Metastable States in High Order Short-Range Spin Glasses

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Abstract. The mean number $\langle N \rangle$ of metastable states in higher order short-range spin glasses is estimated analytically using a variational method introduced by Tanaka and Edwards for very large coordination numbers. For lattices with small connectivities, numerical simulations do not show any significant dependence on the relative positions of the interacting spins on the lattice, indicating thus that these systems can be described by a few macroscopic parameters. As an extremely anisotropic model we consider the low autocorrelated binary spin model and we show through numerical simulations that its landscape has an exceptionally large number of local optima.

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1. Introduction

The notion of an (adaptive) landscape has proved to be a valuable concept in theoretical investigations of evolutionary change, combinatorial optimization, and the physics of disordered systems. From the mathematical point of view, a landscape consists of three ingredients: (i) a set $V$ of “configurations” which we shall assume to be finite but very large, (ii) a cost or fitness function $f : V \to \mathbb{R}$ that evaluates the configurations, and (iii) some sort of additional geometrical, topological, or algebraic structure $X$ on $V$ that allows us to define notions of closeness, similarity, or dissimilarity among the configurations [1, 2, 3]. In the simplest case, $X$ is an adjacency relation. In this contribution we shall consider systems consisting of $N$ Ising spins and we shall assume that two spin configurations $x$ and $x'$ are adjacent when they differ in the orientation of a single spin, $x'_k = -x_k$. We say that $x \in V$ is a local minimum of the landscape $f$ if $f(x) \leq f(y)$ for all adjacent configurations (neighbors) $y$ of $x$. The use of $\leq$ instead of $<$ is conventional [4, 5]; it does not make a significant difference for spin glass models. Local maxima are defined analogously. The number $N$ of local optima in a landscape may serve as a measure for the landscape’s ruggedness [6]. Alternatively, ruggedness can be measured by means of correlation functions such as $r(s)$, defined as the autocorrelation function of the “time series” $f(x_t)$ sampled along an unbiased random walk of $s$ steps on the configuration space [3]. Explicitly, $r(s)$ can be represented as a quadratic form

$$r(s) = (\tilde{f}, (\mathbf{D}^{-1} \mathbf{A})^s \tilde{f})/(\tilde{f}, \tilde{f})$$

(1)

where $\mathbf{A}$ is the adjacency matrix of the configuration space $(V, X)$, $\mathbf{D}$ is the diagonal matrix of its vertex degrees, i.e., $D_{xx}$ is the number of neighbors of each configuration, $\tilde{f}(x) = f(x) - \overline{f}$, and $\overline{f} = |V|^{-1} \sum_x f(x)$ [1]. It is not hard to verify that $r(s)$ is an exponential function if and only if $\tilde{f}$ is an eigenvector of $\mathbf{A}$. Such landscapes have been termed elementary. The importance of elementary landscapes derives in part from the fact that all Ising spin models

$$\mathcal{H}(x) = \sum_{(i_1<i_2< \ldots <i_p)} J_{i_1i_2 \ldots i_p} x_{i_1} x_{i_2} \ldots x_{i_p}$$

(2)

with a fixed interaction order $p$ are elementary, with an eigenvalue $N - 2p$ that depends only on $p$ and not on the details of the index set $(i_1 < i_2 < \ldots < i_p)$ of non-vanishing spin interactions. In the case that the couplings $J_{i_1 \ldots i_p}$ are statistically independent, Gaussian distributed random variables, Eq.(2) defines Derrida’s $p$-spin Hamiltonian [7], which for $p = 2$ reduces to the well-known SK model [8].

The information contained in $r(s)$ is conveniently further condensed into the correlation length $\ell = \sum_{k=0}^{\infty} r(s)$. For elementary Ising spin models we obtain immediately $\ell = N/(2p)$, see e.g. [9, 10]. It would appear that $N$ and $\ell$ are two sides of the same coin, and hence we would expect a close connection between the two measures. Indeed, for Derrida’s $p$-spin Hamiltonian the expected number of local optima $\langle N \rangle$ scales like $\exp(\alpha N)$ with $\alpha$ increasing from 0.199 for $p = 2$ to $\ln 2 \approx 0.692$ for $p \to \infty$ [11].
This increase of $\alpha$, and hence of the number of local optima, matches the decrease of the correlation length $\ell$ with increasing $p$.

