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Nonexistence of metastable states in a one-dimensional Heisenberg model spin-glass

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It is shown that in the classical Heisenberg linear chain with arbitrary nearest-neighbor interactions and nonzero but otherwise arbitrary next-nearest-neighbor interactions there are no metastable states. Since these models include examples with random and strongly competing exchange interactions (i.e., model spin-glasses), this result tends to run counter to the rather widely held notion that such competition aided by randomness causes the existence of a large number of low-energy local minima. In addition, some explicit metastable states are exhibited for a nonrandom planar spin model, and remarks on previous work are given which show that the question of the existence of a large number of low-lying local minima in two- and three-dimensional vector-spin model spin-glasses remains unanswered.

I. INTRODUCTION

The question of the number of local minima in classical vector models of spin-glasses was considered by Edwards and Anderson.[1] Interest in this question and the closely related one concerning metastable states (local minima lying above the ground-state energy) continues.[2–8] It is widely believed[9] that random competing exchange interactions (frustration effects), thought to be essential to spin-glass behavior, cause the existence of a large number of such states of low energy. In addition to the possible implications for equilibrium thermodynamic properties,[1,6,8] there is also the possibility[4] that such states might give rise to the unusual dynamic properties observed[5] in some spin-glasses.

In this paper, a rigorous calculation of the number of metastable states is given for a class of one-dimensional classical Heisenberg models which includes examples with random exchange interactions having arbitrarily large competition or frustration. The number found is zero, showing that large competition plus randomness does not automatically imply the existence of a large number of metastable states. As far as I am aware, this is the first calculation of the number of metastable states in *any* spin model involving many interacting spins, let alone models with the complexity (random, competing interactions) of those considered here.[10] Although one-dimensional models are, of course, special, and the results often do not generalize to two and three dimensions, exact solutions to problems always of course have at least the utility that they serve as check points for methods designed for more general applicability. In addition, a thermodynamically small number of metastable states is exhibited for a system with lattice translational symmetry. This is of some interest because rigorously demonstrated metastable states are rare and because it shows that they are not limited to random systems. Finally, earlier statements[1,7,8] claiming a large number of low-lying minima or important ground-state degeneracy in certain vector-spin models of various dimensionalities (including one), with randomness and/or frustration, are shown to be either erroneous or without foundation. Thus these papers leave unanswered the question of the existence of large numbers of low-lying local minima in two- and three-dimensional vector-spin model spin-glasses.

II. COUNTING OF METASTABLE STATES FOR HEISENBERG CHAINS

Central to the calculations for the spin-glass is a theorem stated without exhibiting the proof by Lyons and Kaplan[11] (LK). Because of its importance here I restate the theorem and present the proof. This LK theorem is, in words differing slightly from the original: Within the classical Heisenberg model, any locally stable coplanar state must be a ground state. The precise definitions of the terms used are as follows. The energy in the classical Heisenberg model is

$$E = -\sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j \equiv E\{\vec{S}_i\} \; , \tag{1}$$

where the spins $\vec{S}_i$ are real three-dimensional unit vectors,

$$\vec{S}_i^2 \equiv \sum_{\nu=1}^{m} S_{i\nu}^2 = 1 \; , \tag{2}$$

with $m=3$, and $J_{ij}=J_{ji}$, $J_{ii}=0$, J_{ij} are real. A locally stable state $\{\vec{S}_i^0\}$ (i.e., a local minimum), is defined as one that has the property

$$E\{\vec{S}_i\} - E\{\vec{S}_i^0\} \geq 0 \tag{3}$$

for sufficiently small, but otherwise arbitrary $\vec{S}_j - \vec{S}_j^0$ for all j.[12] A coplanar state is one that has the property $\vec{y}\cdot\vec{S}_i^0 = 0$ for all i, with $\vec{y}$ being a single real nonzero three vector (in other words the $\vec{S}_i^0$ are all parallel to one plane, the normal to which is $\vec{y}$). A ground state is one for which $E\{\vec{S}_i^0\}$ is the absolute or "global" minimum of E [i.e., Eq. (3) holds for *all* sets $\{\vec{S}_i\}$ satisfying Eq. (2)]. We note that Eq. (3) implies that a local minimum must be a stationary state, i.e.,

$$\left(\frac{\partial E}{\partial S_{i\nu}}\right)_0 = 0 \tag{4}$$

subject to Eq. (2).

