{dx_a}{2\pi} \prod_{a=1}^n \cos^{N-2} x_a \frac{N(N-1)}{2} A^{N-2} (qB_1 T_1 + q^2 B_2 T_2)^2 + O(q^4). \tag{4.10}$$

Since

$$\int T_1 T_2 \prod \cos^{N-2} x_a = 0$$

there is no  $q^3$  contribution from the second term. Because

$$\int T_1^2 \prod \cos^{N-2} x_a = n(n-1) \left( \int_0^{2\pi} \frac{dx}{2\pi} \cos^{N-2} x \right)^{n-2} \left( \int_0^{2\pi} \frac{dx}{2\pi} \cos^{N-4} x \sin^2 x \right)^2 \sim -\frac{n}{e^2 N^2} \tag{4.11}$$

the  $q^2$  contribution is not extensive. We conclude that (4.4) equals

$$\exp nN \left( -\frac{q}{2} + \int Dz \ln \cosh \sqrt{q} z + K - \frac{q^2}{2e^2 N} + \ln 2 \right) \tag{4.12}$$

where

$$K = \frac{1}{N} \int_0^{2\pi} \frac{dx}{2\pi} \cos^N x \sim \frac{2}{\sqrt{\pi}} e^{-N^{3/2}}. \tag{4.13}$$

Therefore

$$-\frac{\beta F}{N} = \frac{q^2}{4\beta^2 v^2} - \frac{q}{2} + \int Dz \ln \cosh \sqrt{q} z. \tag{4.14}$$

The value of the saddle point  $q$  is given by the familiar equation

$$\frac{q}{\beta^2 v^2} = \int Dz \tanh^2 \sqrt{q} z. \tag{4.15}$$

The system undergoes a second-order phase transition at

$$T_c = J_0 [p(1-p)]^{1/2}. \tag{4.16}$$

Above  $T_c$ , the cost function is equal to  $N^2 p/r$ . No effect of optimisation will be seen until  $T < T_c$ . This behaviour was observed in simulated annealing [13].

It is well known [15] that the replica symmetric solution, (4.3) and (4.15), becomes unstable below  $T_c$  in the SK spin glass model. The same instability exists in this problem. We can demonstrate this by showing that the Hessian associated with the saddle point has negative eigenvalues. After some tedious but straightforward algebra similar to that of (4.6)–(4.12) (see appendix 2) we obtain results identical to those of de Almeida and Thouless [15] (see also Bray and Moore [16]). It is therefore necessary to break replica symmetry.

In fact, (4.2) can be calculated for any small but arbitrary matrix  $Q_{ab}$  and large  $N$ . Details of the derivation can be found in appendix 2. It is clear from this calculation that near the transition point the constraints (3.2) are irrelevant; their corrections are all of order  $1/N$  compared with the main part. For large  $N$ ,

$$nf(Q) = \frac{1}{4} \text{Tr} Q^2 - \frac{1}{6} \text{Tr} Q^3 + \frac{1}{8} \text{Tr} Q^4 - \frac{1}{4} \sum_{b \neq c} Q_{ab}^2 Q_{ac}^2 + \frac{1}{12} \sum_{a,b} Q_{ab}^4 + \ln 2 + O(N^{-1}) \tag{4.17}$$

which is the same as that of an SK spin glass. Parisi's solution applies and the ultrametric structure of the solution space follows immediately [2].

We have been unable to establish the irrelevance of the constraints (3.2) at all temperatures. However, in the absence of a second transition the topological structure of solution space should not change drastically. While the quantitative behaviour of the order parameter  $q(x)$  in our problem may differ from that of a spin glass at a lower temperature, the qualitative features are the same.

## 5. Discussion

In this section we discuss some general problems encountered in applying statistical mechanics to optimisation problems.