Although for random landscapes (Hamiltonians with disorder) it is often desirable to determine $\langle \ln N \rangle$, in most cases one has $\langle \ln N \rangle = \ln \langle N \rangle$ (a notable exception is the linear spin chain [12]). The reason for this equality is that the overlap between two randomly chosen metastable states vanishes with probability one and so the replica approach needed to evaluate the average of $\ln N$ reduces to the annealed approximation, which takes the average directly on $N$ [13]. Of course, this is no longer true if one considers specific classes of metastable states (e.g. those possessing a given energy density) or if one adds an external magnetic field to the Hamiltonian (2) [14].

In [1, 2] the notion of an isotropic random landscape was introduced as a “statistically symmetric model”, that is, as a random landscape with a covariance matrix $C_{xy} = \langle f(x)f(y) \rangle - \langle f(x) \rangle \langle f(y) \rangle$ that shares the symmetries of the underlying configuration space. An Ising spin glass is isotropic if and only if all interaction coefficients $J_{i_1...i_p}$ are uncorrelated with mean $\langle J_{i_1...i_p} \rangle = 0$, and those $J_{i_1...i_p}$ that belong to a common interaction order have the same variance, $\langle J_{i_1...i_p}^2 \rangle = \sigma^2(p)$ [2]. In other words, the elementary isotropic Ising models are exactly the $p$-spin Hamiltonians with infinite-range interactions. It is argued at length in [15, 16] that isotropy can be interpreted as a maximum entropy condition. The properties of the infinite-range $p$-spin Hamiltonians are obviously determined exclusively by the number of spins $N$ and the interaction order $p$ or, equivalently, by the correlation length $\ell$.

Short-range spin models, in which only a small fraction of all $\binom{N}{p}$ possible $p$-ary spin interactions contribute to the Hamiltonian, i.e., $\langle J_{i_1...i_p}^2 \rangle = 0$ for most $p$-ary spin patterns ($i_1 < i_2 < \ldots < i_p$), deviate significantly from isotropy. For the SK model ($p = 2$) a slightly larger number of local optima has been found [17, 18] than for the infinite-range case [19]. The deviation is proportional to $1/z$, where $z$ is the number of the nearest-neighboring points in a hypercubic lattice of dimension $d = z/2$.

In this contribution we show that an analogous effect is at work in higher order spin glasses. In addition, numerical simulations for small values of connectivities do not show a substantial dependence on the patterns of interacting spins. The rest of this paper is organized in the following way. In section 2 we generalize the variational method of Tanaka and Edwards [17] to estimate the $1/z$ corrections to the expected number of metastable states of Derrida’s $p$-spin model. The results of numerical simulations of fourth-order spin glasses in two- and three-dimensional cubic lattices with small connectivities are discussed in section 3. In section 4 we investigate the metastable states of a highly frustrated one-dimensional spin model without explicit disorder, namely, the low autocorrelated binary string problem [20]. Finally, in section 5 we present some concluding remarks.
2. Short-Range $p$-spin Models

The coupling strengths $J_{i_1...i_p}$ in Eq. (2) are modeled as statistically independent random variables with the Gaussian distribution

$$P(J_{i_1...i_p}) = \sqrt{\frac{z^{p-1}}{\pi p!}} \exp \left[ -\frac{(J_{i_1...i_p})^2 z^{p-1}}{p!} \right] \Theta[(i_1 < i_2 < \ldots < i_p)]$$

(3)

where $\Theta[(i_1 < i_2 < \ldots < i_p)] = 1$ if $(i_1 < \ldots < i_p)$ is a valid interaction pattern and 0 otherwise. Since in practice it is not feasible to consider a fixed interaction pattern, we consider all interaction patterns with given fixed coordination number $z$. In other words, we sum over all ways of choosing the $p-1$ spins among the $z$ allowed ones.

As an immediate consequence of Eq. (2) the energy cost of flipping the spin $x_j$ is

$$\delta \mathcal{H} = 2 \lambda_j$$

(4)

where

$$\lambda_j = \sum_{(i_2 < \ldots < i_p)} J_{j i_2...i_p} x_j x_{i_2} \ldots x_{i_p}$$

is the stability of $x_i$. Hence any state $x$ that satisfies

$$\lambda_i \geq 0 \quad \forall i$$

(5)

is a local minimum of the random landscape defined in Eq. (2). Thus the number of local minima can be written as

$$\mathcal{N} = \text{Tr}_x \prod_j \int_0^\infty d\lambda_j \delta \left( \lambda_j - \sum_{(i_2 < \ldots < i_p)} J_{j i_2...i_p} x_j x_{i_2} \ldots x_{i_p} \right)$$

(6)

where $\text{Tr}_x$ denotes the summation over the $2^N$ spin configurations and $\delta(x)$ is the Dirac delta function.