The proof is as follows. Put

$$\vec{S}_i = \vec{S}_i^0 + \vec{\epsilon}_i \ . \tag{5}$$

Since $\vec{S}_i$ and $\vec{S}_i^0$ both satisfy Eq. (2) we have

$$2\vec{S}_i^0\cdot\vec{\epsilon}_i + \vec{\epsilon}_i^{\,2} = 0 \ , \tag{6}$$

which gives

$$E\{\vec{S}_i\} = E_0 - 2\sum_i \vec{\epsilon}_i\cdot\sum_j J_{ij}\vec{S}_j^0 - \sum_{ij} J_{ij}\vec{\epsilon}_i\cdot\vec{\epsilon}_j \ , \tag{7}$$

where $E_0 = E\{\vec{S}_i^0\}$. It is easy to see that the necessary and sufficient condition for stationarity of $\{\vec{S}_i^0\}$, i.e., for Eq. (4), is

$$\sum_j J_{ij}\vec{S}_j^0 = \lambda_i^0\vec{S}_i^0 \ , \tag{8}$$

all i, where λ_i^0 are scalars [Eqs. (8) and (2) imply $\lambda_i^0 = \vec{S}_i^0\cdot\sum_j J_{ij}\vec{S}_j^0$, which is + or − the magnitude of the "mean or molecular field" $\sum_j J_{ij}\vec{S}_j^0 \equiv \vec{\lambda}_i^0$ at spin i]. Equation (7) with Eqs. (6) and (8) gives

$$\Delta \equiv E\{\vec{S}_i\} - E_0 = \sum_{ij} W_{ij}\vec{\epsilon}_i\cdot\vec{\epsilon}_j \ , \tag{9}$$

exactly, where

$$W_{ij} = \lambda_i^0\delta_{ij} - J_{ij} \ . \tag{10}$$

Introduce a Cartesian coordinate system for each i with orthonormal vectors $\hat{x}_i, \hat{y}_i, \hat{z}_i$, choosing

$$\hat{z}_i = \vec{S}_i^0 \tag{11}$$

and write

$$\vec{\epsilon}_i = \hat{x}_i\epsilon_{ix} + \hat{y}_i\epsilon_{iy} + \hat{z}_i\epsilon_{iz} \ . \tag{12}$$

For small $|\vec{S}_i - \vec{S}_i^0|$, Eq. (6) gives

$$\epsilon_{iz} = -\tfrac{1}{2}(\epsilon_{ix}^2 + \epsilon_{iy}^2) + O((\epsilon_{ix}^2 + \epsilon_{iy}^2)^2) \ , \tag{13}$$

so

$$\Delta = \sum_{ij} W_{ij}(\hat{x}_i\cdot\hat{x}_j\epsilon_{ix}\epsilon_{jx} + \hat{y}_i\cdot\hat{y}_j\epsilon_{iy}\epsilon_{jy} + 2\hat{x}_i\cdot\hat{y}_j\epsilon_{ix}\epsilon_{jy}) + O(\epsilon^3) \ , \tag{14}$$

where $O(\epsilon^3)$ means third order in the small quantities ϵ_{ix} and ϵ_{iy}. Suppose now the $\vec{S}_i^0$ are coplanar; choose $\hat{x}_i$ to lie in, i.e., parallel to, this plane. Then $\hat{y}_i = \hat{y}$, independent of i, so that Eq. (14) becomes, for the coplanar case,

$$\Delta = \sum_{ij} W_{ij}(\hat{x}_i\cdot\hat{x}_j\epsilon_{ix}\epsilon_{jx} + \epsilon_{iy}\epsilon_{jy}) + O(\epsilon^3) \ . \tag{15}$$

It follows that if the coplanar state $\{\vec{S}_i^0\}$ is locally stable, W_{ij} must be a positive semidefinite matrix [choose in Eq. (15) $\epsilon_{ix} = 0$ for all i]. But this with Eq. (9) shows that $\Delta \geq 0$ for *all* allowed $\vec{\epsilon}_i$, and therefore $E\{\vec{S}_i^0\}$ is the absolute minimum of $E\{\vec{S}_i\}$. That is, this LK theorem is proved.

