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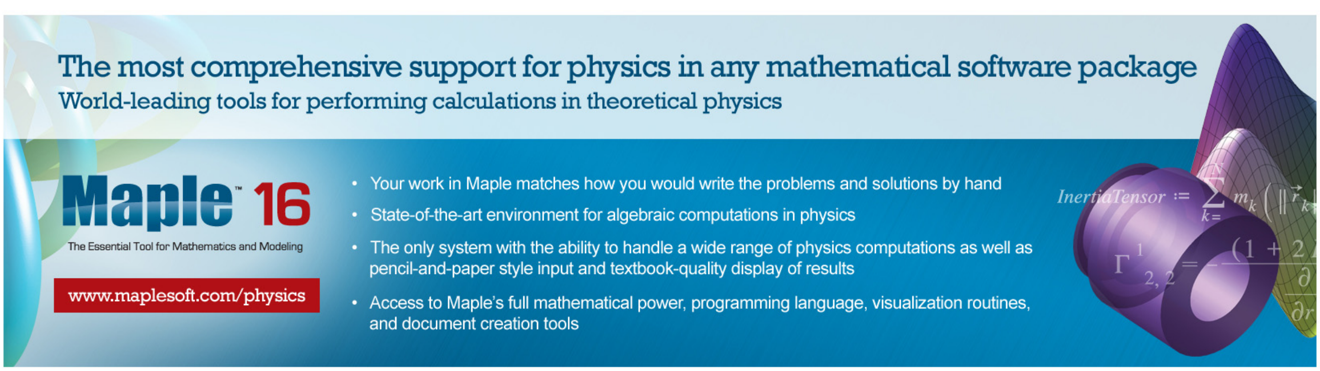

This equation and its simple generalizations are the results Craig needs. But $G_0^{-1}$ has a vanishing eigenvalue so that the solution to Eq. (2) is only given modulo the addition of an arbitrary amount of the solution of the homogeneous equation $G_0^{-1}(1, \bar{1}) \times f(\bar{1}) = 0$. This added term will serve to correct Eq. (3) for the mismatch between the value of the two-particle correlation function implied by the decomposition and that appropriate to the statistical state of interest.[9] These are just the terms which are neglected in Craig's expansion and which are needed to describe the complete effect of the chosen statistical state on the system properties.

[9] This is not to say that Ambegaokar's proof is not valid in the context in which it was introduced. In thermal equilibrium the boundary conditions on the correlation functions are such that no additional terms can be appended to Eq. (3).

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# On Next-Nearest-Neighbor Interaction in Linear Chain. I

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Ground-state properties of the Hamiltonian

$$H = \tfrac{1}{2}J\sum_{i=1}^{N} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+1} + \tfrac{1}{2}J\alpha \sum_{i=1}^{N} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+2}$$

($\boldsymbol{\sigma}_{N+1} \equiv \boldsymbol{\sigma}_1$, $\boldsymbol{\sigma}_{N+2} \equiv \boldsymbol{\sigma}_2$) are studied for both signs of $J$ and $-1 \leq \alpha \leq 1$ to gain insight into the stability of the ground state with nearest-neighbor interactions only ($\alpha = 0$) in the presence of the next-nearest-neighbor interaction. Short chains of up to 8 particles have been exactly studied. For $J > 0$, the ground state for even $N$ belongs always to spin zero, but its symmetry changes for certain values of $\alpha$. For $J < 0$, the ground state belongs either to the highest spin (ferromagnetic state) or to the lowest spin and so to zero for even $N$. The trend of the results suggests that these facts are true for arbitrary $N$ and that the critical value of $\alpha$ is probably zero. Upper and lower bounds to the ground-state energy per spin of the above Hamiltonian are obtained. Such bounds can also be obtained for the square lattice with the nearest- as well as the next-nearest-neighbor interaction.

## I. INTRODUCTION

The Heisenberg linear chain with the Hamiltonian

$$H = \tfrac{1}{2}J\sum_{i=1}^{N} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+1} \tag{1}$$

($J < 0$ ferromagnetic, $J > 0$ antiferromagnetic) was thoroughly investigated by Bethe[1] and the ground-state energy determined by Bethe and Hulthén.[2] des Cloizeaux and Pearson[3] discussed the low-lying excitation spectrum and Griffiths[4] calculated the magnetization at zero temperature. While the 1-dimensional version is an interesting many-body problem, the general Heisenberg Hamiltonian as a description of magnetic phenomena belongs, to quote Herring,[5] "more to the world of thought." An extensive criticism of the exchange integral and its relevance to magnetic properties of solids is given by Herring.[6]

Two obvious criticisms leveled against (1) or its 3-dimensional analog are the neglect of anisotropy and the restriction to nearest-neighbor interaction only. Taking the isotropic Hamiltonian, Mermin and Wagner[7] showed that there was no spontaneous magnetization in one and two dimensions. In three dimensions, spontaneous magnetization is believed to exist. An attempt to incorporate anisotropy is the study of the Hamiltonian considered in detail by Orbach[8]:

$$H = \tfrac{1}{2}J\sum_{i=1}^{N} (\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \Delta\sigma_i^z\sigma_{i+1}^z). \tag{2}$$

Many interesting properties of this Hamiltonian are known from the recent extensive work by Yang and Yang,[9] who give references to earlier works. One might expect that in two dimensions, for sufficiently large $\Delta$, a spontaneous magnetic moment exists, although in the 1-dimensional case, at finite temperatures, it probably does not.

[1] H. Bethe, Z. Physik **71**, 205 (1931).
[2] L. Hulthén, Arkiv Mat. Astron. Fysik **26A**, No. 11 (1938).
[3] J. des Cloizeaux and J. J. Pearson, Phys. Rev. **128**, 2131 (1962).
[4] R. B. Griffiths, Phys. Rev. **133**, A768 (1964).
[5] C. Herring, Rev. Mod. Phys. **34**, 631 (1962).
[6] C. Herring, in *Magnetism*, G. T. Rado and H. Suhl, Eds. (Academic Press Inc., New York, 1966), Vol. IV.
[7] N. D. Mermin and H. Wagner, Phys. Rev. Letters **17**, 1133 (1966).
[8] R. Orbach, Phys. Rev. **112**, 309 (1958); **115**, 1181 (1959).
[9] C. N. Yang and C. P. Yang, Phys. Rev. **147**, 303 (1966); **150**, 321, 327 (1966); **151**, 258 (1966).

Our purpose is to direct attention to the second of the two restrictions—only nearest-neighbor interactions. We propose to study the Hamiltonian

$$H = \tfrac{1}{2}J \sum_{i=1}^{N} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+1} + \tfrac{1}{2}J\alpha \sum_{i=1}^{N} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+2} \tag{3}$$

($N + 1 \equiv 1,\ N + 2 \equiv 2$), where the next-nearest neighbors interact with a strength $\alpha J$, $-1 \leq \alpha \leq 1$. In general, the next-nearest-neighbor interaction will be smaller than the nearest-neighbor interaction. However, their ratio may not be completely negligible.[10] An exact solution of this Hamiltonian, not to speak of its 3-dimensional variant, is probably very difficult. We shall, however, present lower and upper bounds on the ground-state energy per spin in one dimension for any $J$ and for $\alpha$ in $[-1, 1]$. To get an idea of the possibilities involved we have studied short chains of 4, 6, 8 and 3, 5, 7 spins and we shall present the data with the corresponding conjectures about large $N$.