In the following we will calculate analytically the expected number of metastable states $\langle \mathcal{N} \rangle$ in the limit of large $N$ and $z$ with $N \gg z$. Here $\langle \ldots \rangle$ stands for an average over the coupling strengths in all possible interaction patterns with fixed coordination number $z$. Using the integral representation of the delta function, the average over the couplings as well as the summation over the spin configurations can be easily performed [14], yielding

$$\langle \mathcal{N} \rangle = \prod_i \int_0^\infty d\lambda_i \int_\infty^{-\infty} \frac{d\phi_i}{\pi} \exp \left( i \lambda_i \phi_i \right) \times \exp \left[ -\frac{p!}{4 z^{p-1}} \sum_{(i_1 < i_2 < \ldots < i_p)} (\phi_{i_1} + \phi_{i_2} + \ldots + \phi_{i_p})^2 \right] .$$

(7)

Clearly, the expansion of the quadratic term in the argument of the exponential function will lead to interactions terms of second order in the auxiliary fields $\phi_i$. More precisely, using

$$\frac{p!}{z^{p-1}} \sum_{(i_1 < \ldots < i_p)} \phi_{i_1}^2 = \frac{1}{z^{p-1}} z (z-1) \ldots (z-p+2) \sum_i \phi_i^2$$

$$= \left[ 1 - \frac{1}{2z} (p-1)(p-2) + \mathcal{O}(z^{-2}) \right] \sum_i \phi_i^2$$

(8)
and
\[ \frac{p!}{z^{p-1}} \sum_{i_1<\ldots<i_p} \phi_{i_1}\phi_{i_p} = \frac{2}{z^{p-1}} (z-1)(z-2)\ldots(z-p+2) \sum_{(i<j)} \phi_i\phi_j \]
\[ = \left[ \frac{2}{z} + O(z^{-2}) \right] \sum_{(i<j)} \phi_i\phi_j, \tag{9} \]
we write Eq.(7) as
\[ \langle N \rangle = \int_{-\infty}^{\infty} \prod_i d\phi_i \, D(\phi_i) \exp \left[ -\frac{p(p-1)}{2z} \sum_{(i<j)} \phi_i\phi_j \right] \tag{10} \]
where
\[ D(\phi_i) = \left[ 1 + \frac{p(p-1)(p-2)}{8z} \phi_i^2 + O(z^{-2}) \right] \int_0^{\infty} \frac{d\lambda}{\pi} e^{-\lambda \phi_i^2 - \frac{p}{\sqrt{4\pi}} \phi_i} \tag{11} \]
is the field’s weight function. As mentioned before, Eqns.(8) and (9) follow from the sum over all possible interaction patterns with coordination number \( z \). More precisely, for each site \( i \) there are precisely \( z \) sites \( k \) such that \((i, k, i_3, \ldots, i_p)\) is a valid interaction pattern for some choice of \( i_3, \ldots, i_p \). This notion of site connectivity is independent of the lattice dimensionality; in fact, it is not necessary to assume that the sites are arranged on a lattice at all: Eq.(10) remains valid as long as \( z \) is site independent. Hence we will refer to \( z \) simply as the connectivity of our model.

To proceed further we must evaluate the integrals in Eq.(10) taking the care to collect all terms of first order in \( 1/z \). In particular, note that \( \sum_{(i<j)} 1 = Nz/2 \). This can be achieved through an ingenious variational method introduced by Tanaka and Edwards in their analysis of the case \( p = 2 \) [17]. The idea is to add an auxiliary single-particle term to the effective Hamiltonian of Eq.(10) which is then rewritten as
\[ \langle N \rangle = [\Phi(t)]^N \left\langle \exp \left[ -\frac{p(p-1)}{2z} \sum_{(i<j)} \phi_i\phi_j - it p^{1/2} \sum_i \phi_i \right] \right\rangle_t, \tag{12} \]
where the average \( \langle \ldots \rangle_t \) is defined by
\[ \langle \ldots \rangle_t = \frac{\int \prod_i d\phi_i \, D(\phi_i) \langle \ldots \rangle \exp \left( it p^{1/2} \sum_i \phi_i \right)}{\int \prod_i d\phi_i \, D(\phi_i) \exp \left( it p^{1/2} \sum_i \phi_i \right)} \tag{13} \]
and
\[ \Phi(t) = \int_{-\infty}^{\infty} d\phi \, D(\phi) \exp \left( it p^{1/2} \phi \right) = \text{erfc}(-t) + \frac{1}{z \sqrt{4\pi}} (p-1)(p-2) e^{-t^2} + O(z^{-2}) \tag{14} \]
For example, we find
\[ it^{p^{1/2}} \langle \phi_k \rangle_t = \Phi'(t)/\Phi(t) \tag{15} \]
\[ -p \langle \phi_k^2 \rangle_t = \Phi''(t)/\Phi(t) \tag{16} \]
for \( k = 1, \ldots, N \). Here \( t \) is a variational parameter which will be determined so as to maximize \( \langle \mathcal{N} \rangle \). At this point we can note that the \( 1/z \) expansion is valid provided that \( z \gg p^2 \).