Statistical mechanics is valid only in the thermodynamic limit. The meaning of such a limit is not clear in an optimisation problem. Intuitively, the system must be sufficiently large, but it is difficult to be more specific. While empirically in every problem there is always one quantity which measures the size of the system most naturally, the choice is by no means unique. Although the thermodynamic functions of physical systems are extensive, the entropy and cost function of an optimisation

problem can in principle have quite arbitrary dependence on this equally arbitrarily chosen measure of size.

In general, the free energy of the system can be decomposed into the energy part and the entropy part. At high temperature the entropy is determined by the number of states  $\Omega$ :

$$S \sim \ln \Omega \propto g(N) \quad (5.1)$$

and hence has a well defined  $N$  dependence (although not necessarily a linear dependence). On the other hand, the energy part will depend on certain 'counting variables' (the  $J$  in (2.5); the characteristic step length in the travelling salesman problem). These variables are arbitrary, and can be chosen to have the appropriate dependence on  $N$  so that the energy part will scale with  $N$  in a similar way as that of the entropy part. A generalised thermodynamic limit can then be defined. The free energy is extensive in the sense that the limit

$$\lim_{N \rightarrow \infty} F/g(N) \quad (5.2)$$

exists. The ground state energy can then be calculated. Eliminating the counting variables we recover the cost function with the correct  $N$  dependence. This procedure also guarantees that the phase transition temperature is  $N$  independent and finite.

Another common feature of optimisation problems is the existence of certain constraints. It is customary to replace the constraints by some additive penalty functions in the Hamiltonian (see, for example, the discussion of the travelling salesman problem [6]). This is a convenient device for the practical implementation of optimisations by simulated annealing or other techniques. As a tool for theoretical discussion, however, it has obvious drawbacks. In principle one should tune these penalty functions so that no illegal solution is included. This is achieved by taking the coupling constants in front of the penalty functions to large values, preferably infinity. But this leads to serious problems of exchanging limits. To recover information from a Hamiltonian with too many penalty terms is very difficult. Since the penalty function and the cost function are usually additive in the Hamiltonian, there may be trade-offs between these two terms. For multiple constraints this is a particularly serious problem. Ideally one should use the elements of the appropriate permutation group as the variable. The constraints can be strictly enforced; the permissible solutions form a subgroup. The partition function could then be calculated by a sum over this subgroup. Future development in the relevant mathematical techniques will be welcome.

While our discussion has focused on the theoretical side of the problem, spin glass theory can also help us to deal with specific instances [17]. In particular, the coupling constants of model 2 form a sparse matrix, which can be easily diagonalised. The localised eigenmodes corresponding to high eigenvalues can be first satisfied, producing local clusters. These clusters represent good features of the solution and can be preserved when one proceeds to deal with eigenmodes of lower eigenvalues. Because of frustration, it is impossible to satisfy all modes, and the Ising nature of the spins introduces strong interactions between the modes, making it impossible to carry this program to the end. As the Kernighan-Lin algorithm runs in time of order  $N^2 \ln N$ , it is also unlikely that one can gain much by this procedure. Nevertheless, since most of the localised modes can be treated locally, it opens new roads to parallel processing. It will be interesting to test these ideas by direct implementation. Some heuristic algorithms actually use ideas of block spin transformation [18] (see also [11]).

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**Appendix 1**

In this appendix we show that the constraints (3.2) are irrelevant at  $T = 0$ . Introducing the antiferromagnetic term (3.8), we have

$$[Z^n]_{av} = \exp(\beta J_1 n/2) \exp(-n^2 \beta^2 J_0^2/4) \exp(nN\beta^2 J^2/4) \times \text{Tr} \exp \left[ -\frac{\beta J_1}{2N} \sum_{a=1}^n \left( \sum_{i=1}^N S_i^a \right)^2 + \frac{\beta^2 J_0^2}{2N} \sum_{a < b} \left( \sum_i S_i^a S_i^b \right)^2 \right]. \tag{A1.1}$$

