Dependence of ground-state energy of classical *n*-vector spins on *n*

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We study the ground state energy $E_G(n)$ of N classical $O(n)$ vector spins with the Hamiltonian $\mathcal{H}=-\Sigma_{i>j}J_{ij}\vec{S}_i\cdot\vec{S}_j$ where the coupling constants $\{J_{ij}\}$ are arbitrary. We prove that $E_G(n)$ is independent of n for all $n>n_{\max}(N)=\lfloor(\sqrt{8N+1}-1)/2\rfloor$. We show that this bound is the best possible. We also derive an upper bound for $E_G(m)$ in terms of $E_G(n)$, for $m<n$. We obtain an upper bound on the frustration in the system, as measured by $F(n)\equiv[\Sigma_{i>j}|J_{ij}|+E_G(n)]/\Sigma_{i>j}|J_{ij}|$. We describe a procedure for constructing a set of J_{ij}'s such that an arbitrary given state, $\{\vec{S}_i\}$, is the ground state. We show that the problem of finding the ground state for the special case $n=N$ is equivalent to finding the ground state of a corresponding soft-spin problem.

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I. INTRODUCTION

In this paper, we study the ground states of N unit classical $O(n)$ spins, $\vec{S}_i$, having a hamiltonian of the form

$$\mathcal{H}=-\sum_{i>j}J_{ij}\vec{S}_i\cdot\vec{S}_j \tag{1}$$

where J_{ij}'s are arbitrary real numbers—positive, negative, or zero. Such Hamiltonians with arbitrary bonds and couplings are of interest in the context of disordered systems, especially spin glasses [1]. One of the interesting questions is the behavior of the ground state energy as the spin space dimension, n, is increased. For example one can study the behavior of such models when n is large. In this context, Hastings [2] proved that for N spins beyond a spin space dimension of $n_{\max}(N)=\lfloor(\sqrt{8N+1}-1)/2\rfloor$ the ground state energy does not decrease any further and also that this bound is saturated. Aspelmeier and Moore [3] have then used this bound in accelerating their numerical simulations of spin glasses. We provide an alternate proof for this bound. A similar analysis has been done earlier in the context of correlation matrices by Grone *et al.* [4] and for a relaxed version of maxcut problem of theoretical computer science [5].

An interesting question is the behavior of the *average* number of nonzero spin space components (average over disorder) in the ground state as a function of the number of spins, N. For the infinite range model with gaussian distributed J_{ij}'s, this number increases as N^{μ} where $\mu=\frac{2}{5}$ [2,3]. Lee, Dhar, and Young [6] have numerically determined μ for several different models.

We also derive both upper and lower bounds on the ground state energy of $O(m)$ spins in terms of the ground state energy when they are replaced by $O(n)$ spins $(m\neq n)$ keeping the couplings, J_{ij}'s, the same. A stronger bound is also provided for Ising spins $(m=1)$ when all couplings are antiferromagnetic and $E_G(n)$ is low.

We also consider the problem of finding the ground state of such a Hamiltonian [7]. We study the inverse problem—how to find a (nontrivial) Hamiltonian of the form in Eq. (1) so that a given spin state $\{\vec{S}_i\}$ is the ground state. This question is trivial for Ising spins. One just assigns a non-negative J_{ij} if the spins are parallel, and a nonpositive J_{ij} if they are antiparallel. However with $O(n)$ spins $(n>1)$ the problem is nontrivial and in some cases there is no (nonzero) solution, for example, $N=3$, $n\geq 3$, with the three spins noncoplanar. In general, to find the desired set of couplings, J_{ij}'s, we can express the Hamiltonian in terms of the angles of the spherical polar coordinates of the spins and set the derivatives with respect to the angles equal to zero at the angles corresponding to the desired ground state. This gives a set of linear relations between the couplings, J_{ij}'s. In addition, to ensure that this extremum is a minimum, and not a maximum or a saddle point, we have the additional constraint of the Hessian being positive semidefinite. Finding J_{ij}'s which simultaneously satisfy the linear relations as well as the positive semidefiniteness constraint on the Hessian is nontrivial. It is a semidefinite programming problem [8] for which fast algorithms and their software implementations are available.

We provide a simple procedure for obtaining a large class of such Hamiltonians. However, not all Hamiltonians with $\{\vec{S}_i\}$ as the ground state are obtained by this procedure. We conjecture a characterization of the Hamiltonians obtained and give proof of a part of the conjecture.

The special case $n=N$ is of interest as it is equivalent to the "large-N" models studied earlier [2]. We show an equivalence between the problem of finding the ground state when $n=N$ and the ground state of a corresponding soft spin problem. While this duality is interesting in itself, it also clarifies the conceptual relation between the proof given in this paper of $n_{\max}(N)=\lfloor(\sqrt{8N+1}-1)/2\rfloor$ and the one given by Hastings [2].

The plan of the paper is as follows. In Sec. II we summarize some properties of the correlation matrices of classical spin states which are found useful in the later sections. In Sec. III, we prove that for N spins beyond a spin space dimension of $n_{\max}(N)$ the ground state energy becomes independent of n. That this is the best bound is proved by providing a sequence of graphs and couplings, one for each N, such that $E_G(n_{\max}-1)>E_G(n_{\max})$. In Sec. IV, we derive both upper and lower bounds on the ground state energy of $O(m)$ spins in terms of the ground state energy when they are replaced by $O(n)$ spins $(m\neq n)$ keeping the couplings, J_{ij}'s, the same. For Ising spins with all couplings antiferromagnetic, in a special case, a stronger bound is derived. We obtain an

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upper bound on spin frustration, as measured by $F(n) \equiv [\Sigma_{i>j}|J_{ij}| + E_G(n)]/\Sigma_{i>j}|J_{ij}|$—we show that $F(n) - F(\infty) \leq \beta_n$ where β_n is a constant, independent of J_{ij}'s. In Sec. V, we provide a procedure for constructing Hamiltonians of the form in Eq. (1) with arbitrary given state $\{\vec{S}_i\}$ as the ground state. In Sec. VI we demonstrate a duality between the problem of finding the ground state for the special case of $n=N$ and a corresponding soft-spin problem. Section VII summarizes the results.