As usual, the average in Eq.(12) can be evaluated through the cumulant expansion. In particular, we assume that only the first cumulant contains terms of zeroth order in \( 1/z \) and it is solely these terms that determine the value \( t = t_m \) that maximizes \( \langle \mathcal{N} \rangle \) [17]. Of course, this assumption must be verified \textit{a posteriori} through the explicit calculation of the higher order cumulants. Evaluating the first cumulant we find that \( t_m \) maximizes the expression

\[
\ln \Phi(t) - \frac{p(p-1)}{4} \langle \phi_k \rangle_t^2 - i \ t \ p^{1/2} \langle \phi_k \rangle_t
\]

and so it is given by the solution of the equation

\[
t_m = \frac{1}{2} (p-1) i \ p^{1/2} \langle \phi_k \rangle_{t_m}.
\]

The usefulness of the variational approach becomes transparent only when we rewrite Eq.(12) replacing \( t \) by \( t_m \) and rearranging the terms:

\[
\langle \mathcal{N} \rangle = \exp \left[ N \ln \Phi(t_m) + N \frac{p(p-1)}{4} \langle \phi_k \rangle_{t_m}^2 \right] \times \langle \exp(\Xi) \rangle_{t_m}
\]

where

\[
\Xi = -\frac{p(p-1)}{2z} \sum_{(i<j)} (\phi_i - \langle \phi_i \rangle_{t_m}) (\phi_j - \langle \phi_j \rangle_{t_m}).
\]

Since \( \langle \Xi \rangle_{t_m} = 0 \), it is now straightforward to evaluate the higher order cumulants in the cumulant expansion

\[
\langle \exp(\Xi) \rangle_{t_m} = \exp \left( \sum_{n=1}^{\infty} \frac{1}{n!} \langle \Xi^n \rangle_{t_m,c} \right).
\]

In particular, we find

\[
\langle \Xi^1 \rangle_{t_m,c} = 0,
\]

\[
\langle \Xi^2 \rangle_{t_m,c} = N \frac{p^2(p-1)^2}{8z} \langle (\phi_k - \langle \phi_k \rangle_{t_m})^2 \rangle_{t_m},
\]

\[
\langle \Xi^3 \rangle_{t_m,c} = -N \frac{p^3(p-1)^3}{16z^2} \langle (\phi_k - \langle \phi_k \rangle_{t_m})^3 \rangle_{t_m}.
\]

More generally, we can easily show that \( \langle \Xi^n \rangle_{t_m,c} \) is of order \( z^{1-n} \). Therefore, to keep terms up to \( 1/z \) we need to consider only the second cumulant in Eq.(19). Moreover, the leading terms of the \( 1/z \) expansion (i.e., the terms of zeroth order in \( 1/z \)) are those outside the average symbol in Eq.(19). Clearly, these results remain unchanged by the fact that for \( p > 2 \) the averages \( \langle \phi_k^n \rangle_{t_m} \) also contribute to the \( 1/z \) corrections, see Eqns.(14-16). Hence

\[
\frac{1}{N} \ln \langle \mathcal{N} \rangle = \ln \Phi(t_m) + \frac{p(p-1)}{4} \langle \phi_k \rangle_{t_m}^2
\]

\[
+ \frac{p^2(p-1)^2}{16z} \left( \langle \phi_k^2 \rangle_{t_m} - \langle \phi_k \rangle_{t_m}^2 \right)^2 + O(z^{-2}).
\]
Table 1. Values of $\alpha_0$ and $\alpha_1$ obtained from Eqns.(26), (28), and (29).