The question that we hope to answer by studying (3) in this way is the following: How stable are the ground states of (1) with regard to the presence of the next-nearest-neighbor interaction? In particular, if the "classical" ground states become unstable, what is the nature of instability and what is the new ground state? Another purpose is to examine the mathematical difficulties one might encounter in the extension to a realistic situation of forces of intermediate range.

The sign of the exchange integral is a difficult question and without any prior prejudice we should allow both possibilities for next-nearest-neighbor interactions. We thus have the following four different cases:

(i) $J < 0$, $\alpha > 0$: all the interactions are ferromagnetic, and the classical ground state of aligned spins is expected to be stable;

(ii) $J > 0$, $\alpha < 0$: the nearest neighbors interact antiferromagnetically, while the next-nearest neighbors tend to align themselves—again a stabilization of the classically accepted picture;

(iii) $J < 0$, $\alpha < 0$: the next-nearest-neighbors have a tendency to align in opposite direction and the ferromagnetic alignment is likely to be destroyed for large $|\alpha|$ (An interesting question here is: what is this critical $\alpha$?);

(iv) $J > 0$, $\alpha > 0$: the alignment of the next-nearest neighbors is opposing that of the nearest-neighbor interaction and the ground state, although of spin zero, may have alignments different from that of the classical ground state, that is, different symmetry.

[10] J. S. Smart, in *Magnetism*, G. T. Rado and H. Suhl, Eds. (Academic Press Inc., New York, 1963), Vol. III.

The study of short linear chains corroborates the expectations. In cases (i) and (ii), nothing untoward happens. In the presence of strong antiferromagnetic next-nearest-neighbor interaction, the ferromagnetic ground state becomes unstable and the lowest state has spin zero ($N$ even). When all interactions are antiferromagnetic, the ground state definitely has spin zero, but the symmetry of the ground state changes for strong antiferromagnetic next-nearest-neighbor interaction.

Concerned with this last point we have a theorem due to von Neumann and Wigner[11] about Hamiltonians such as (3) that depend on a single parameter. The theorem forbids crossing of two levels of identical symmetry. By symmetry all possible symmetries are to be included. The levels that cross in the case of all interactions antiferromagnetic, differ by a kind of permutation symmetry, which we shall describe in detail for the short chains. We must also recall a theorem of Lieb and Mattis[12] for the ground state when $J > 0$. According to this theorem, the ground state always has spin zero. This we have found to be true.

## II. SHORT LINEAR CHAINS. NOTATION

Let us start with a few generalities and notations. We note that the total spin $S^2$ as well as its $z$ component $S_z$ are constants of motion. Hence, to get a complete picture of the eigenvalues, it will be enough to investigate the $S_z = 0$ subspace ($N$ even) since every state can be rotated to this subspace without change in energy. The number of states with $S_z = 0$ for $N$ spin-$\frac{1}{2}$ particles is given by $\binom{N}{\frac{1}{2}N}$. It is also desirable to know the number of states with total spin $S = 0$, which is

$$\binom{N}{\frac{1}{2}N} \Big/ (\tfrac{1}{2}N + 1).$$

This is obtained by considering the difference in the total number of states in the $S_z = 0$ subspace and in the $S_z = 1$ subspace, a procedure with obvious generalization.[13] It is possible to derive it in a somewhat circuitous way, which, however, has certain advantages in that this new method gives also the structure of $S = 0$ states. Consider the problem group-theoretically. Each particle of spin $\frac{1}{2}$ is associated with the basic representation of the $SU_2$ group. For $N$ particles, the possible spins can be obtained by constructing direct products of the basic representations of the $SU_2$ group, the spin $\frac{1}{2}$ representation.

[11] E. P. Wigner and J. von Neumann, Physik. Z. **30**, 467 (1929).
[12] E. H. Lieb and D. C. Mattis, J. Math. Phys. **3**, 749 (1962).
[13] F. Bloch, Z. Physik **59**, 208 (1930).

The various representations are characterized by Young's tableaux, with at most two rows. It is well known that, because of the nature of the special unitary group $SU_2$, only one number may be used to characterize the representation. However, the tableaux with two rows are also certain special representations of the symmetric or permutation group of $N$ particles. The dimensionality of the representation is obviously the possible number of linearly independent states with the spin characteristic of the tableau. This dimensionality is nothing but the character of the unit element in that representation and can also be obtained as the number of ways of filling up the tableaux in the standard order.[14] All this simply depends on the correspondence of the representations of the permutation groups and the general linear group discussed extensively by Weyl.[15] Now the two-rowed tableaux with numerical characters filling them obviously suggest a way of writing down the spin $S = 0$ states. The number of total $S = 0$ states are fewer than the number of $S_z = 0$ states and the states in $S = 0$ subspace may be studied for slightly longer chains than those possible for $S_z = 0$ subspace. Hulthén,[2] who first studied short linear chains, used the construction suggested by the above procedure, but found it convenient not to use the states of the tableaux filled in the standard fashion. Rather he used a set of states which had the same structure, but took better advantage of the cyclic nature of the Hamiltonian with only nearest-neighbor interaction. We shall use the same set of states used by Hulthén, but we shall find that the presence of next-nearest-neighbor interaction introduces certain difficulties in the computations as soon as the chain becomes moderately long.

We shall follow Hulthén's article[2] closely in notation. Let $\alpha$ and $\beta$ be the up- and down-spin states and $\sigma_k^x$, $\sigma_k^y$, $\sigma_k^z$ be the usual Pauli spinors for the particle numbered $k$. Now introduce

$$[l, m] = \alpha(l)\beta(m) - \beta(l)\alpha(m),$$
$$\{l, m\} = \alpha(l)\beta(m) + \beta(l)\alpha(m). \tag{4}$$

In general, a symmetric function in particles $k, l, m, \cdots$ is $\{k, l, m \cdots\}$. The basic functions of (4) fulfil certain algebraic relations:

$$[k, l]\{m, n\} + [l, m]\{n, k\} + [m, n]\{k, l\} + [n, k]\{l, m\} = 0,$$
$$[k, l]\,[m, n] + [k, n]\,[l, m] + [k, m]\,[n, l] = 0. \tag{5}$$

[14] D. Littlewood, *The Theory of Group Characters* (Oxford University Press, London, 1940).
[15] H. Weyl, *Classical Groups* (Princeton University Press, Princeton, N.J., 1946).

Hulthén's basis functions are constructed out of such units as (4). Hence it is important to know the following properties for calculating eigenvalues of the Hamiltonian:

$$\tfrac{1}{2}(1 - \boldsymbol{\sigma}_l \cdot \boldsymbol{\sigma}_m)[l, m] = 2[l, m],$$
$$\tfrac{1}{2}(1 - \boldsymbol{\sigma}_l \cdot \boldsymbol{\sigma}_m)\{l, m, k, \cdots\} = 0,$$
$$\tfrac{1}{2}(1 - \boldsymbol{\sigma}_l \cdot \boldsymbol{\sigma}_m)[k, l]\{m, n\} = -[l, m]\{k, n\},$$
$$\tfrac{1}{2}(1 - \boldsymbol{\sigma}_l \cdot \boldsymbol{\sigma}_m)[k, l]\,[m, n] = [l, m]\,[n, k]. \tag{6}$$

## III. EVEN NUMBER OF SPINS

### A. 4 Spins

We shall start by considering 4 spins. This is a somewhat degenerate case since the next-nearest-neighbor interactions are not fully developed. Nevertheless, certain interesting features are present. The Hamiltonian is

$$H = \tfrac{1}{2}J \sum_{i=1}^{4} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+1} + \tfrac{1}{2}J\alpha \sum_{i=1}^{2} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+2}. \tag{7}$$

Here the particle 5 is equivalent to particle numbered 1. Define now

$$H' = -\frac{H - \alpha J - 2J}{J} = \sum_{i=1}^{4} \tfrac{1}{2}(1 - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+1}) + \alpha \sum_{i=1}^{2} \tfrac{1}{2}(1 - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+2}). \tag{8}$$

There are 6 states with $S_z = 0$, and are of the forms $\alpha(1)\,\beta(2)\,\alpha(3)\,\beta(4)$, $\alpha(1)\,\alpha(2)\,\beta(3)\,\beta(4)$, etc. The $6 \times 6$ matrix of the Hamiltonian can easily be constructed. The diagonalization problem is trivial and can be done by inspection. We shall rather follow Hulthén's construction procedure described above, so as to illustrate our remarks in Sec. II.