II. SOME PROPERTIES OF CORRELATION MATRICES OF CLASSICAL SPIN STATES

Summarized below are some properties of correlation matrices which will be useful in the later sections. These properties are well known in computer science literature [5].

For an arbitrary state $\{\vec{S}_i\}$ of $O(n)$ spins define the $(N \times N)$ correlation matrix, $C=[\vec{S}_i \cdot \vec{S}_j]$. Explicitly,

$$C = S^T S, \tag{2}$$

where S is the $(n \times N)$ matrix with vector of the ith spin as the ith column. Clearly, C is real, symmetric, has diagonal elements unity, and can be written as $C=\mathcal{O}D\mathcal{O}^T$, where $\mathcal{O}$ is an orthogonal matrix and D diagonal.

C is positive semidefinite, i.e., all eigenvalues of C are non-negative, since for every $x \in R^N$, $x^T C x = (Sx)^T(Sx) \geq 0$.

The number of nonzero (and hence positive) eigenvalues of C is at most n. This can be seen as follows: Each row of C is a linear combination of the n rows of S implying that the number of linearly independent rows of C is at most n. Diagonalizing C, let $C=\mathcal{O}D\mathcal{O}^T$ where $\mathcal{O}$ is an orthogonal matrix and D diagonal with (let us say) first k eigenvalues positive and rest zero. The rows (columns) of $\mathcal{O}$ are mutually orthogonal and hence linearly independent. $(D\mathcal{O}^T)$ now has k linearly independent rows and thus $\mathcal{O}D\mathcal{O}^T$ also has k linearly independent rows. The number of linearly independent rows of C we have already argued to be at most n. Hence the number of positive eigenvalues of C is at most n.

Conversely, if C is a real, symmetric matrix with diagonal elements unity and having n or fewer positive eigenvalues and rest zero, then there exists a spin state of classical $O(n)$ unit spins for which it is the correlation matrix. To see this, C being real and symmetric, can be diagonalized as $C = \mathcal{O}D\mathcal{O}^T = (\mathcal{O}\sqrt{D})(\mathcal{O}\sqrt{D})^T$ where $\mathcal{O}$ is an orthogonal matrix and D diagonal with first $k(\leq n)$ diagonal entries positive. The last $(N-n)$ rows of $(\mathcal{O}\sqrt{D})^T$ are known to be zero and we drop them to define an $(n \times N)$ matrix S such that $C = S^T S$. Since $c_{ii}=1 \; \forall \, i$ each column of S can be interpreted as a unit classical $O(n)$ spin, C being their correlation matrix.

III. INDEPENDENCE OF THE GROUND STATE ENERGY FROM n FOR $n \geq n_{\max}(N)$

Consider the variation of the ground state energy $E_G(n)$ as a function of the spin space dimension n of the $O(n)$ spins keeping the couplings, J_{ij}'s, the same. For $n' > n$ we have $E_G(n) \geq E_G(n')$ because for any state of $O(n)$ spins we can construct a corresponding state of $O(n')$ spins with the same value of energy by adding $(n'-n)$ zero components to each $O(n)$ vector. Also for any $n > N$ we have $E_G(n)=E_G(N)$ because N spins span an at most N dimensional subspace of the n dimensional spin space implying that by an appropriate choice of basis we can make all coordinates after the first N coordinates zero and by dropping them we get an $O(N)$ spin state with the same value of energy.

Theorem 1. For N classical unit $O(n)$ vector spins with Hamiltonian $\mathcal{H} = -\Sigma_{i>j} J_{ij} \vec{S}_i \cdot \vec{S}_j$, where $\{J_{ij}\}$ are any real numbers, the ground state energy $E_G(n)=E_G(n_{\max})$ for all $n > n_{\max}$ where

$$n_{\max}(N) = \left\lfloor \frac{\sqrt{8N+1}-1}{2} \right\rfloor. \tag{3}$$

Here $\lfloor x \rfloor$ for $x \in \mathbf{R}$ is the greatest integer not greater than x.

Proof. Let us summarize the idea of the proof before getting into the details. Suppose we have a ground state which has more than $n_{\max}(N)$ dimensions. Starting from the correlation matrix of this state we construct another matrix which is the correlation matrix of a spin state which is embedded in one less spin space dimension but has the same energy. This construction always works whenever the spin state is embedded in more than $n_{\max}(N)$ dimensions. Since, as shown above, $E_G(n) \geq E_G(n')$ for $n' > n$ this implies that for $n > n_{\max}$, $E_G(n)=E_G(n_{\max})$, as desired.

We now discuss the proof. When the spins are $O(N)$ vectors let $\{\vec{S}_i\}$ be a ground state. Consider the correlation matrix, C, with elements $c_{ij}=\vec{S}_i \cdot \vec{S}_j$ for all i, j. Diagonalizing C, we can write $C=\mathcal{O}^T D \mathcal{O}$ with D a diagonal matrix and $\mathcal{O}$ an orthogonal matrix. Let

$$D = \begin{bmatrix} d_1 & \ldots & 0 & 0 & \ldots & 0 \\ \ldots & & \ldots & 0 & \ldots & 0 \\ 0 & \ldots & d_k & 0 & \ldots & 0 \\ 0 & \ldots & 0 & 0 & & 0 \\ \ldots & \ldots & \ldots & & & \ldots \\ 0 & \ldots & \ldots & & & 0 \end{bmatrix}, \tag{4}$$

where the first k diagonal entries of D are positive and rest zero.