| $p$ | 2   | 3   | 4   | 5   | 6   | 10  |
|-----|-----|-----|-----|-----|-----|-----|
| $\alpha_0$ | 0.1992 | 0.2956 | 0.3552 | 0.3965 | 0.4273 | 0.5001 |
| $\alpha_1$ | 0.0656 | 0.3393 | 0.7789 | 1.3411 | 1.9985 | 5.2894 |

The next step is to separate the contributions of zeroth and first order in $1/z$. To achieve this we note that $t_m$ is determined only by the zeroth order term in the $1/z$ expansion so that Eq.(18) reduces to

$$t_m = \frac{p - 1}{\sqrt{\pi}} \exp \left( -\frac{t_m^2}{p} \right) \text{erfc} \left( -\frac{t_m}{p} \right).$$ (26)

Inserting this result in Eqns.(14), (15) and (16), we rewrite Eq.(25) as

$$\lim_{N \to \infty} \frac{1}{N} \ln \langle N \rangle = \alpha = \alpha_0 + \frac{1}{z} \alpha_1 + \mathcal{O} (z^{-2})$$ (27)

with

$$\alpha_0 = \ln \left[ \text{erfc} \left( -t_m \right) \right] - \frac{t_m^2}{p - 1}$$ (28)

$$\alpha_1 = p^2 t_m^2 \left[ \frac{t_m^2}{(p - 1)^2} + \frac{p - 2}{2p^2} \right].$$ (29)

In Table 1 we summarize the values of $\alpha_0$ and $\alpha_1$ obtained from a numerical solution of Eq.(26). For $p \to \infty$ we find $t_m \approx \sqrt{\ln p}$ and so $\alpha_0 \to \ln 2$ while $\alpha_1$ diverges like $p \ln p$. Of course, $\alpha_1/z \ll 1$ since, as mentioned before, the $1/z$ expansion is consistent only if $z \gg p^2$. We note that our results for $p = 2$ are in agreement with those of ref. [17]; the values of $\alpha_0$ agree with the TAP solution [11], and with a numerical survey [21].

3. Simulations

The analytical results in section 2 are valid for very large connectivities, $z \gg p^2$, and for superimposed interaction patterns. Actually, the later restriction amounts to consider all interactions patterns as equivalent, in the sense that they have on the average the same number of local minima. In order to investigate the effect of distinct interaction patterns we consider in this section a variety of 4-spin models with small connectivities.

For the sake of computational simplicity we consider only translation invariant interaction patterns $P$ on two- and three-dimensional cubic lattices with periodic boundary conditions. We identify each spin by its $d$-dimensional lattice coordinates and take all indices modulo the lattice sizes $m_1$ through $m_d$. In two dimensions, for instance, translation invariance means $(i_1, j_1; i_2, j_2; i_3, j_3; i_4, j_4) \in P$ if and only if $(i_1 + p, j_1 + q; i_2 + p, j_2 + q; i_3 + p, j_3 + q; i_4 + p, j_4 + q) \in P$ for all integers $p \mod m_1$ and $q \mod m_2$. The Hamiltonian (2) becomes

$$\mathcal{H}(x) = \sum_{(i_1,j_1;i_2,j_2;i_3,j_3;i_4,j_4) \in P} J_{i_1,j_1;i_2,j_2;i_3,j_3;i_4,j_4} x_{i_1,j_1} x_{i_2,j_2} x_{i_3,j_3} x_{i_4,j_4}$$ (30)
in this example. A variety of interaction patterns on a square lattice, compiled in Figure 1 and named according to the number and type of combinations (patterns) of spins that contribute to the Hamiltonian (30), have been used. In addition, we have considered three patterns on a cubic lattice: (i) The “positive orthant”, coupling each spin $x_{i,j,k}$ with its lattice neighbors along $x_{i+1,j,k}$, $x_{i,j+1,k}$ and $x_{i,j,k+1}$, (ii) the pattern $S$ restricted to a fixed plane, i.e., $x_{i,j,k}$ coupled with $x_{i,j+1,k}$, $x_{i,j,k+1}$, and $x_{i,j+1,k+1}$, and (iii) the couplings with the neighbors in all eight orthants.