With 4 spin-$\frac{1}{2}$ particles we have three tableaux to consider corresponding to partitions [4], [31], [22]. [4] corresponds to only completely symmetric states of spin 2, $\psi_6 = \{1\ 2\ 3\ 4\}$ and using (6) one has

$$H'\psi_6 = H'\{1\ 2\ 3\ 4\} = 0. \tag{9}$$

The tableau [31] can be filled in the standard order in 3 different ways:

$$\begin{matrix} 1 & 3 & 4 \\ 2 & & \end{matrix}, \quad \begin{matrix} 1 & 2 & 4 \\ 3 & & \end{matrix}, \quad \text{and} \quad \begin{matrix} 1 & 2 & 3 \\ 4 & & \end{matrix}.$$

These have spin 1. As Hulthén remarked, it is convenient to choose a function suggested by the first labeling and then use the nearest-neighbor interaction part of the Hamiltonian (7) to generate the other states. Hence we take as the basis

$$\psi_3 = [12]\{34\},$$
$$\psi_4 = [23]\{41\}, \tag{10}$$
$$\psi_5 = [34]\{12\}.$$

It is especially important to notice that the basis functions are not normalized and are not necessarily orthogonal. Using (6) to operate with $H'$ and using (5), we get

$$\begin{aligned} H'\psi_3 &= 3\psi_3 + \psi_5 + \alpha(\psi_3 - \psi_5), \\ H'\psi_4 &= -\psi_3 + 2\psi_4 - \psi_5 + \alpha(\psi_3 + 2\psi_4 + \psi_5), \\ H'\psi_5 &= \psi_3 + 3\psi_5 - \alpha(\psi_3 - \psi_5). \end{aligned} \tag{11}$$

Hence, we obtain the eigenfunctions

$$\begin{aligned} H'(\psi_3 + \psi_5) &= 4(\psi_3 + \psi_5), \\ H'(\psi_3 + \psi_4) &= (2 + 2\alpha)(\psi_3 + \psi_4), \\ H'(\psi_4 + \psi_5) &= (2 + 2\alpha)(\psi_4 + \psi_5). \end{aligned} \tag{12}$$

We have also the scalar product $(\psi_3, \psi_3) = (\psi_4, \psi_4) = (\psi_5, \psi_5) = 4, (\psi_3, \psi_4) = (\psi_4, \psi_5) = -2,$ and $(\psi_3, \psi_5) = 0$. Hence, the eigenfunctions $(\psi_3 + \psi_5)$, $(\psi_3 + \psi_4)$, and $(\psi_4 + \psi_5)$ are mutually orthogonal.

The tableau [22] can be filled in two ways:

$$\begin{matrix} 1 & 3 \\ 2 & 4 \end{matrix} \quad \text{and} \quad \begin{matrix} 1 & 2 \\ 3 & 4 \end{matrix}.$$

They have spin zero. Again we choose Hulthén's basis functions, cyclically generated:

$$\varphi_1 = [12]\,[34], \quad \varphi_2 = [23]\,[41]. \tag{13}$$

Then, by (6) and (5),

$$\begin{aligned} H'\varphi_1 &= 4\varphi_1 + 2\varphi_2 + 2\alpha[13]\,[24], \\ H'\varphi_2 &= 2\varphi_1 + 4\varphi_2 - 2\alpha[13]\,[24], \end{aligned} \tag{14}$$

so that

$$\begin{aligned} H'(\varphi_1 + \varphi_2) &= 6(\varphi_1 + \varphi_2), \\ H'(\varphi_1 - \varphi_2) &= (2 + 4\alpha)(\varphi_1 - \varphi_2). \end{aligned} \tag{15}$$

In deriving the last equation we have used (5). We have obtained all the eigenvalues which are given in Fig. 1. It must be pointed out that this is not a "spectrum of the chain" of 4 spin-$\frac{1}{2}$ particles. As des Cloizeaux and Pearson[3] have explained, the spectrum of the chain necessarily implies a consideration of the wave vector $k$. (Identical remarks hold for Figs. 3 and 5.)

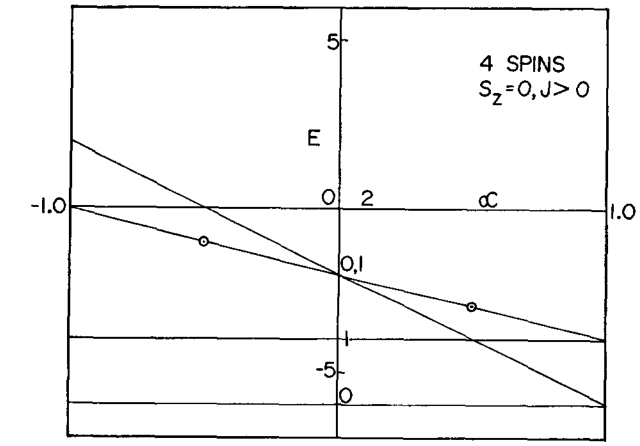



FIG. 1. Eigenvalues of $-H'$ for 4 spins as functions of $\alpha$. The small circle denotes a doubly degenerate level. Spins of the levels are also indicated.

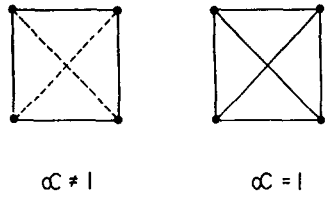



FIG. 2. Symmetries of the 4-spin complex. ($\alpha = 1$) is a complete graph and represents a tetrahedron.

Figure 1 has been drawn for the $S_z = 0$ subspace, with $J > 0$, antiferromagnetic case. For ferromagnetic case ($J < 0$) the picture should be inverted (same for Figs. 3 and 5). For antiferromagnetic case the ground state always has spin zero. For ferromagnetic case, however, the ground state changes from one having spin 2 to one having spin zero at $\alpha = -\frac{1}{2}$.

There are certain interesting multiplet structures and level crossings in the diagram, which may be related to the symmetries of the problem. Since we have already taken full rotational symmetry into account by going over to $S_z = 0$ subspace, we must look for the explanation of the multiplet structure to certain other invariances. In particular, the structure at $\alpha = 1$, where all states of the same spin come together, is really interesting. To investigate the symmetries, it is convenient to have geometrical pictures, which make the permutation symmetries inherent in (7) rather intuitive. So let us place the 4 spins at the corners of a square and imagine that the sides represent bonds of strength $J$ connecting nearest neighbors. Join the diagonals with dotted lines to represent the next-nearest-neighbor bonds of strength $\alpha J$. When $\alpha = 1$, the dotted lines are replaced by full lines. In the language of graph theory we have now the "square of the original graph."[16] If we call two vertices connected by a nearest-neighbor bond to be at a "distance" 1, the next-nearest-neighbor interaction inserts a bond between vertices at distance 2. For the square diagram of 4 spins, the square of the graph is a "complete" graph,[17] a somewhat degenerate situation from the physical stand point. To obtain the symmetries of our Hamiltonian, consider the automorphisms of the graphs in Fig. 2, which leave the connections invariant. For $\alpha = 1$, the

[16] A. Mukhopadhyaya, J. Combinatorial Theory **2**, 290 (1967).