The two quadratic terms can be decoupled by two independent Gaussian transformations with auxiliary variables  $x_a$  and  $Q_{ab}$ . The trace part is

$$\int (\text{D}x_a)(\text{D}Q_{ab}) \left[ \text{Tr} \exp \left( i \sum_{a=1}^n x_a S^a + \sum_{a < b} Q_{ab} S^a S^b \right) \right]^N \tag{A1.2}$$

where

$$\begin{aligned} \text{D}x_a &= \prod_a dx_a \left( \frac{N}{2\pi\beta J_1} \right)^{1/2} \exp \left( -\frac{N x_a^2}{2\beta J_1} \right) \\ \text{D}Q_{ab} &= \prod_{a < b} dQ_{ab} \left( \frac{N}{2\pi\beta^2 J_0^2} \right)^{1/2} \exp \left( -\frac{N Q_{ab}^2}{2\beta^2 J_0^2} \right). \end{aligned} \tag{A1.3}$$

For simplicity we assume that the replica symmetry is unbroken. (A1.2) can be calculated using saddle point expansion. Standard manipulation leads to

$$\frac{\beta F}{N} \equiv f = -\lim_{n \rightarrow 0} \frac{[Z^n]_{av} - 1}{n} = \frac{x^2}{2\beta J_1} - \frac{q^2}{4\beta^2 J_0^2} - \frac{\beta^2 J_0^2}{4} + \frac{q}{2} - \ln 2 - \int \text{D}z \ln \cosh(ix + \sqrt{q} z) \tag{A1.4}$$

$$\text{D}z = (dz/\sqrt{2\pi}) e^{-z^2/2}.$$

The saddle points are given by

$$\partial f / \partial x = 0 \quad \partial f / \partial q = 0 \tag{A1.5}$$

or

$$\frac{x}{\beta J_1} = - \int \text{D}z \frac{\sin 2x}{\cos 2x + \cosh 2\sqrt{q} z} \tag{A1.6}$$

$$\frac{q}{\beta^2 J_0^2} = \int \text{D}z \frac{\sinh^2 2\sqrt{q} z - \sin^2 2x}{(\cosh 2\sqrt{q} z + \cos 2x)^2}. \tag{A1.7}$$

$x = 0$  is the only solution if  $q = 0$ . In general there will be many solutions. We are interested in the local maxima of  $f$ . The second derivative

$$\frac{\partial^2 f}{\partial^2 x} = -\frac{1}{\beta J_1} - \int Dz \frac{1 + \cosh 2\sqrt{q} z \cos 2x}{(\cosh 2\sqrt{q} z + \cos 2x)^2} \tag{A1.8}$$

is periodic in  $x$  with periodicity  $\pi$ , and diverges at  $2x = (2n + 1)\pi$ , where the right-hand side of (A1.6) jumps from  $\pi/q$  to  $-\pi/q$ . In the limit  $\beta$  goes to infinity, the local maximal solutions are given by

$$2x_m = 2m\pi \quad |m| \leq l \tag{A1.9}$$

where  $l \sim \beta J_1/q$  since the right-hand side of (A1.6) is bounded by  $\pi/q$ . We should sum up all their contributions to  $f$ . They are

$$\frac{\pi^2}{2\beta J_1} \sum_{m=1}^l m^2 \tag{A1.10}$$

and

$$- \int Dz \sum_{m=1}^l \ln \cos x_m \tag{A1.11}$$

neither of which contributes to the cost function. The constraints are therefore irrelevant.

### Appendix 2

In this appendix we derive (4.17). From (4.2),

$$\begin{aligned} \exp[nNf(Q)] &= \int Dx [\text{Tr} \exp(\frac{1}{2} Q_{ab} S^a S^b + i x_a S^a)]^N \\ &= 2^{nN} \int Dx \left[ \text{Tr} \exp\left(-\frac{1}{2} Q_{ab} \frac{\partial}{\partial x_a} \frac{\partial}{\partial x_b}\right) \prod_{a=1}^n \cos x_a \right]^N \end{aligned} \tag{A2.1}$$

where

$$\int Dx \equiv \int_0^{2\pi} \prod_{a=1}^n \frac{dx_a}{2\pi} \tag{A2.2}$$

$$Q_{aa} = 0 \quad a = 1, 2, \dots, n \tag{A2.3}$$

and summation over repeated indices is assumed.