Consider $C' = \mathcal{O}^T(D + rB)\mathcal{O}$ where B is symmetric with $B_{ij}=0$ if $i > k$ or $j > k$. This leaves $\frac{1}{2}k(k+1)$ free parameters in B and ensures that C' is also symmetric and the zero eigenvalues of C and the corresponding eigenvectors are not perturbed. Also, let B satisfy

$$[\mathcal{O}^T B \mathcal{O}]_{tt} = 0 \tag{5}$$

for all $t=1,2,\ldots,N$. This ensures that the diagonal elements of C' remain unchanged.

The $\frac{1}{2}k(k+1)$ free parameters of B must satisfy the N linear homogenous equations (5). Hence whenever $\frac{1}{2}k(k+1) > N$ such a nonzero B will exist and we can increase r till one of the first k eigenvalues of C becomes zero. Thus we obtain a matrix C' which is the correlation matrix of a spin state embedded in $(k-1)$ dimensions. (The same argument

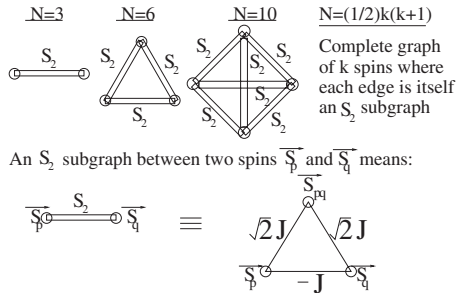

FIG. 1. Sequence of examples for which $E_G(n_{\max}(N)) < E_G(n_{\max}(N)-1)$. Shown are three of those members of the sequence for which $(\sqrt{8N+1}-1)/2$ is an integer [such N's are $3,6,10,\ldots=\frac{1}{2}k(k+1)$]. The rest of the members are obtained by adding appropriate number of free spins to the example of the last N for which $(\sqrt{8N+1}-1)/2$ is an integer, e.g., $N=8$ example has two more free spins added to the $N=6$ example.

goes through if r is negative and we increase $|r|$.) As shown in the next paragraph, this spin state is a ground state. Thus applying this procedure repeatedly we obtain a ground state embedded in at most $\lfloor(\sqrt{8N+1}-1)/2\rfloor$ dimensions.

The matrix B chosen above is such that for r small enough $C'=C\pm r\mathcal{O}^T B\mathcal{O}$ are *both* correlation matrices of valid spin states with energy $-\Sigma_{i>j}J_{ij}c_{ij}\pm r[\Sigma_{i>j}J_{ij}(\mathcal{O}^T B\mathcal{O})_{ij}]$. Since we started from a C which was a ground state this can happen only if $\Sigma_{i>j}J_{ij}(\mathcal{O}^T B\mathcal{O})_{ij}=0$, i.e., if $\mathcal{O}^T B\mathcal{O}$ was a "neutral direction." Thus the correlation matrix C' also corresponds to a ground state.

Hence we have provided a construction for continuously deforming a ground state and bringing it to lie in an at most $n_{\max}(N)$ dimensional subspace of the spin space without changing the energy, thus proving the desired result.

Theorem 2. The bound in theorem 1 is the best possible, i.e., there exist values of $\{J_{ij}\}$ such that $E_G(n_{\max})<E_G(n_{\max}-1)$ where $n_{\max}(N)=\lfloor(\sqrt{8N+1}-1)/2\rfloor$.

Proof. Consider three spins $\vec{S}_p$, $\vec{S}_q$, and $\vec{S}_{pq}$ with $J_{pq}=-J$ and $J_{p(pq)}=J_{q(pq)}=\sqrt{2}J$; see Fig. 1. It is easy to see that for this system of three spins, in the ground state $\vec{S}_p$ is perpendicular to $\vec{S}_q$ (and $\vec{S}_{pq}$ is along their angle bisector).

Now consider a complete graph of k spins such that each edge is itself an S_2 subgraph, as shown in Fig. 1. While constructing the ground state of such a system we need to consider only the k spins at the joints of these S_2 subgraphs because in the minimum energy configuration each of the spins which are internal to the S_2 subgraphs will lie along the angle bisector of its two neighbors. The contribution of any of the S_2 subgraphs, let us say consisting of the spins $\vec{S}_p$, $\vec{S}_q$ and $\vec{S}_{pq}$, will get minimized if $\vec{S}_p$ and $\vec{S}_q$ are perpendicular to each other. The k spins at the joints between S_2 subgraphs can be arranged perpendicular to each other only in an at least $n_{\max}=k$ dimensional spin space thus completing the proof.

We note that at finite temperature the free energy does not remain independent of n even for large n. This may be seen in, both, the high as well as low temperature expansions for the free energy.

IV. BOUNDS ON THE GROUND STATE ENERGY

We have seen that $E_G(m)\geq E_G(n)$ for $m<n$. Now we will derive an *upper* bound on $E_G(m)$ in terms of $E_G(n)$. This result (theorem 3) generalizes a known result on the performance of Goemans-Williamson algorithm for maxcut problem of theoretical computer science [5]. The result by Goemans and Williamson, when translated into statistical physics language, would correspond to the special case of $m=1$. Theorem 4 is a translation of a known result on maxcut problem into statistical physics language [5]. The connection between the problem of finding the ground states of Ising spins and maxcut problem has been known before [9].