[17] G. Uhlenbeck and G. W. Ford, in *Statistical Mechanics*, J. de Boer and G. E. Uhlenbeck, Eds. (North-Holland Publishing Co., Amsterdam, 1962), Vol. I, p. 119.

graph is complete and the automorphisms constitute the full symmetric group $S_4$. The representations of the group are well known[14] and the degeneracies of the states at $\alpha = 1$ are immediately explained. In fact, the very construction of our states $\varphi_1$, $\varphi_2$, $\psi_3$, $\psi_4$, $\psi_5$, and $\psi_6$ make their transformation properties obvious. When $\alpha \neq 1$, the group of automorphisms is clearly the group of the square. It is a subgroup of $S_4$ with 8 elements and is, in fact, the dihedral group $D_4$. The irreducible representations of $D_4$ fall into five classes $A_1$, $A_2$, $B_1$, $B_2$, and $E$ with dimensions 1, 1, 1, 1, 2 (see the Appendix for the character table). It is easy to verify that the doubly degenerate states $(\psi_3 + \psi_4)$ and $(\psi_4 + \psi_5)$ form the representation of dimension 2. The ground state $(\varphi_1 + \varphi_2)$ belongs to the representation $A_1$, as also the completely symmetric state $\psi_6$. The state $(\varphi_1 - \varphi_2)$ belongs to the representation $B_1$. The state $(\psi_3 + \psi_5)$ transforms as $B_2$. The triple degeneracy at $\alpha = 0$ of the eigenvalues is accidental.

### B. 6 Spins

Henceforth we shall concentrate on the $S_z = 0$, $S = 0$ subspace. For 6 spin-$\frac{1}{2}$ particles there are five $S = 0$ states, which we take as

$$\begin{aligned}
&\varphi_1 = [12]\,[34]\,[56], \quad \varphi_2 = [23]\,[45]\,[61], \\
&\psi_3 = [23]\,[41]\,[56], \quad \psi_4 = [12]\,[45]\,[63], \\
&\psi_5 = [34]\,[61]\,[25].
\end{aligned} \tag{16}$$

The Hamiltonian is written as

$$\begin{aligned}
H' &= -\frac{H - 3J - 3\alpha J}{J} \\
&= \tfrac{1}{2}\sum_{i=1}^{6}(1 - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+1}) + \tfrac{1}{2}\alpha\sum_{i=1}^{6}(1 - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+2}),
\end{aligned} \tag{17}$$

with usual identification $\boldsymbol{\sigma}_7 \equiv \boldsymbol{\sigma}_1$, $\boldsymbol{\sigma}_8 \equiv \boldsymbol{\sigma}_2$. With (6) and (5) we get

$$\begin{aligned}
H'\varphi_1 &= (6 + 6\alpha)\varphi_1 + (1 - 2\alpha)(\psi_3 + \psi_4 + \psi_5), \\
H'\varphi_2 &= (6 + 6\alpha)\varphi_2 - (1 - 2\alpha)(\psi_3 + \psi_4 + \psi_5), \\
H'\psi_3 &= 4\psi_3 + 2\varphi_1 - 2\varphi_2 \\
&\quad + 2\alpha\{-\varphi_1 + \varphi_2 + 3\psi_3 - [25]\,[14]\,[63]\}, \\
H'\psi_4 &= 4\psi_4 + 2\varphi_1 - 2\varphi_2 \\
&\quad + 2\alpha\{-\varphi_1 + \varphi_2 + 3\psi_4 - [25]\,[14]\,[63]\}, \\
H'\psi_5 &= 4\psi_5 + 2\varphi_1 - 2\varphi_2 \\
&\quad + 2\alpha\{-\varphi_1 + \varphi_2 + 3\psi_5 - [25]\,[14]\,[63]\}.
\end{aligned} \tag{18}$$

From (18), after some obvious manipulations, we get

$$\begin{aligned}
H'(\varphi_1 + \varphi_2) &= (6 + 6\alpha)(\varphi_1 + \varphi_2), \\
H'(\varphi_1 - \varphi_2) &= (6 + 6\alpha)(\varphi_1 - \varphi_2) \\
&\quad + 2(1 - 2\alpha)(\psi_3 + \psi_4 + \psi_5), \\
H'(\psi_3 - \psi_4) &= (4 + 6\alpha)(\psi_3 - \psi_4), \\
H'(\psi_3 - \psi_5) &= (4 + 6\alpha)(\psi_3 - \psi_5), \\
H'(\psi_3 + \psi_4 + \psi_5) &= (4 + 6\alpha)(\psi_3 + \psi_4 + \psi_5) \\
&\quad + (6 - 6\alpha)(\varphi_1 - \varphi_2) \\
&\quad - 6\alpha[25]\,[14]\,[63].
\end{aligned} \tag{19}$$

We have found 3 eigenvalues $(6 + 6\alpha)$, $(4 + 6\alpha)$, and $(4 + 6\alpha)$. The remaining 2 must be found by studying the secular equation connecting $(\varphi_1 - \varphi_2)$ and $(\psi_3 + \psi_4 + \psi_5)$. The first difficulty of using the next-nearest-neighbor interaction is apparent in the existence of the state [25] [14] [63]. With $\alpha = 0$, the five linearly independent states of the Hulthén basis (16) were the only ones regenerated by the operation of the Hamiltonian. However, now another state [25] [14] [63] appears which has to be re-expressed in terms of the basis (16). The basis functions (16) were neither normalized nor mutually orthogonal in general. Hence we write

$$\begin{aligned}
\psi &\equiv [25]\,[14]\,[63] \\
&= c_1\varphi_1 + c_2\varphi_2 + c_3\psi_3 + c_4\psi_4 + c_5\psi_5,
\end{aligned} \tag{20}$$

and consider the set of linear equations for the $c$'s:

$$\begin{aligned}
(\varphi_1, \psi) &= c_1(\varphi_1, \varphi_1) + c_2(\varphi_1, \varphi_2) + c_3(\varphi_1, \psi_3) \\
&\quad + c_4(\varphi_1, \psi_4) + c_5(\varphi_1, \psi_5),
\end{aligned} \tag{21}$$

etc. The matrix of the scalar product is easy to construct:

$$\begin{aligned}
&(\varphi_i, \varphi_i) = (\psi_i, \psi_i) = 8, \\
&(\varphi_1, \varphi_2) = -2, \\
&(\varphi_1, \psi_i) = -(\varphi_2, \psi_i) = 4, \\
&(\psi_i, \psi_j) = 2 \quad (i \neq j), \\
&(\varphi_1, \psi) = -(\varphi_2, \psi) = 2, \quad (\psi_i, \psi) = 4.
\end{aligned}$$