We will need  $f(Q)$  up to  $Q^4$  order. Defining a set of operators  $L$ :

$$L_{ab} = -\frac{1}{2} \frac{\partial}{\partial x_a} \frac{\partial}{\partial x_b} \tag{A2.4}$$

and the function

$$R = \prod_{a=1}^n \cos x_a \tag{A2.5}$$

we have

$$\begin{aligned}
 [\exp(QL)R]^N &= \left( R + (QL)R + \frac{(QL)^2}{2} R + \dots \right)^N \\
 &= R^N + NR^{N-1} \left( (QL)R + \frac{(QL)^2}{2} R + \frac{(QL)^3}{3!} R + \frac{(QL)^4}{4!} R + \dots \right) \\
 &\quad + \binom{N}{2} R^{N-2} \left( (QL)R + \frac{(QL)^2}{2} R + \frac{(QL)^3}{3!} R \right)^2 \\
 &\quad + \binom{N}{3} R^{N-3} \left( (QL)R + \frac{(QL)^2}{2} R \right)^3 + \binom{N}{4} R^{N-4} [(QL)R]^4 + O(Q)^5.
 \end{aligned}
 \tag{A2.6}$$

$Q^0$  order:

$$\int Dx R^N = \left( \int_0^{2\pi} \frac{dx}{2\pi} \cos^N x \right)^n = \left[ 2 \left( \frac{e}{\pi N} \right)^{1/2} \right]^n \equiv W.
 \tag{A2.7}$$

$Q^1$  order:

$$-\frac{1}{2} \sum_{c_1 \neq c_2} Q_{c_1 c_2} \int Dx \left( \prod_{a=1}^n \cos^{N-1} x_a \right) \left( \prod_{b \neq c_1, c_2} \cos x_b \right) \sin x_{c_1} \sin x_{c_2} = 0.
 \tag{A2.8}$$

$Q^2$  order:

$$N \int Dx R^{N-1} \frac{(QL)^2}{2} R + \binom{N}{2} \int Dx R^{N-2} [(QL)R]^2.
 \tag{A2.9}$$

The integral in the second term:

$$\begin{aligned}
 &\frac{1}{4} \sum_{c_1 \neq c_2, d_1 \neq d_2} Q_{c_1 c_2} Q_{d_1 d_2} \int Dx \prod_{a=1}^n \cos^{N-2} x_a \prod_{b \neq c, d} \cos^2 x_b \sin x_{c_1} \dots \sin x_{d_2} \\
 &= \frac{1}{2} \text{Tr} Q^2 \left( \int_0^{2\pi} \cos^N x \frac{dx}{2\pi} \right)^{n-2} \left( \int_0^{2\pi} \cos^{N-2} x \sin^2 x \frac{dx}{2\pi} \right)^2 \propto N^{-2}.
 \end{aligned}
 \tag{A2.10}$$

Here and below we use

$$\int_0^{2\pi} \cos^{N-2l} x \sin^{2l} x \, dx / 2\pi = \sqrt{2/\pi} (l - \frac{1}{2})^l e^{-l+1/2} (2/N)^{l+1/2}.
 \tag{A2.11}$$

Therefore the second term in (A2.9) is not extensive and can be neglected. Similarly every term except those in the first square bracket can be neglected. The only extensive contributions are those coming from terms containing

$$\int Dx R^N.
 \tag{A2.12}$$

The rest of the calculation is straightforward. One notices that the operators  $(QL)^l$  must act in such a way as to leave  $R$  invariant. This is not possible for the  $l = 1$  term since the two derivatives must act on different  $x_a$ . The rest of the expression can be evaluated using graphical rules similar to those of the linked graph expansion for Ising



systems [19], with a common factor

$$W = 1 + n \ln[2(e/\pi N)^{1/2}] \sim 1 \quad (\text{A2.13})$$

from which we obtain (4.17).

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