It will be helpful to summarize the overall strategy before getting into the details. Suppose the various possible orientations of $O(m)$ spins occur according to an arbitrary given probability distribution. Then the energy is also a random variable and the expected value of the energy will always be greater than or equal to the ground state energy, i.e., $E_G(m)\leq E[\mathcal{H}_m]$, where $E[\mathcal{H}_m]$ denotes the expected value of the energy of $O(m)$ spins. If we choose the probability distribution in such a way that we are able to bound $E[\mathcal{H}_m]$ in terms of $E_G(n)$ from above we would have obtained the desired result.

Now we give the derivation in detail. First we define a randomized procedure for obtaining an $O(m)$ state, say $\{\vec{S}_{i(m)}\}$, from the ground state $\{\vec{S}'_{i(n)}\}$ of $O(n)$ spins. In the spin space of $O(n)$ spins randomly choose an m-dimensional subspace and project all the spins onto it. Normalize the $O(m)$ vectors thus obtained. Clearly different $O(m)$ states are obtained by this procedure depending on which m-dimensional subspace was chosen for projection. The expectation value of the $O(m)$ energy is $E[\mathcal{H}_m]=-\Sigma_{i>j}J_{ij}E[\vec{S}_{i(m)}\cdot\vec{S}_{j(m)}]$. Now if $\mathcal{P}_{mn}$ denotes a projection operator from n to m dimensions

$$E[\vec{S}_{i(m)}\cdot\vec{S}_{j(m)}]=\int\frac{\mathcal{P}_{mn}\vec{S}'_{i(n)}\cdot\mathcal{P}_{mn}\vec{S}'_{j(n)}}{|\mathcal{P}_{mn}\vec{S}_{i(n)}||\mathcal{P}_{mn}\vec{S}_{j(n)}|}d\mathcal{P}_{mn}\equiv f_{mn}(\theta_{ij}), \tag{6}$$

where θ_{ij} is the angle between $\vec{S}'_{i(n)}$ and $\vec{S}'_{j(n)}$ and the integral is over all projection operators $\mathcal{P}_{mn}$ with equal measure. As an example, in spherical polar coordinates,

$$f_{23}(\theta)=\int_{\phi_2=0}^{\pi}\int_{\phi_1=0}^{2\pi}\frac{\sin\phi_2(\cos\theta-\cos\phi_1\sin^2\phi_2\cos(\phi_1-\theta))}{4\pi\sqrt{1-\cos^2\phi_1\sin^2\phi_2}\sqrt{1-\sin^2\phi_2\cos^2(\phi_1-\theta)}}d\phi_2 d\phi_1. \tag{7}$$

By reversing the direction of $\vec{S}'_{i(n)}$ we observe that

$$f_{mn}(\pi - \theta_{ij}) = -f_{mn}(\theta_{ij}). \tag{8}$$

Also $[1-f_{mn}(\theta)]/(1-\cos\theta) \geq 0$ for all $\theta \in (0,\pi]$. Hence we can find a lower bound on $[1-f_{mn}(\theta)]/(1-\cos\theta)$, denoted by α_{mn}, which gives

$$f_{mn}(\theta) \leq (1-\alpha_{mn}) + \alpha_{mn}\cos\theta. \tag{9}$$

Also replacing θ by $(\pi-\theta)$ in this inequality we get

$$-f_{mn}(\theta) \leq (1-\alpha_{mn}) - \alpha_{mn}\cos\theta. \tag{10}$$

For $J_{ij}<0$, using Eq. (9), we get

$$-J_{ij}f_{mn}(\theta_{ij}) \leq -(1-\alpha_{mn})J_{ij} - \alpha_{mn}J_{ij}\cos\theta_{ij}. \tag{11}$$

For $J_{ij}>0$, using Eq. (10), we get

$$-J_{ij}f_{mn}(\theta_{ij}) \leq (1-\alpha_{mn})J_{ij} - \alpha_{mn}J_{ij}\cos\theta_{ij}. \tag{12}$$

Summing Eq. (11) over all those ij pairs for which $J_{ij}<0$ and Eq. (12) over all those ij pairs for which $J_{ij}>0$ and adding we get

$$E[\mathcal{H}_m] = -\sum_{i>j} J_{ij}f_{mn}(\theta_{ij}) \leq (1-\alpha_{mn})\sum_{i>j}|J_{ij}| + \alpha_{mn}E_G(n). \tag{13}$$

Now the minimum value of a random variable is always less than or equal to its expectation value. Therefore, we have the following.

Theorem 3. For $(m<n)$

$$E_G(n) \leq E_G(m) \leq (1-\alpha_{mn})\sum_{i>j}|J_{ij}| + \alpha_{mn}E_G(n), \tag{14}$$

where α_{mn} is the minimum value of $[1-f_{mn}(\theta)]/(1-\cos\theta)$ over the interval $\theta \in (0,\pi]$ and $f_{mn}(\theta)$ has been defined above or, rearranging the inequality, $(1/\alpha_{mn})E_G(m) - [(1-\alpha_{mn})/\alpha_{mn}]\Sigma_{i>j}|J_{ij}| \leq E_G(n) \leq E_G(m)$.

As an example, it is easy to show [5] that for $m=1$ and n arbitrary, $f_{1n}(\theta_{ij}) = 1-2(\theta_{ij}/\pi)$ and $\alpha_{1n} \approx 0.878\,56$. We have determined f_{23} and f_{34} numerically by representing them as integrals in spherical polar coordinates; see Eq. (7), for instance. The graphs of $f_{34}(\theta)$ and $q_{34}(\theta) = [1-f_{mn}(\theta)]/(1-\cos\theta)$ are shown in Fig. 2. We find that $\alpha_{23} \approx 0.96$ and $\alpha_{34} \approx 0.98$.