Solving (21), we obtain

$$\psi = -(\varphi_1 - \varphi_2) + (\psi_3 + \psi_4 + \psi_5), \tag{22}$$

so that

$$\begin{aligned}
H'(\varphi_1 - \varphi_2) &= (6 + 6\alpha)(\varphi_1 - \varphi_2) \\
&\quad + 2(1 - 2\alpha)(\psi_3 + \psi_4 + \psi_5), \\
H'(\psi_3 + \psi_4 + \psi_5) &= 6(\varphi_1 - \varphi_2) + 4(\psi_3 + \psi_4 + \psi_5),
\end{aligned} \tag{23}$$

and the secular equation is

$$\begin{vmatrix} 6+6\alpha-\lambda & 2(1-2\alpha) \\ 6 & 4-\lambda \end{vmatrix} = 0, \tag{24}$$

with the roots

$$\lambda = (5+3\alpha) \pm (13-18\alpha+9\alpha^2)^{\frac{1}{2}}. \tag{25}$$

We have therefore determined all the eigenvalues of $S=0$ levels. The eigenvalue of the spin $S=3$ levels is of course 0. Hence a spin-zero state crosses the ferromagnetic ground state when $\alpha=-0.25$. For the antiferromagnetic case a new possibility shows itself at $\alpha=\frac{1}{2}$. A spin-zero state $(\varphi_1+\varphi_2)$, which was higher than the ground state at $\alpha=0$, crosses the ground state and becomes the new ground state for $\alpha>\frac{1}{2}$. By the Wigner–von Neumann theorem, the two states must differ in symmetry, which we shall examine below.

We have also determined the exact eigenvalues for all states in the $S_z=0$ subspace. There are 20 $S_z=0$ states, and, rather than proceeding analytically as above, the matrix of the Hamiltonian can be easily diagonalized on a CDC 3600 computer. Figure 3 presents the eigenvalues of the 20 states. Their spins can be determined by comparing our eigenvalues with those given by Orbach[8] for 6 spins, or directly by analytic computation. The point to observe is the following. In the antiferromagnetic case the ground state is always of spin zero. In the ferromagnetic case $(J<0)$ the ground state is either of maximum spin 3 or spin zero. States of lower spin do cross the spin-3 state, but they all do so at values of $\alpha$ more negative than that necessary for spin-zero-level crossing.

The symmetries of the 6-spin complex can be described by placing them at the six corners of a

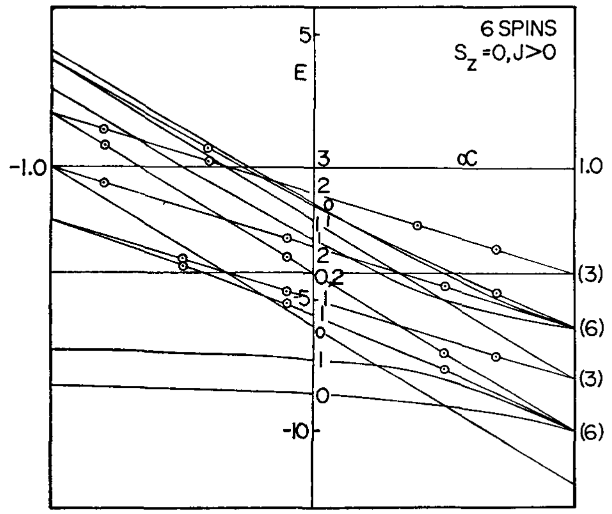
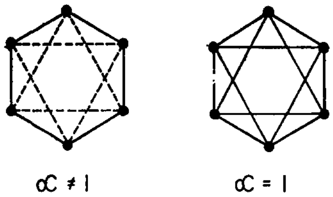



FIG. 3. Eigenvalues of $-H'$ for 6 spins. The small circle implies a degeneracy of 2. Level spins are indicated. The numbers on the right indicate the total number of levels of the cluster.

FIG. 4. Symmetries of the 6-spin complex. ($\alpha=1$) represents an octahedron.




regular hexagon (Fig. 4). The next-nearest neighbors can be joined by dotted lines, which are replaced by full lines for $\alpha=1$, and we get the square graph of the hexagon, which, unlike the 4-spin case, is not complete. The next-nearest-neighbor interactions are already fully developed. For $\alpha\neq 1$, the symmetry of the graph is obviously that of the dihedral group $D_6$ of the hexagon. Therefore the corresponding permutation group that leaves the Hamiltonian invariant has 6 irreducible representations: $A_1'$, $A_2'$, $A_1''$, $A_2''$, $E'$, and $E''$ of dimensions 1, 1, 1, 1, 2, and 2, respectively. The maximum degeneracy of the states is 2, which is the case in Fig. 3 excepting a few points of accidental degeneracy. Since two spin-zero states cross for the ground state, it is necessary that they must have different symmetry, according to von Neumann and Wigner. It is easy to verify that the state $a(\varphi_1-\varphi_2)+b(\psi_3+\psi_4+\psi_5)$ (with $a$ and $b$ constants) has the symmetry $A_1''$, while the state $(\varphi_1+\varphi_2)$ transforms as the representation $A_2''$. For $\alpha=1$, the graph obviously represents an octahedron. The automorphisms of the graph constitute the well-known group $O_h$ with 48 elements. The corresponding permutation group for 6 spins can easily be written down and be verified to leave the Hamiltonian invariant. The irreducible representations of $O_h$ have dimensions 1, 2, and 3. Figure 3, however, shows that at $\alpha=1$, besides triply degenerate levels, we have two levels of degeneracy 6. No group bigger than $O_h$ has been found so far. Hence we may say that there are accidental degeneracies present at $\alpha=1$.

### C. 8 Spins

For 8 spins there are 70 states in the $S_z=0$ subspace and 14 of them have spin $S=0$. Following Hulthén, we take the 14 basis functions as

$$\begin{gathered}
\varphi_1=[12]\,[34]\,[56]\,[78],\quad \varphi_2=[23]\,[45]\,[67]\,[81],\\
\psi_1=[23]\,[41]\,[56]\,[78],\quad \psi_2=[34]\,[52]\,[67]\,[81],\\
\chi_1=[23]\,[41]\,[67]\,[85],\\
\psi_3=[12]\,[45]\,[63]\,[78],\quad \psi_4=[23]\,[56]\,[74]\,[81],\\
\chi_3=[81]\,[27]\,[45]\,[63],\\
\psi_5=[12]\,[34]\,[67]\,[85],\quad \psi_6=[23]\,[45]\,[78]\,[16],\\
\chi_2=[78]\,[16]\,[34]\,[52],\\
\psi_7=[34]\,[56]\,[81]\,[27],\quad \psi_8=[45]\,[67]\,[12]\,[38],\\
\chi_4=[12]\,[38]\,[56]\,[74].
\end{gathered} \tag{26}$$

The operation of the Hamiltonian

$$H' = -\frac{H - 4(1+\alpha)J}{J}$$
$$= \sum_{i=1}^{8} \tfrac{1}{2}(1 - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+1}) + \alpha \sum_{i=1}^{8} \tfrac{1}{2}(1 - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+2}) \qquad (27)$$

(with $\boldsymbol{\sigma}_9 \equiv \boldsymbol{\sigma}_1$ and $\boldsymbol{\sigma}_{10} \equiv \boldsymbol{\sigma}_2$) gives

$$\begin{aligned}
H'\varphi_1 &= 8\varphi_1 + \psi_1 + \psi_3 + \psi_5 + \psi_7 \\
&\quad + \alpha(8\varphi_1 - 2\psi_1 - 2\psi_3 - 2\psi_5 - 2\psi_7), \\
H'\psi_1 &= 6\psi_1 + 2\varphi_1 + \psi_4 + \psi_6 + \chi_1 \\
&\quad + \alpha(8\psi_1 - 2\varphi_1 - \psi_4 - \psi_6 - 2\chi_1 - x_2 - x_1), \\
H'\psi_2 &= 6\psi_2 + 2\varphi_2 + \psi_5 + \psi_7 + \chi_2 \\
&\quad + \alpha(8\psi_2 - 2\varphi_2 - \psi_5 - \psi_7 - 2\chi_2 - x_5 - x_6), \\
H'\chi_1 &= 4\chi_1 + 2\varphi_2 + 2\psi_1 + 2\psi_5 \\
&\quad + \alpha(8\chi_1 - 2\psi_1 - 2\psi_5 - 2x_5 - 2x_7). \qquad (28)
\end{aligned}$$