Consider now an open linear chain with first- and second-neighbor interactions J_{ij} only, containing N spins:

$$E = -2\sum_{i=1}^{N-1} J_i^{(1)}\vec{S}_i\cdot\vec{S}_{i+1} - 2\sum_{i=1}^{N-2} J_i^{(2)}\vec{S}_i\cdot\vec{S}_{i+2} \ . \tag{16}$$

This, with the $J_i^{(n)}$ chosen according to some probability distribution, defines the class of one-dimensional spin-glasses (and nonglasses) that will be studied here.[13] Since both positive and negative values of $J_i^{(1)}$ and $J_i^{(2)}$ are allowed, the model is seen to contain important *competition* between different exchange interactions.[11,14] For example if $J_i^{(1)}$ and $J_{i+1}^{(1)}$ have the same sign and $J_i^{(2)} < 0$, the spins $\vec{S}_i$, $\vec{S}_{i+1}$, $\vec{S}_{i+2}$ cannot be chosen to minimize each "bond" individually, that is, each of the three terms $-J_i^{(1)}\vec{S}_i\cdot\vec{S}_{i+1}$, $-J_{i+1}^{(1)}\vec{S}_{i+1}\cdot\vec{S}_{i+2}$, $-J_i^{(2)}\vec{S}_i\cdot\vec{S}_{i+2}$. It is this competition that is thought to be an essential ingredient in giving so-called spin-glass behavior, the other essential ingredient being randomness.[3,5,6,8,15] Recently a new word, "frustration," has been introduced[15] (attributed[15] to Anderson) and claimed to represent a new concept.[8,15] In fact the concept described[15,16] was not new, being identical to the idea of competition studied extensively[11,14,17] in 1959 and the early 60's—see in particular the detailed description of the concept in the introduction of the Lyons-Kaplan paper cited in Ref. 14.

It will now be shown that in every stationary state for our linear chain the spins must be coplanar for all distributions with zero probability of a zero value of the second-neighbor interaction $J_i^{(2)}$. Let spins $\vec{S}_1$ and $\vec{S}_2$ in a particular stationary state define a plane P (if they are collinear the plane will not be unique). The mean field acting on $\vec{S}_1$ is $\vec{\lambda}_1 = J_1^{(1)}\vec{S}_2 + J_1^{(2)}\vec{S}_3$ and therefore Eq. (8) with $i = 1$ demands $\vec{S}_3$ must be in P (for $J_1^{(2)} \neq 0$). Similarly $\vec{\lambda}_2 = J_1^{(1)}\vec{S}_1$

$+J_2^{(1)}\vec{S}_3+J_2^{(2)}\vec{S}_4$, so that Eq. (8) forces $\vec{S}_4$ to be in P (for $J_2^{(2)}\neq 0$). Now $\vec{\lambda}_3$ involves the four spins $\vec{S}_1$, $\vec{S}_2$, $\vec{S}_4$, $\vec{S}_5$, three of which are coplanar; since $\vec{\lambda}_3$ is parallel to $\vec{S}_3$, also in P, it follows (for $J_3^{(2)}\neq 0$) that $\vec{S}_5$ is in P. This process obviously continues (for $J_n^{(2)}\neq 0$ all n), since for $i\geq 3$ the general case where $\vec{\lambda}_i$ is a linear combination of at most four spins holds. (In the case where $\vec{S}_1$ and $\vec{S}_2$ are collinear the above considerations show that the spins must all be collinear.)

Combining this result with the LK theorem gives the result, an open-ended one-dimensional Heisenberg model with only nearest neighbor $J_i^{(1)}$, and second-nearest-neighbor interactions $J_i^{(2)}$ such that none of the $J_i^{(2)}$ are zero (but $J_i^{(1)}$ and $J_i^{(2)}$ are otherwise arbitrary) has no metastable states.