As a specific instance, for the triangular lattice antiferromagnet $E_G(1) = -\frac{1}{3}J$ implying that $-(0.52)J \leq E_G(2) \leq -\frac{1}{3}J$. It is known that $E_G(2) = -(0.5)J$ which compares very well with the *nontrivial part* of the inequality. Now, we prove a stronger bound for a special case of Ising antiferromagnets.

Theorem 4. For the special case of $m=1$, let all couplings, J_{ij}, be antiferromagnetic. Then for the case $(E_G(n) \leq \delta\Sigma_{i>j}|J_{ij}|)$ $(\delta \approx -0.69)$ we have the stronger bound

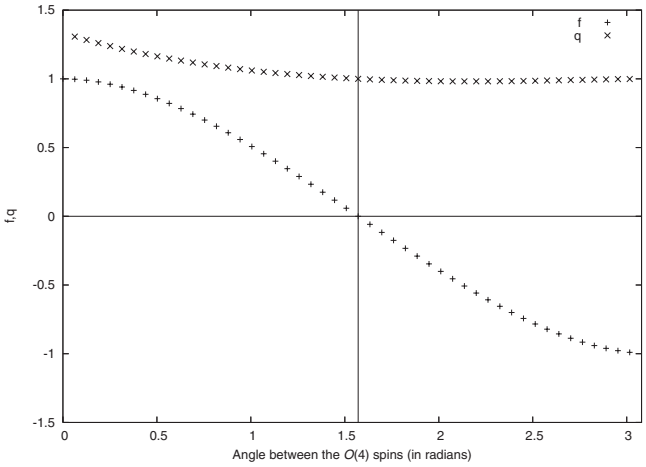

FIG. 2. Functions $f_{34}(\theta)$ and $q_{34}(\theta) = [1-f_{34}(\theta)]/(1-\cos\theta)$.

$$E_G(n) \tag{15}$$

$$\leq E_G(1) \tag{16}$$

$$\leq \left(-\sum_{i>j}|J_{ij}|\right)\frac{2}{\pi}\arccos\left(\frac{E_G(n)}{\sum_{i>j}|J_{ij}|}\right) + \sum_{i>j}|J_{ij}|. \tag{17}$$

Proof. Again using the randomized procedure in the derivation of theorem 3, from the ground state $\{\vec{S}'_{i(n)}\}$ of $O(n)$ model, various Ising states are obtained with different probabilities such that $E[\mathcal{H}_1] = -\Sigma_{i>j}J_{ij} + \Sigma_{i>j}J_{ij}(2/\pi)\arccos x_{ij}$ where $x_{ij} = \vec{S}'_{i(n)}\cdot\vec{S}'_{j(n)}$ [using $f_{1n}(\theta_{ij}) = 1-2(\theta_{ij}/\pi)$].

Consider the function $\arccos x$. Draw the *oblique* tangent from (1,0) to the curve, intersecting the curve tangentially at $(\delta, \arccos\delta)$. Consider the function $h(x)$ which is the same as $\arccos x$ for $x<\delta$ and the same as the tangent for $x \in [\delta,1]$.

Clearly, $\arccos x_{ij} \geq h(x_{ij})$ and since all $J_{ij} \leq 0$,

$$E[\mathcal{H}_1] \tag{18}$$

$$\leq \frac{2}{\pi}\sum_{i>j}J_{ij}h(x_{ij}) - \sum_{i>j}J_{ij} \tag{19}$$

$$\leq -\frac{2}{\pi}\left(\sum_{i>j}|J_{ij}|\right)h\left(\sum_{i>j}\frac{|J_{ij}|}{\sum_{p>q}|J_{pq}|}x_{ij}\right) - \sum_{i>j}J_{ij}, \tag{20}$$

where the last inequality uses the convexity of $h(x)$.

Since the minimum value of a random variable is less than or equal to its expectation value, we have $E_G(n) \leq E_G(1) \leq E[\mathcal{H}_1]$. Also, for $x<\delta$ we have $h(x) = \arccos x$ and the desired inequality is proved.

In the presence of antiferromagnetic J_{ij}'s, there may not exist any spin configuration that minimizes the energy of each individual bond to $-|J_{ij}|$. One of the possible measures of the frustration of spins is

$$F(n) \equiv \frac{\sum_{i>j} |J_{ij}| + E_G(n)}{\sum_{i>j} |J_{ij}|}. \tag{21}$$

We can consider spin frustration as arising in two steps: First we choose the J_{ij}'s but do not put any restriction on the dimensionality of the spin space—it is allowed to be as large as desired for the minimization of energy. The frustration of this system will be $F(\infty)$ which will be the same as $F(n_{\max}(N))$, where $n_{\max}(N)=\lfloor(\sqrt{8N+1}-1)/2\rfloor$, because $E_G(n)=E_G(n_{\max}(N))$ for $n>n_{\max}(N)$. To obtain the actual $O(n)$ system we *now* restrict the number of dimensions in the spin space to n, thus increasing the spin frustration from $F(n_{\max}(N))$ [same as $F(\infty)$] to $F(n)$.

Theorem 5. If $(m<n)$

$$\frac{E_G(m)-E_G(n)}{\sum_{i>j} |J_{ij}|} \le 2(1-\alpha_{mn}). \tag{22}$$

As a particular case,

$$F(n)-F(n_{\max}(N)) \le 2(1-\alpha_{nN}), \tag{23}$$

where α_{mn} are the same as in theorem 3.