The relevant quantity for comparing the simulations with the analytical theory is the connectivity $z$ of a lattice site $j$, that is, the number of spins $k \neq j$ such that $J_{j_3 j_4 i_3 i_4} \neq 0$ for some $i_3$ and $i_4$. The value of $z$ depends of course strongly on the interaction pattern, see Table 2. Note that $z$ is independent of the lattice dimensionality and of the number $X$ of non-zero interaction strengths per site.

Numerical simulations were performed by sampling up to $10^8$ spin configurations from at least $10^5$ different instances (random assignments of the coupling constants) for each model and values of $N = \prod_{k=1}^{d} m_k$ between 8 and 60. The standard deviations listed in Table 2 are statistical errors from fitting the curve $\ln \langle N \rangle$ versus $N$ to a straight line. With the exception of the cubic models, where we have only few data points, and the models $q_1 q$, $q_2 q$, which show quite strong finite size effects, the correlation coefficient of the linear regression is $\rho > 0.9998$.

By comparison with the numerical estimates for the infinite-range 4-spin glass we suspect that systematic errors might be slightly larger than the statistical errors. A conservative estimate appears to be an over all accuracy of at least $\pm 0.012$. We also note that replacing the Gaussian distribution of $J_{i_1 \ldots i_p}$ by a uniform distribution with mean 0 apparently does not significantly influence the number of metastable states.

The results of Table 2 show a clear tendency of decrease of $\alpha$ with increasing connectivities $z$, as expected from the calculations of section 2. Moreover, for fixed $z$ and within the estimated accuracy, the values of $\alpha$ seem to be independent of the geometry of the interaction patterns. This interesting result indicates that the properties of short-range $p$-spin Hamiltonians may be fully characterized by a few macroscopic parameters,
Table 2. Estimated values of $\alpha$ for various short-range 4-spin models.
For each pattern we list the number $X$ of non-zero interaction coefficients per spin, the site connectivity $z$, the best numerical estimate for $\alpha$ and standard deviation estimated from the linear regression.

| Model | Pattern | $X$ | $z$ | $\alpha$ | sdev  |
|-------|---------|-----|-----|----------|-------|
| q     | S       | 1   | 8   | 0.4056   | 0.0027|
| qdq   | D       | 1   | 8   | 0.4058   | 0.0017|
| q1Tq  | T1      | 1   | 10  | 0.3820   | 0.0024|
| q1q   | B       | 1   | 8   | 0.3885   | 0.0266|
| q2q   | S,D     | 2   | 12  | 0.3830   | 0.0049|
| qpq   | T3,T4   | 2   | 12  | 0.3830   | 0.0013|
| q3q   | S,D,B   | 3   | 16  | 0.3695   | 0.0014|
| q4q   | T1-T4   | 4   | 12  | 0.3807   | 0.0009|
| q5q   | T1-T4,D | 5   | 12  | 0.3744   | 0.0012|
| q6q   | T1-T4,D,B| 6  | 16  | 0.3746   | 0.0012|
| q8q   | T1-T4,L1-L4| 8 | 20  | 0.3744   | 0.0014|
| qAq   | T,L,D,B | 10  | 24  | 0.3757   | 0.0026|
| c     | octant  | 1   | 12  | 0.3911   | 0.0053|
| cp    | planar S| 1   | 8   | 0.4181   | 0.0076|
| c8    | 8 octants| 8  | 18  | 0.4058   | 0.0174|
| 4-spin numerical | $\infty$ | $\infty$ | 0.3509 | 0.3509 [21] |
| TAP   |         |     |     | 0.3552   | 0.3552 [11] |
| LABSP | open    |     |     | $O(N^2)$ | $O(N)$ 0.4634 | 0.4634 [20] | 0.0011 |
| LABSP | periodic|     |     | $O(N^2)$ | $O(N)$ 0.4713 | 0.4713 [22] | 0.0020 |

namely, $N$, $p$ and $z$. Indeed, the error between our theoretical predictions for $p = 4$ (see Table 1) and the numerical data for the two-dimensional model with the largest connectivity, $qAq$ ($z = 24$), is only 3.2%. (Comparison of the simulation data with the TAP solution for $z \to \infty$ yields an error of 5.4%.) Since the estimated systematic error is 1.2% the agreement between theory and simulations is quite good and provides additional evidence of the minor role played by the geometry of the interaction patterns on the landscape properties of $p$-spin models.