It is interesting to note that if there are (in addition) third neighbor interactions, or periodic boundary conditions, the above proof that all stationary states are coplanar fails.

One can easily prove the following similar theorem by a very slightly different argument for coplanarity. A one-dimensional Heisenberg (open or closed) chain with nearest-neighbor interactions only, none of which are zero, has no metastable states. The open ended case here has no competing interactions, of course.

III. EXPLICIT METASTABLE STATES FOR A PLANAR MODEL

Having exhibited a class of models in which there are no metastable states, I now present some explicit metastable states for a particular model. Consider the (classical) planar-spin model (the spins are coplanar by definition), with energy (1) which can be written

$$E=-\sum_{ij}J_{ij}\cos(\phi_i-\phi_j)\ , \tag{17}$$

where the ϕ_i, whose range is 0 to 2π, are the angles made by the spins relative to an axis fixed in the spin plane. Further put the spin-sites $i=1,\ldots,N$ on a regular linear chain with periodic boundary conditions and take the $J_{ij}=J>0$ for nearest neighbors, zero otherwise (the ground state is ferromagnetic). Clearly any simple spiral, i.e., any state with the angles $\phi_i^0=QR_i$, is stationary (the periodic boundary conditions require $Q=2\pi n/N$, where n is an integer). Local stability requires the matrix

$$\left(\frac{\partial^2 E}{\partial\phi_p\partial\phi_s}\right)_0=\begin{cases}-2J_{ps}\cos(\phi_p^0-\phi_s^0), & p\neq s\\ 2\sum_t J_{pt}\cos(\phi_p^0-\phi_t^0), & p=s\end{cases} \tag{18}$$

to be positive semidefinite. But the eigenvalues of Eq. (18) are easily found to be

$$\lambda_k=2J(1-\cos k)\cos Q\ , \tag{19}$$

where $k=2\pi m/M$, $m=0,\pm 1,\ldots$. Thus any spiral with $|Q|<\pi/2$ is locally stable. Since the energy of such a spiral is $E(Q)=-2NJ\cos Q$, it follows that spirals with $0<Q<\frac{1}{2}\pi$ are metastable. Although these metastable states clearly owe their existence to the boundary conditions, and are therefore not of interest in connection with bulk properties, they nevertheless are of some interest. Aside from their mere existence (interesting because rigorously demonstrated metastable states in infinite systems are very rare), they probably are relevant to calculations for finite systems.[2,5,18]

IV. COMMENTS ON PREVIOUS WORK

The number of locally stable states in the planar spin model was calculated by Edwards and Anderson[1]; they found a very large number ($\approx 2^N$) for random J_{ij}, independent of lattice structure and dimensionality. However there is a series of errors, which I now note, which invalidates their argument. The first error is the statement including their Eq. (3.2), namely, that a stationary state $\{\phi_\alpha^0\}$ will be a minimum if[19] (in the notation of the present paper) $\sum_j J_{ij}\cos(\phi_i^0-\phi_j^0)>0$. The latter is simply the requirement that λ_i^0, Eq. (8) above, be positive; i.e., each spin points in the same direction as the mean field $\vec{\lambda}_i^0$ at its site. A counterexample is $\phi_i^0=0$ for all i on a linear chain with strong ferromagnetic 2nd neighbor J_{ij} and weak antiferromagnetic nearest neighbor J_{ij} (an infinitesimal uniform rotation of all even-numbered spins will lower the energy, and yet $\lambda_i^0=\sum_i J_{ij}>0$). In fact $\lambda_i^0>0$ is a necessary but not always sufficient condition for local stability, $2\lambda_i^0$ being a diagonal element of Eq. (18) ($\lambda_i^0>0$ is the condition for stability under deviation, small or large, of one spin at a time).[20] The next error is the statement, below their Eq. (3.14), to the effect that for any stationary solution $\{\phi_i^0\}$, there are 2^N solutions based on combinations of choices like ϕ_i^0 and $\pi-\phi_i^0$. This statement is easily seen to be incorrect for a collinear spin state with $\phi_i^0=\phi^0$ independent of i and nonzero. Probably $\phi_i^0\rightarrow\pi+\phi_i^0$ was intended since in this case their statement is correct for collinear spin states; however, then the statement is easily seen to be incorrect by considering a spiral with general $\vec{Q}$. The last error to be discussed here is the statement (page 1934 of Ref. 1) that there are 4^N stationary states, contradicting the result $N_e=2^N$ obtained just previously[1] by the authors. It seems that they have assumed that their earlier "result" [that there are 2^N solutions for each solution of Eq. (3.3)] says to multiply N_e by 2^N to obtain the number of stationary states—however this is not so since their counting formula, (3.15), includes *all* solutions.