Proof. In theorem 3, subtract $E_G(n)$ throughout, divide by $\Sigma_{i>j}|J_{ij}|$ and observe that $E_G(n)/\Sigma_{i>j}|J_{ij}| \ge -1$ thus completing the proof.

In particular, for all n, $F(n)-F(n_{\max}(N)) \le F(1)-F(n_{\max}(N)) \le 2(1-\alpha_{1N}) \approx 0.242\,88$ (independent of N, as discussed at the end of theorem 3).

V. PROCEDURE FOR CONSTRUCTING A MODEL WITH AN ARBITRARY GIVEN GROUND STATE

For N classical spins of $O(n)$ type let $\{\vec{S}_i'\}$ be a given state. We want to construct a Hamiltonian with only two-spin Heisenberg type interactions which has $\{\vec{S}_i'\}$ as the ground state. The following procedure constructs a Hamiltonian of the form in Eq. (1) (up to a constant) which has $\{\vec{S}_i'\}$ as the ground state.

(1) For the given ground state $\{\vec{S}_i'\}$ construct the correlation matrix, C', such that $c_{ij}'=\vec{S}_i'\cdot\vec{S}_j' \; \forall\, i,j=1,2,\ldots,N$.

(2) Let $C'=O'D'O'^T$ where O' is an orthogonal matrix and D' diagonal with, let us say, the first k diagonal entries nonzero and the rest entire matrix zero.

(3) Construct an $(N\times N)$ auxilliary matrix G as follows:

$$G=\begin{bmatrix} G_1 & G_2 \\ G_3 & G_4 \end{bmatrix}, \tag{24}$$

where G_1 is a $(k\times k)$ matrix, etc. Moreover, choose $G_1=0$, $G_2=0$, $G_3=0$, and G_4 to be any $(N-k)\times(N-k)$ real, symmetric matrix with all eigenvalues *nonpositive*.

(4) Define $J=[J_{ij}]=O'GO'^T$.

Theorem 6. For the Hamiltonian $\mathcal{H}=-\Sigma_{i,j=1}^{N} J_{ij}\vec{S}_i\cdot\vec{S}_j$ thus constructed, the spin state $\{\vec{S}_i'\}$ is the ground state.

Proof. For any spin state $\{\vec{S}_i\}$, construct the correlation matrix $C=[c_{ij}]=[\vec{S}_i.\vec{S}_j]$ and diagonalize it,

$$C=\mathcal{O}D\mathcal{O}^T, \tag{25}$$

where $\mathcal{O}$ is an orthogonal matrix and D is diagonal with all eigenvalues non-negative.

Also for the matrix J defined above let

$$(-J)^T=\hat{O}\hat{D}\hat{O}^T, \tag{26}$$

where $\hat{O}$ is an orthogonal matrix and $\hat{D}$ is diagonal. Since J is negative semidefinite, $(-J)$ is positive semidefinite, thus the entries of $\hat{D}$ are non-negative.

Now $\mathcal{H}=\mathrm{Tr}((-J)^TC)$. Using Eqs. (25) and (26) and repeatedly using $\mathrm{Tr}(AB)=\mathrm{Tr}(BA)$ we get $\mathcal{H}=\mathrm{Tr}[W^TW]\ge 0$ where $W=\sqrt{\hat{D}}\hat{O}^T\mathcal{O}\sqrt{D}$. Therefore, for any state $\{\vec{S}_i\}$,

$$\mathcal{H}\ge 0. \tag{27}$$

For $\{\vec{S}_i'\}$, by construction, $\mathcal{H}=\mathrm{Tr}((-J)^TC')=0$ implying that $\{\vec{S}_i'\}$ is a ground state of $\mathcal{H}$.

Although a large number of Hamiltonians with arbitrary given state $\{\vec{S}_i'\}$ as the ground state can be obtained by this procedure, not all the Hamiltonians with this property are obtained. For instance, it can be easily checked that for three Ising spins, one up and the other two down happens to be a ground state when all three couplings are antiferromagnetic with equal strength, but this set of couplings can not be obtained by the above procedure for any allowed choice of the matrix G_4. Thus we would like to characterize which Hamiltonians can be obtained by this procedure for a given ground state and which Hamiltonians cannot be obtained.

We expect that a Hamiltonian with $\{\vec{S}_i'\}$ as the ground state is obtained by this procedure if and only if upon replacing the given spins by spins with any higher spin space dimension, keeping J_{ij}'s the same, the ground state energy remains the same. The *if* part is our conjecture while the *only if* part is proved as follows: for any $\tilde{n}>n$, by augmenting each vector of $\{\vec{S}_i'\}$ by $(\tilde{n}-n)$ zeroes, we can obtain a state with the value of the Hamiltonian $\mathcal{H}_{\tilde{n}}=0$. Since the Hamiltonian is expressible as the trace of the product of two symmetric positive semidefinite matrices its value cannot be negative as in Eq. (27), implying that the $\tilde{n}$ dimensional state thus obtained is the ground state of $O(\tilde{n})$ spins. Therefore, for $\tilde{n}>n$ we have $E_G(\tilde{n})=E_G(n)$ thus completing the proof. This proof is consistent with the case of three Ising spins with antiferromagnetic couplings discussed above because if we replace three Ising spins by XY spins the ground state energy decreases from $-\frac{1}{3}J$ per bond to $-\frac{1}{2}J$ per bond.

VI. DUALITY OF THE PROBLEM OF FINDING THE GROUND STATE WHEN $n=N$

It is interesting to compare Hastings' proof of theorem 1 [2] with the proof given here. We make this comparison by demonstrating a close relation between the problem of finding the ground state when $n=N$ and a corresponding soft spin

problem. The case of $n=N$ is equivalent to the "large-N" model studied by Hastings and others [2]. Apart from providing an understanding of the relation between the two proofs of theorem 1, this duality is interesting in itself. The duality derived below is a special case of semidefinite programming duality. We follow the approaches in [8,10]. The analysis leading to theorems 7 and 8 below amounts to specializing the general approach of [8,10] to the case of our interest.