4. The Low Autocorrelated Binary String Problem

The Low Autocorrelated Binary String Problem (LABSP) [20, 22] consists of finding binary strings $x$ of length $N$ over the alphabet $\{\pm 1\}$ with low aperiodic off-peak autocorrelation $R_k(x) = \sum_{i=1}^{N-k} x_i x_{i+k}$ for all lags $k$. These strings have technical applications such as the synchronization in digital communication systems and the modulation of radar pulses. In the periodic variant of this model, one considers $R_k(x) = \sum_{i=1}^{N} x_i x_{i+k}$ with indices taken mod$N$. The quality of a string $x$ is measured
by the fitness function

$$f(x) = \sum_{k=1}^{N-1} R_k(x)^2.$$ (31)

In most of the literature on the LABSP the merit factor $F(x) = N^2/(2f(x))$ is used (see [20]): using $f$ instead is more convenient for explicit computations.

Recently there has been much interest in frustrated models without explicit disorder. The LABSP and related bit-string problems have served as model systems for this avenue of research [23, 24, 25]. These investigations have shown that LABSP has a golf-course type landscape structure, which explains the fact that it has been identified as a particularly hard optimization problem for heuristic algorithms such as simulated annealing (see [26, 27] and the references therein). In this section we show that LABSP has by far more local optima than one would expect from its correlation length or interaction order.

We use the fact that every function on the hypercube $\{+1, -1\}^N$ can be written as a linear combination of the $p$-spin functions $\varepsilon_{i_1, i_2, ..., i_p}(x) = x_{i_1}x_{i_2}x_{i_3} \ldots x_{i_p}$ to translate LABSP into explicit spin glass form. Explicitly, we have for the aperiodic model [1]

$$f(x) = a_0 + \sum_{k=1}^{\left\lfloor \frac{N}{2} \right\rfloor - 1} \sum_{i=1}^{N-2k} 2\varepsilon_{i, i+k}(x) + \sum_{k=1}^{N-1} \sum_{i=1}^{N-1} \sum_{j \neq i-k, i, i+k} \varepsilon_{i, i+k, j, j+k}(x),$$ (32)

where $a_0$ is a constant factor which does not depend on $N$. A similar expression can be derived for the periodic model. There are roughly $N^2/4$ non-zero second order contributions and on the order of $N^3$ non-zero fourth order contributions. Thus the relative weights (amplitudes) of the 2-spin and the 4-spin contributions are $B_2 = O(1/N)$ and $B_4 = 1 - O(1/N)$, respectively. For the general definition of $B_p$ see [1]. The landscape of LABSP thus consists of a (dominant) 4-spin Hamiltonian plus an asymptotically negligible quadratic component. The correlation length $\ell$ is therefore given by $\ell = N/8 + O(1)$, which is in excellent agreement with the estimate $\ell \approx 0.123 \cdot N - 0.983$ from numerical simulations [28]. We note that the generic 4-spin landscape is Derrida’s 4-spin Hamiltonian [7] which is a linear combination of all $\left(\begin{array}{c} N \\ 4 \end{array}\right)$ distinct 4-spin functions, while Eq.(32), on the other hand, only contains $O(N^3)$ non-vanishing 4-spin contributions. The landscape of the LABSP thus corresponds to a dilute 4-spin glass.

Table 2 summarizes a numerical survey of the local minima of the LABSP. For $N \leq 70$ we have generated up to $10^8$ spin configurations at random and checked whether they are local minima. As expected, the number of spin configurations that are local minima increases exponentially as $\exp(\alpha N)$. The non-exponential pre-factor depends strongly on $N \mod 4$: separate estimates of $\alpha$ from data for $N \mod 4 = 0, 1, 2, 3$ show deviations of up to $\pm 0.005$ within each of the variants of the LABSP, while the standard deviations from linear regression within each data set is almost an order magnitude smaller. We conclude that the discrepancy of 0.008 between the best estimates for $\alpha_{\text{periodic}}$ and $\alpha_{\text{open}}$, is not significant, since it is about the same size as the $N \mod 4$ dependence.
5. Conclusion

Metastable states are an important aspect of a landscape’s ruggedness. In this contribution we have shown that anisotropies, that is, deviations from a maximum entropy condition, significantly influence the frequency of metastable states, even when the interaction order $p$ of the spin glass model, and therefore the correlation length of the resulting landscape, is kept constant.

The correlation length $\ell$ was introduced as an easy-to-compute measure of ruggedness. Later on, it turned out that it has desirable algebraic properties, in particular in the context of Fourier transformation theory for fitness landscapes [1]. The inability of $\ell$ to reflect the $z$-dependence of $\langle N \rangle$ is certainly a weakness of this measure, in particular when ruggedness measures are used to predict the performance of optimization heuristics.