A related question concerns a statement made by José.[8] Namely, the spins in a frustrated plaquette do not have a unique way of lowering their energy by changing their orientations. A plaquette is a square with a spin at each corner; a frustrated plaquette is one in which the product of the four (nearest-neighbor) exchange interactions J is negative. The model considered[8] is either the classical Heisenberg or the planar model. It is clear from the context that the nonuniqueness intended is only nonuniqueness beyond that implied by (the trivial) *uniform* spin rotations, which occurs even in nonfrustrated systems. In fact the claim of nonuniqueness is incorrect as seen by an example, the Heisenberg model with three of the J's $=1$, the fourth one $=-1$. Let the spins be labeled $\vec{S}_1, \vec{S}_2, \vec{S}_3, \vec{S}_4$ going successively clockwise around the square. That the spins are coplanar in the ground state follows from the discussion above. Let $\vec{S}_1$ and $\vec{S}_2$ share the antiferromagnetic bond and ϕ be the angle between them. If θ_i is the angle made by $\vec{S}_i$ with $\vec{S}_1+\vec{S}_2$, so $\theta_1=\frac{1}{2}\phi=-\theta_2$, the minimum energy occurs when[21] $\theta_4=-\theta_3=\frac{1}{6}\phi$ and $\phi=\frac{1}{4}3\pi$. The uniqueness follows from the fact the (only) other solution, $\phi=-\frac{1}{4}3\pi$, is merely a uniform rotation of the spins from the first. (For the planar model, this does yield a true twofold degeneracy beyond uniform rotations, as described by the two-valued "chirality" τ[21]; nevertheless, even in this case the ground-state degeneracy for a macroscopic square net is probably insignificant—Villain[6] argues that there is merely a twofold degeneracy.)

A similar statement is the one by Marland and Betts[7] to the effect that the ground state is highly degenerate in classical spin systems (which includes according to them the $S=\frac{1}{2}$ Ising model and the planar model) with competing interactions. A particular example with competing interactions discussed[7] is the triangular lattice (in either the planar or Heisenberg models) with nearest-neighbor antiferromagnetic interactions. However, it is known[11] that the ground state for the classical planar and Heisenberg models in this case is a spiral (the turn angle between nearest-neighbor spins is 120°). Furthermore, one can show that this state is essentially nondegenerate (no thermodynamically significant degeneracy beyond that due to uniform rotations) by means of an argument along the lines of the one used by Villain[6] to prove the nondegeneracy for his "odd-rule" square net. Thus, the statement[7] that the classical ground state is highly degenerate is incorrect. It follows that the general import of that paper,[7] that it is quantum effects which are responsible for the lack of degeneracy in the ground state, is without foundation.[22]

V. SUMMARY

In summary, I have demonstrated errors in statements in the literature which claim for spin-glasses a large number of low-lying local minima or a large ground-state degeneracy. I have presented the first calculation of the number of metastable states in any spin model; the models considered are one-dimensional, and include a class of spin-glasses (Heisenberg models with random competing interactions). The number of metastable states was found to be zero in all those models. I also exhibited some metastable states for a model with translational symmetry. It should not be concluded from this that, in general, vector spin-glasses possess no metastable states—numerical work[2,18] has already indicated the existence of some. A proper conclusion is that *random competing exchange interactions alone are not sufficient to cause the existence of metastable states.* In any case I would remark that obviously the important related question is not whether a spin-glass model has low-lying local minima, but rather, if it does, how does the number and nature of these states compare with similar states that might exist in *crystalline* spin models (which presumably show "ordinary" phase transitions, differing profoundly from observed spin-glass behavior) for which the question of the existence of local minima is unanswered, to my knowledge.