The problem of finding the ground state of N classical $O(n)$ spins having a Hamiltonian of the form $\mathcal{H}=-\Sigma_{i>j}J_{ij}\vec{S}_i.\vec{S}_j$ is

Problem $P_1(n)$

$$\text{minimize} - \sum_{i>j} J_{ij}\vec{S}_i \cdot \vec{S}_j$$

subject to constraints

$$\vec{S}_i \cdot \vec{S}_i = 1 \text{ and } \vec{S}_i \in R^n \; \forall \; i = 1 \ldots N$$

By the properties of correlation matrices discussed in Sec. II, for each state $\{\vec{S}_i\}$ of N classical $O(n)$ unit vectors the corresponding correlation matrix, C, satisfies the constraints of problem $P_2(n)$, below, and conversely, any matrix, C, satisfying the constraints of $P_2(n)$ is a correlation matrix of a state $\{\vec{S}_i\}$ of N classical $O(n)$ unit vectors. Moreover, this correspondence is such that $-\Sigma_{i>j}J_{ij}\vec{S}_i.\vec{S}_j=-\Sigma_{i>j}J_{ij}c_{ij}$ implying that the problems $P_1(n)$ and $P_2(n)$ are equivalent.

Problem $P_2(n)$

$$\text{minimize} - \sum_{i>j} J_{ij}c_{ij}$$

subject to constraints

$$c_{ii} = 1 \; \forall \; i = 1 \ldots N$$

$C^T = C$ and has all eigenvalues non-negative

number of positive eigenvalues of $C \leq n$

$C = [c_{ij}]$ being an $(N \times N)$ matrix

Consider the special case of $n=N$, i.e., the number of spin space dimensions being equal to the number of spins. For this case the constraint in $P_2(n)$, that the number of positive eigenvalues of the matrix C be at most n, becomes redundant and can be dropped.

The constraints in the remaining problem $P(n=N)$ can be accounted for by taking the matrix C to be of the form

$$C = I + \sum_{i>j} c_{ij}M_{ij} \tag{28}$$

with all eigenvalues of C non-negative, I being the identity matrix and M_{ij} the matrix with (ij)th and (ji)th entries 1 and rest zero, i.e.,

Problem $P_2(n=N)$

$$\text{minimize} - \sum_{i>j} J_{ij}c_{ij}$$

subject to constraints

C is a real $(N \times N)$ matrix

$$C = I + \sum_{i>j} c_{ij}M_{ij}$$

C has all eigenvalues non-negative

Define a symmetric matrix $C_D=C_D^T$ and a Lagrangian, $\mathcal{L}$ as

$$\mathcal{L}(c_{ij}, c_{D(kl)})_{i>j,k\geq l} \tag{29}$$

$$= - \sum_{i>j} J_{ij}c_{ij} - \text{Tr}(C_D C) \tag{30}$$

$$= - \sum_{i>j} J_{ij}c_{ij} - \left[\left(\sum_{i=1}^{N} c_{D(ii)} \right) + 2 \sum_{i>j} c_{ij}c_{D(ij)} \right] \tag{31}$$

$$= - \sum_{i>j} (2c_{D(ij)} + J_{ij})c_{ij} - \sum_{i=1}^{N} c_{D(ii)}. \tag{32}$$

The problem $P_2(n=N)$ is then equivalent to

$$E_G(n=N) \tag{33}$$

$$= \min_{\text{all } c_{ij}} \max_{C_D \succeq 0, C_D^T = C_D} \mathcal{L}(c_{ij}, c_{D(kl)})_{i>j,k\geq l}, \tag{34}$$

where $C_D \succeq 0$ means that all the eigenvalues of C_D are non-negative.

To see this equivalence, observe that for any C having a negative eigenvalue (let us say the first) we can choose C_D to be $C_D=\alpha^2 v_1 v_1^T$ where v_1 is the eigenvector of C corresponding to the first eigenvalue and then $Tr(C_D C)=\alpha^2 Tr(v_1^T C v_1) \leq 0$. By choosing α to be large, the maximization over C_D results in $\mathcal{L}$ becoming $+\infty$. Thus all C's with any eigenvalue negative will get ignored when we minimize over c_{ij}'s and we need to consider only C's with all eigenvalues non-negative. When C has all eigenvalues non-negative, let $C=\mathcal{O}D\mathcal{O}^T$ and for any allowed C_D let $C_D=\tilde{\mathcal{O}}\tilde{D}\tilde{\mathcal{O}}^T$. Then

$$\text{Tr}(C_D C) \tag{35}$$

$$= \text{Tr}[(\sqrt{\tilde{D}}\tilde{\mathcal{O}}^T\mathcal{O}\sqrt{D})(\sqrt{\tilde{D}}\tilde{\mathcal{O}}^T\mathcal{O}\sqrt{D})^T] \tag{36}$$

$$\geq 0. \tag{37}$$

Thus for a C with all eigenvalues non-negative

$$\max_{C_D \succeq 0, C_D^T = C_D} \mathcal{L}(c_{ij}, c_{D(kl)})_{i>j,k\geq l} = - \sum_{i>j} J_{ij}c_{ij} \tag{38}$$

proving the desired equivalence.