The structure of the remaining ten equations that we have not written down can be surmized from these. There are 8 extra states denoted by $x_1, \cdots, x_8$:

$$\begin{aligned}
x_1 &= [25]\,[36]\,[41]\,[78], & x_5 &= [14]\,[83]\,[52]\,[67], \\
x_2 &= [14]\,[83]\,[56]\,[27], & x_6 &= [47]\,[36]\,[52]\,[81], \\
x_3 &= [12]\,[63]\,[58]\,[47], & x_7 &= [23]\,[74]\,[61]\,[58], \\
x_4 &= [34]\,[85]\,[61]\,[72], & x_8 &= [83]\,[72]\,[45]\,[16].
\end{aligned} \qquad (29)$$

The appearance of these states accentuates the difficulties of having the next-nearest-neighbor interactions. We have now to express these extra states in terms of our nonorthogonal basis (26). This is an extremely tedious but straightforward calculation along the line of Eqs. (20), (21), and (22). Hence, we get

$$\begin{aligned}
x_1 &= -\tfrac{5}{7}\varphi_1 - \tfrac{15}{28}\varphi_2 + \tfrac{6}{7}\psi_1 + \tfrac{4}{7}\psi_3 - \tfrac{1}{28}\psi_5 - \tfrac{3}{7}\psi_7 \\
&\quad + \tfrac{3}{14}\psi_2 + \tfrac{15}{56}\psi_4 - \tfrac{41}{56}\psi_6 + \tfrac{3}{14}\psi_8 + \tfrac{1}{56}\chi_1 + \tfrac{25}{28}\chi_2 \\
&\quad + \tfrac{9}{14}\chi_3 - \tfrac{3}{28}\chi_4, \\
x_2 &= -\varphi_1 + \psi_1 + \psi_7 - \psi_4 + \chi_4, \qquad (30)
\end{aligned}$$

and six similar equations. Thus the operation of the Hamiltonian gives us, finally,

$$\begin{aligned}
H'\varphi_1 &= 8\varphi_1 + \psi_1 + \psi_3 + \psi_5 + \psi_7 \\
&\quad + \alpha[8\varphi_1 - 2\psi_1 - 2\psi_3 - 2\psi_5 - 2\psi_7], \\
H'\psi_1 &= 6\psi_1 + 2\varphi_1 + \psi_4 + \psi_6 + \chi_1 \\
&\quad + \alpha[-\tfrac{2}{7}\varphi_1 + \tfrac{15}{28}\varphi_2 + \tfrac{43}{7}\psi_1 - \tfrac{4}{7}\psi_3 + \tfrac{1}{28}\psi_5 \\
&\quad - \tfrac{4}{7}\psi_7 - \tfrac{3}{14}\psi_2 - \tfrac{15}{56}\psi_4 - \tfrac{15}{56}\psi_6 - \tfrac{3}{14}\psi_8 \\
&\quad - \tfrac{113}{56}\chi_1 - \tfrac{25}{28}\chi_2 - \tfrac{9}{14}\chi_3 - \tfrac{25}{28}\chi_4], \qquad (31)
\end{aligned}$$

and 12 similar equations for the other functions. For $\alpha = 0$, Hulthén was able, by taking proper linear combinations, to decompose the $14 \times 14$ subspace

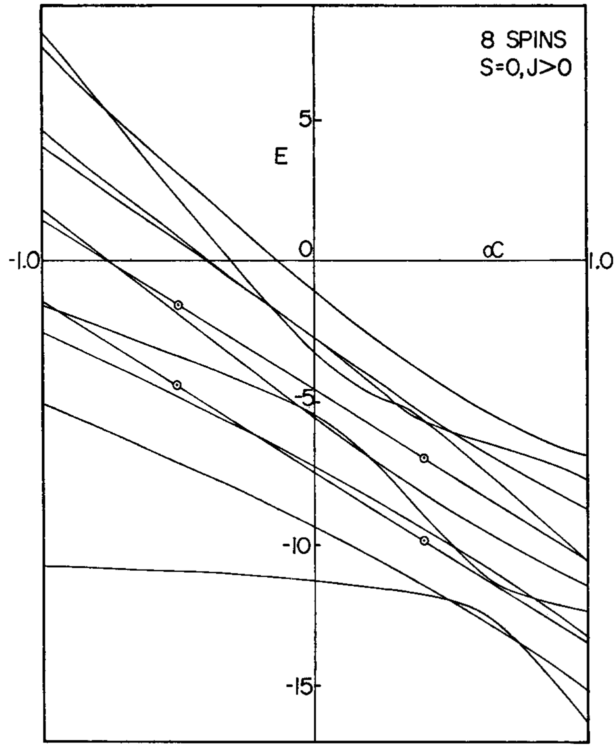



FIG. 5. Eigenvalues of $-H'$ for 8 spins. Two levels are indistinguishably close (the third excited state at $\alpha = 0$). The circles denote degeneracy of 2.

into smaller subspaces. Because of the complicated nature of our coefficients, it is somewhat difficult to use the same technique; in fact the decomposition cannot be pushed as far as Hulthén did, while it was still feasible for the 6 spins. We have therefore diagonalized the $14 \times 14$ nonsymmetric matrix arising from Eq. (31) directly on a CDC 3600 computer, using the known values due to Orbach[8] at $\alpha = 0$ and the four analytically computed values $6 + 6\alpha \pm (2)^{\frac{1}{2}}$, $5 + 6\alpha \pm (5 + 4\alpha^2 - 4\alpha)^{\frac{1}{2}}$ as checks. Figure 5 represents the result. Only one new feature is present: in the case $J < 0$, $\alpha < 0$, the ferromagnetic ground state is first crossed by a spin-zero state which in turn is crossed by another spin-zero state. We have also analyzed the entire $S_z = 0$ subspace of 70 states and verified that the ferromagnetic ground state becomes unstable first with respect to a spin-zero state and that the ground state in all cases belong to either $S = 0$ or $S = 4$. The symmetry group is dihedral group $D_8$, with maximum allowed degeneracy 2. Nothing particularly striking happens at $\alpha = 1$.