The anisotropy of short-range spin glass models is the consequence of a large number of vanishing coupling constants compared with the corresponding infinite-range $p$-spin model. Following earlier work by Tanaka and Edwards [17] we have determined the influence of a finite connectivity $z$ on the mean number $\langle N \rangle$ of metastable states. Our result shows that, to first order in $1/z$, the number of metastable states increases, i.e., short-range spin glasses are in general more rugged than their infinite-range counterparts. Moreover, the finite $z$ effect becomes much more pronounced as $p$ increases since the coefficient of $1/z$ diverges like $p \ln p$. Of course, large anisotropies due to very small lattice connectivities cannot be dealt with by our approach, which is also based on the assumption that all interaction patterns with fixed connectivity are equivalent. However, numerical simulations of several fourth-order spin glasses show that in these cases $\langle N \rangle$ seems to depend only on the lattice connectivity and not on the detailed geometry of the spin interactions.

The low-autocorrelated binary string problem may be regarded as a strongly anisotropic 4-spin model, where the interaction strength can assume only the values 0 and 1. This model is a particularly hard optimization problem [20, 27]. In this contribution we have shown that it exhibits a number of local optima that is by far larger than expected for a 4-spin model, even taking into account the reduced number of non-zero coefficients.

Our results indicate that a large class of generic short-range $p$-spin Hamiltonians may be fully characterized by a few macroscopic parameters, namely, $N$, $p$ and $z$. Particular anisotropic (non-generic) constructions, on the other hand, need not conform to this picture, as the example of the LABSP shows.

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References

[1] Stadler P F 1996 J. Math. Chem. 20 1
[2] Stadler P F and Happel R 1999 J. Math. Biol. 38 435
[3] Weinberger E D 1990 Biol. Cybern. 63 325
[4] Kern W 1993 Discr. Appl. Math. 43 115
[5] Ryan J 1995 Discr. Appl. Math. 56 75
[6] Palmer R 1991 Molecular Evolution on Rugged Landscapes: Proteins, RNA, and the Immune System ed A S Perelson and S A Kauffman (Redwood City: Addison Wesley)
[7] Derrida B 1980 Phys. Rev. Lett. 45 79
[8] Sherrington D and Kirkpatrick S 1975 Phys. Rev. Lett. 35(26) 1792
[9] Weinberger E D and Stadler P F 1993 J. Theor. Biol. 163 255
[10] Stadler P F 1994 J. Phys. I France 4 681
[11] Gross D J and Mézard M 1984 Nucl. Phys. B 240 431
[12] Derrida B and Gardner E 1986 J. Physique 47 959
[13] Roberts S A 1981 J. Phys. C: Solid St. Phys. 14 3015
[14] Oliveira V M and Fontanari J F 1997 J. Phys. A: Math. Gen. 30 8445
[15] García-Pelayo R and Stadler P F 1997 Physica D 107 240
[16] Stadler P F 1999 Evolutionary Dynamics; to appear in: Exploring the Interplay of Selection, Neutrality, Accident, and Function, ed J P Crutchfield and P Schuster (Oxford: Oxford University Press).
[17] Tanaka F and Edwards S F 1980 J. Phys. F: Met. Phys. 10 2769
[18] Bray A J and Moore M A 1981 J. Phys. C: Solid St. Phys. 14 1313
[19] Bray A J and Moore M A 1980 J. Phys. C: Solid St. Phys. 13 L469
[20] Bernasconi J 1987 J. Physique 48 559
[21] Stadler P F and Krakhofer B 1996 Rev. Mex. Fis. 42 355
[22] Golay M J E 1977 IEEE Trans. Inform. Th. IT-23 43
[23] Marinari E, Parisi G and Ritort F 1994 J. Phys. A: Math. Gen. 27 7615
[24] Marinari E, Parisi G and Ritort F 1994 J. Phys. A: Math. Gen. 27 7647
[25] Migliorini G and Ritort F 1994 J. Phys. A: Math. Gen. 27 7669
[26] Militzer B, Zamparelli M and Beule D 1998 IEEE Trans. Evol. Comp. 2 34
[27] Mertens S 1996 J. Phys. A: Math. Gen. 29 L473
[28] Stadler P F 1992 Europhys. Lett. 20 479
[29] Stadler P F and Schnabl W 1992 Phys. Lett. A 161 337