It is easy to see that if in Eq. (34) we instead perform the minimization before the maximization, the resulting value

can only decrease. We will call this resulting problem as the dual problem and denote its value by $-E_G^D$:

$$-E_G^D \tag{39}$$

$$=\max_{C_D\succeq 0, C_D^T=C_D} \min_{\text{all } c_{ij}} \mathcal{L}(c_{ij}, c_{D(kl)})_{i>j,k\geq l} \tag{40}$$

$$\leq \min_{\text{all } c_{ij}} \max_{C_D\succeq 0, C_D^T=C_D} \mathcal{L}(c_{ij}, c_{D(kl)})_{i>j,k\geq l} \tag{41}$$

$$=E_G(n=N). \tag{42}$$

By arguments similar to the equivalence between $P_2(n=N)$ and Eq. (34) the dual problem Eq. (40) can easily be shown to be equivalent to

$$\max \; -\sum_{i=1}^N c_{Dii}$$

subject to constraints

$$c_{Dij} = -\tfrac{1}{2} J_{ij} \; \forall \; i>j$$

$C_D = C_D^T$ and has all eigenvalues non-negative

C_D being a real $(N \times N)$ matrix.

By arguments similar to those given above this is the same as

Problem dual

$$\min \sum_{i=1}^N \vec{S}_i^{D2}$$

subject to constraints

$$\vec{S}_i^D \cdot \vec{S}_j^D = -\tfrac{1}{2} J_{ij} \; \forall \; i>j$$

$$\vec{S}_i^D \in R^N \; \forall \; i = 1 \ldots N$$

The problem $P(n=N)$ and the dual satisfy the requirements of the strong duality theorem of semidefinite programming (see, for instance, theorem 3.1 of [8]) which then implies the following.

Theorem 7:

$$E_G(n=N) = -E_G^D. \tag{43}$$

Using this in Eqs. (30), (32), and (38), we also conclude that if $\{\vec{S}_i^*\}$ is the ground state of the unit spin problem with $n=N$ and $\{\vec{S}_i^{D*}\}$ is the ground state of the dual problem then the corresponding correlation matrices satisfy

$$\mathrm{Tr}(C^* C_D^*) = 0. \tag{44}$$

Since C^* and C_D^* both have all eigenvalues non-negative, rewriting the trace as in Eq. (36) above, Eq. (44) implies that

$$C^* C_D^* = 0 \tag{45}$$

or in terms of the spins

$$\sum_{j=1}^N (\vec{S}_i^* \cdot \vec{S}_j^*)(\vec{S}_j^{D*} \cdot \vec{S}_k^{D*}) = 0 \; \forall \; i,k. \tag{46}$$

So we have seen that the problems of finding the ground states $P(n=N)$ and dual are closely related. If $\{\vec{S}_i^*\}$ is the ground state of $P(n=N)$ and $\{\vec{S}_i^{D*}\}$ of dual then $E_G(n=N) = -E_G^D$ and Eqs. (46) hold. Conversely, if for some $\vec{S}_i \in R^N$, $\vec{S}_i \cdot \vec{S}_i = 1 \; \forall \; i$ and $\vec{S}_i^D \in R^N$ with $\vec{S}_i^D \cdot \vec{S}_j^D = -\frac{1}{2} J_{ij} \; \forall \; i>j$ and the corresponding correlation matrices satisfy $C^* C_D^* = 0$ then we also have $\mathrm{Tr}(C^* C_D^*) = 0$ which means that $-\Sigma_{i=1}^N \vec{S}_i^{D2} = -\Sigma_{i>j} J_{ij} \vec{S}_i \cdot \vec{S}_j$. Since $E_G(n=N) \geq -E_G^D$ the only possibility is that $\{\vec{S}_i\}$ and $\{\vec{S}_i^D\}$ are the respective ground states. Thus for any pair of valid states of $P(n=N)$ and dual if the product of the correlation matrices is zero then they are respective ground states.

Therefore, we have

Theorem 8. $\{\vec{S}_i^*\}$ is the ground state of $P(n=N)$ and $\{\vec{S}_i^{D*}\}$ of dual if and only if the corresponding correlation matrices satisfy

$$C^* C_D^* = 0. \tag{47}$$

Remarks

(1) The connection between our proof of theorem 1 above and Hasting's proof in [2] can now be seen in light of this duality. Our proof counted the number of *nonzero* eigenvalues of the correlation matrix C while Hasting's approach amounts to counting the *zero* eigenvalues of the correlation matrix C_D of the dual (see theorem 8 above). The parameters λ_i in [2] may be identified with c_{Dii} in the above discussion.

(2) The parameters λ_i in Hasting's treatment [2] (which correspond to c_{Dii} in our treatment at zero temperature) continue to remain defined even at finite temperature. Moreover, the expression for average energy at finite temperature in Hasting's treatment is $VkT - \Sigma_{i=1}^V \lambda_i$ [Eq. (9) in [2], the V in this expression is the same as N in our notation]. Recognizing that λ_i are the same as c_{Dii} this form is the same as the Hamiltonian of our dual problem except for the term linear in T. It would therefore be interesting if some form of this duality holds at finite temperatures also.

VII. SUMMARY

We showed that as we increase the spin space dimension, n, the ground state energy, $E_G(n)$, becomes independent of n beyond a spin space dimension of $n_{\max}(N)$, and this bound is the best possible. For $m<n$ we derived an upper bound for $E_G(m)$ in terms of $E_G(n)$, the lower bound was trivial. A stronger version for a special case of $m=1$ was also proved. Similar bounds on $E_G(m) - E_G(n)$ and a measure of spin frustration, $F(n)$, were derived. A procedure was given for constructing a hamiltonian with an arbitrary given spin state, $\{\vec{S}_i'\}$, as the ground state. For the special case $n=N$, the problem of finding the ground state was shown to be equivalent to another soft-spin problem.

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