## IV. ODD NUMBER OF SPINS (3, 5, 7)

We shall summarize the results for odd number of spins briefly. For 3 spins there is no question of next-nearest-neighbor interactions. For odd number of spins, the total spin can only be half integral, so we

TABLE I. Ground-state energy per spin for 5, 6, 7, and 8 particles.

| No. of spins | 5 | | 6 | | 7 | | 8 | |
|---|---|---|---|---|---|---|---|---|
| $\alpha$ | $J>0$ | $J<0$ | $J>0$ | $J<0$ | $J>0$ | $J<0$ | $J>0$ | $J<0$ |
| −1.0 | −0.8944 | −0.8944 | −1.3875 | −0.7280 | −1.1093 | −0.7674 | −1.3496 | −1.0120 |
| −0.9 | −0.8797 | −0.8197 | −1.3402 | −0.6737 | −1.0787 | −0.6901 | −1.3033 | −0.9091 |
| −0.8 | −0.8650 | −0.7450 | −1.2930 | −0.6263 | −1.0483 | −0.6137 | −1.2574 | −0.8185 |
| −0.7 | −0.8503 | −0.6703 | −1.2463 | −0.5947 | −1.0180 | −0.5380 | −1.2119 | −0.7499 |
| −0.6 | −0.8355 | −0.5955 | −1.2000 | −0.5333 | −0.9878 | −0.4639 | −1.1669 | −0.6943 |
| −0.5 | −0.8208 | −0.5208 | −1.1540 | −0.4873 | −0.9582 | −0.4248 | −1.1226 | −0.6361 |
| −0.4 | −0.8061 | −0.4461 | −1.1087 | −0.4420 | −0.9287 | −0.4026 | −1.0788 | −0.5784 |
| −0.3 | −0.7914 | −0.3714 | −1.0640 | −0.3972 | −0.8996 | −0.3802 | −1.0359 | −0.5219 |
| −0.2 | −0.7765 | −0.4000 | −1.0200 | −0.4000 | −0.8710 | −0.4000 | −0.9938 | −0.4600 |
| −0.1 | −0.7619 | −0.4500 | −0.9770 | −0.4500 | −0.8430 | −0.4500 | −0.9527 | −0.4500 |
| 0 | −0.7472 | −0.5000 | −0.9340 | −0.5000 | −0.8158 | −0.5000 | −0.9128 | −0.5000 |
| 0.1 | −0.7325 | −0.5500 | −0.8930 | −0.5500 | −0.7896 | −0.5500 | −0.8743 | −0.5500 |
| 0.2 | −0.7178 | −0.6000 | −0.8540 | −0.6000 | −0.7648 | −0.6000 | −0.8376 | −0.6000 |
| 0.3 | −0.7030 | −0.6500 | −0.8167 | −0.6500 | −0.7419 | −0.6500 | −0.8034 | −0.6500 |
| 0.4 | −0.6889 | −0.7000 | −0.7820 | −0.7000 | −0.7217 | −0.7000 | −0.7730 | −0.7000 |
| 0.5 | −0.6736 | −0.7500 | −0.7500 | −0.7500 | −0.7051 | −0.7500 | −0.7500 | −0.7500 |
| 0.6 | −0.6589 | −0.8000 | −0.8000 | −0.8000 | −0.6936 | −0.8000 | −0.7729 | −0.8000 |
| 0.7 | −0.6442 | −0.8500 | −0.8500 | −0.8500 | −0.7366 | −0.8500 | −0.7988 | −0.8500 |
| 0.8 | −0.6294 | −0.9000 | −0.9000 | −0.9000 | −0.8099 | −0.9000 | −0.8529 | −0.9000 |
| 0.9 | −0.6174 | −0.9500 | −0.9500 | −0.9500 | −0.8851 | −0.9500 | −0.9399 | −0.9500 |
| 1.0 | −0.6000 | −1.0000 | −1.0000 | −1.0000 | −0.9615 | −1.0000 | −1.0326 | −1.0000 |

always have states with finite nonzero spin and the interesting question is whether the state of maximum or that of the minimum spin lies lowest. For 5 spins, we find that a state of spin $\frac{1}{2}$ has always the lowest energy for $J>0$, $-1\leq\alpha\leq 1$.

With $J<0$, $\alpha>0$, the state of maximum spin $\frac{5}{2}$ lies lowest; as the next-nearest-neighbor interaction becomes more and more antiferromagnetic, a state of spin $\frac{1}{2}$ becomes the lowest state and remains so. The symmetries of 5-spin system are analogous to those of 4-spin case, as the graph of 5 spins on a pentagon becomes a complete graph for $\alpha=1$. For $\alpha\neq 1$, the group of symmetries has 10 elements divided into 4 classes, with representations of order 1, 1, 2, and 2. For $\alpha=1$ we have the full symmetric group $S_5$.

The situation with 7 spins is similar. The ferromagnetic ground state becomes unstable at a value of $|\alpha|$ smaller than that for 5 spins.

In Table I we collected the ground-state energy per spin for all values of $\alpha$ for 5, 6, 7, and 8 spins. The cases of 3 and 4 spins are trivial and in any case can be determined from known results.

## V. BOUNDS FOR THE GROUND-STATE ENERGY FOR LARGE $N$

In this section we shall present upper and lower bounds of the ground-state energy for arbitrarily large $N$, for the Hamiltonian of equation (3). Similar bounds can also be found for the square lattice, where the interactions between the nearest neighbors is $J$ and that between next-nearest-neighbors is $\alpha J$.

Consider Eq. (3). Let $NzF(\alpha,J)$ be the ground-state energy, $z$ is the coordination number or the number of nearest neighbors. Let $\psi_0$ be the exact ground-state wavefunction of the Hamiltonian (3). Then

$$\begin{aligned}NzF(\alpha,J)&=\langle\psi_0|\,H\,|\psi_0\rangle\\&=\langle\psi_0|\,\tfrac{1}{2}J\sum_i \boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_{i+1}\,|\psi_0\rangle\\&\quad+\langle\psi_0|\,\tfrac{1}{2}J\alpha\sum_i \boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_{i+2}\,\langle\psi_0\rangle\\&=\langle\psi_0|\,H_1\,|\psi_0\rangle+\langle\psi_0|\,H_2\,\langle\psi_0\rangle,\end{aligned}\tag{32}$$

with

$$H_1=\tfrac{1}{2}J\sum_i \boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_{i+1},\quad N+1\equiv 1,\tag{33}$$

$$H_2=\tfrac{1}{2}J\alpha\sum_i \boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_{i+2},\quad N+1\equiv 1,\quad N+2\equiv 2.\tag{34}$$

Since $\psi_0$ is a variational function for $H_1$ as well as $H_2$, we have

$$NzF(\alpha,J)\geq\langle H_1\rangle_{\text{g.s.}}+\langle H_2\rangle_{\text{g.s.}}.\tag{35}$$

$H_1$ is precisely the Hamiltonian treated by Bethe and Hulthén and its ground-state energy is known. If $J$ is negative, the ground state is ferromagnetic and has energy $-\frac{1}{4}Nz\,|J|$. If $J$ is positive, the ground-state energy is the celebrated Bethe–Hulthén result, $-NJ(2\ln 2-\frac{1}{2})=-\frac{1}{2}NzJ(0.88629)$. As for $\langle H_2\rangle_{\text{g.s.}}$, if $\alpha J$ is negative, i.e., $J$ and $\alpha$ have opposite sign. we have

$$\begin{aligned}\langle H_2\rangle_{\text{g.s.}}&=\Big\langle -\tfrac{1}{2}\,|J|\,|\alpha|\sum_j \boldsymbol{\sigma}_j\cdot\boldsymbol{\sigma}_{j+2}\Big\rangle_{\min}\\&=-\tfrac{1}{2}\,|J|\,|\alpha|\Big\langle\sum_j \boldsymbol{\sigma}_j\cdot\boldsymbol{\sigma}_{j+2}\Big\rangle_{\max}\\&=-\tfrac{1}{2}\,|J|\,|\alpha|\,\tfrac{1}{2}Nz.\end{aligned}\tag{36}$$