An interesting question remaining with the one-dimensional spin-glass model studied above is the ground-state degeneracy. Preliminary considerations suggest there is none of thermodynamic significance—but the problem has not yet been solved.

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[3]P. W. Anderson and Caroline Morgan Pond, Phys. Rev. Lett. 40, 903 (1978).

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[6]Jacques Villain, J. Phys. C 10, 1717 (1977).

[7]L. G. Marland and D. D. Betts, Phys. Rev. Lett. 43, 1618 (1979).

[8]J. V. José, in Proceedings of the 1979 Kyoto Summer Institute (in press).

[9]See, e.g., Refs. 7 and 8 for explicit statements.

[10]The definitions (see text) of local minimum and metastable state (i.e., state of metastable equilibrium) used here are consistent with the papers referred to above, and conform to previous usage [see, e.g., *Dictionary of Physics and Mathematics* (McGraw-Hill New York, 1978), pp. 572, 619, and *Thermodynamics,* H. B. Callen (Wiley, New York 1960)]. These definitions require stability under spin deviations from those in the state of interest in which *arbitrary numbers* of spins take part. As such, they differ seriously from recent usage by some authors. For example, I. Morgenstern and K. Binder, Phys. Rev. Lett. 43, 1615 (1979), use the term "metastable state" within the Ising model to mean a state for which flipping small enough clusters of spins raises the energy, but flipping larger clusters lowers the energy. Somewhat similarly, Bray and Moore, J. Phys. C 13, L469 (1980), define metastable, within an Ising model, as "one spin-flip stable." F. Tanaka and S. F. Edwards (TE) (unpublished), use the term "local minimum" within both Ising and continuous-vector-spin models to mean a state for which single-spin flips raise the energy, and the term "local minimum" for what I (and other sources) call simply a local minimum. It should be realized that these single-spin-flip "local minima" include states which would not be long-lived in real materials involving Heisenberg- or XY-like spins. This is so since such "local minima," would have highly accessible decay channels via single-magnon processes, no energy barrier to lowering the energy being involved.

[11]D. H. Lyons and T. A. Kaplan, Phys. Rev. 120, 1580 (1960).

[12]The equality must occur for any uniform rotation of all the spins. Although in a final definition one probably would want to limit the equality to such deviations and perhaps others of zero measure, it is sufficient for our purpose here to accept the weaker definition given.

[13]One-dimensional spin-glasses are not without precedent—see J. Villain, Z. Phys. B 33, 31 (1979).

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[17]For a brief review of early theoretical work see T. A. Kaplan, Bull. Acad. Sci. USSR, Phys. Ser. 28, 328 (1964).

[18]D. L. Huber, W. Y. Ching, and M. Fibich, J. Phys. C 12, 3535 (1979).

[19]Equations (3.1) and (3.2) contain a misprint, namely, the sum over α and β should be a sum over α or over β.

[20]In unpublished work, Tanaka and Edwards (Ref. 10) recognized the fact that $\lambda_i^0 > 0$ is only a necessary condition for local stability.

[21]J. Villain, J. Phys. C 10, 4793 (1977).

[22]It should perhaps be noted that in Ref. 7, the term "frustration" is used in the sense that a "frustrated system" or a model that "experiences frustration" is, *by definition,* a system or model in which the ground state is highly degenerate (beyond that related to uniform spin rotations). This is a very different sense from that of the other sources of which I am aware (e.g., Refs. 8 and 15), where frustration is defined in terms of the interactions J_{ij}. Thus, e.g., the antiferromagnetic, nearest-neighbor XY model (quantum or classical), on the triangular lattice, would be called frustrated by the definition of Refs. 8 and 15, but is said in Ref. 7 to experience no frustration (in the quantum case).