Hence, for $J$ negative, $\alpha$ positive,

$$NzF(|\alpha|, -|J|) \geq -\tfrac{1}{4}Nz\,|J| - \tfrac{1}{4}\,|J|\,|\alpha|\,Nz$$

or

$$F(|\alpha|, -|J|) \geq -\tfrac{1}{4}\,|J| - \tfrac{1}{4}\,|J|\,|\alpha|. \qquad (37)$$

For $J$ positive, $\alpha$ negative,

$$NzF(-|\alpha|, |J|) \geq -\tfrac{1}{2}Nz\,|J|\,(0.88629) - \tfrac{1}{4}Nz\,|J|\,|\alpha|$$

or

$$F(-|\alpha|, |J|) \geq -\tfrac{1}{2}\,|J|\,(0.88629) - \tfrac{1}{4}\,|J|\,|\alpha|. \qquad (38)$$

The case $\alpha J \geq 0$, i.e., $\alpha$ and $J$ have the same sign, is more interesting. We have now to determine ground state of $H_2$ for $\alpha J \geq 0$. But taking $N$ even, $H_2$ is the sum of two Hamiltonians of spins that interact only with nearest neighbors [odd-numbered spins interact only among themselves, so do the even-numbered ones, Fig. 6(a)], each sub-Hamiltonian containing $\tfrac{1}{2}N$ particles. As the two sub-Hamiltonians are not coupled, the ground-state energy follows directly from Hulthén's work:

$$\langle H_2\rangle_{\text{g.s.}} = -\tfrac{1}{2}Nz\,|J\alpha|\,(0.88629). \qquad (39)$$

The result is also valid for odd $N$, as then the chain with next-nearest-neighbor interaction can be unfolded into a single chain with nearest-neighbor interactions (Fig. 6b). Thus, from (35) for $J < 0$, $\alpha < 0$,

$$NzF(-|\alpha|, -|J|) \geq -\tfrac{1}{4}Nz\,|J| - \tfrac{1}{2}Nz\,|J|\,|\alpha|\,(0.88629)$$

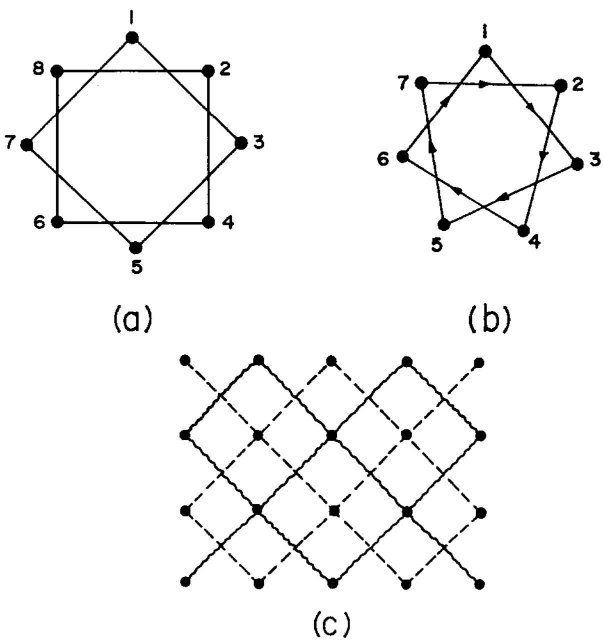



FIG. 6. (a) Decomposition of a linear chain into two independent chains (even $N$); (b) unfolding of a linear chain into a single chain by following the arrow (odd $N$); (c) decomposition of the square lattice.

or

$$F(-|\alpha|, -|J|) \geq -\tfrac{1}{4}\,|J| - \tfrac{1}{2}\,|J|\,|\alpha|\,(0.88629). \qquad (40)$$

Similarly, for $J > 0$, $\alpha > 0$,

$$NzF(\alpha, J) \geq -\tfrac{1}{2}NzJ(0.88629) - \tfrac{1}{2}NzJ\alpha(0.88629)$$

or

$$F(\alpha, J) \geq -\tfrac{1}{2}J(0.88629)(1 + \alpha). \qquad (41)$$

To obtain an upper bound, consider a state $\psi_s$ completely symmetric in all spins:

$$\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+1}\psi_s = \psi_s,$$
$$\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+2}\psi_s = \psi_s. \qquad (42)$$

Then for any $J$ and $\alpha$

$$NzF(\alpha, J) \leq \langle\psi_s|\,H\,|\psi_s\rangle = \tfrac{1}{4}JNz + \tfrac{1}{4}\alpha JNz$$

or

$$F(\alpha, J) \leq \tfrac{1}{4}J + \tfrac{1}{4}J\alpha. \qquad (43)$$

Since for $J < 0$, $\alpha > 0$ the upper and the lower bounds coincide, we have an exact solution for the situation when all interactions are ferromagnetic. For $J > 0$, the upper bound (43) is trivial. To get an improved upper bound, we consider as a variational function the following alternating function ($N$ even):

$$\psi_A = \alpha(1)\beta(2)\alpha(3)\beta(4)\cdots. \qquad (44)$$

Then,

$$NzF(\alpha, |J|) \leq \langle\psi_A|\,H\,|\psi_A\rangle = -\tfrac{1}{4}Nz\,|J| + \tfrac{1}{4}Nz\,|J|\alpha$$

or

$$F(\alpha, |J|) \leq -\tfrac{1}{4}\,|J| + \tfrac{1}{4}\,|J|\,\alpha = -\tfrac{1}{4}J(1 - \alpha). \qquad (45)$$

For large odd $N$, this result will also hold. Table II contains all the bounds for various cases.

The particular topological property of the linear chain which enabled us to determine the lower bound is shared by the square lattice [Fig. 6(c)]; that is, the square lattice with *purely* next-nearest-neighbor interaction can be decomposed into two mutually noninteracting square lattices with half as many particles and nearest-neighbor interactions only. The exact ground-state energy of the Hamiltonian with nearest-neighbor interaction for a square lattice is not known. However, an inequality of the type (35) still holds if we know the lower bounds to the ground-state energy. Such lower bounds can be obtained from the work of Yang and Yang.[9]

Write for a square lattice

$$H = \tfrac{1}{2}J\sum \boldsymbol{\sigma}\cdot\boldsymbol{\sigma}' + \tfrac{1}{2}J\alpha\sum{}' \boldsymbol{\sigma}\cdot\boldsymbol{\sigma}'; \qquad (46)$$

the second sum goes over next-nearest-neighbor pairs only. Call $NzF^s(\alpha, J)$ the ground-state energy, with $z$ the number of nearest- as well as next-nearest

TABLE II. Upper and lower bounds for the ground-state energy for large $N$. When comparing with Table I, note the difference that the coordination number $z$ appears in the definition of $F$.

| $J < 0, \quad \alpha > 0$ | $J > 0, \quad \alpha > 0$ |
|---|---|
| $F(\alpha, J) \geq -\frac{1}{4}\|J\|(1+\alpha)$.<br>$F(\alpha, J) \leq -\frac{1}{4}\|J\|(1+\alpha)$. | $F(\alpha, J) \geq -\frac{1}{2}(0.88629)J(1+\alpha)$.<br>$F(\alpha, J) \leq -\frac{1}{4}J + \frac{1}{4}J\alpha$. |
| $J < 0, \quad \alpha < 0$ | $J > 0, \quad \alpha < 0$ |
| $F(\alpha, J) \geq -\frac{1}{4}\|J\| - \frac{1}{2}\|J\|\,\|\alpha\|\,(0.88629)$.<br>$F(\alpha, J) \leq -\frac{1}{4}\|J\| + \frac{1}{4}\|J\|\,\|\alpha\|$. | $F(\alpha, J) \geq -\frac{1}{2}(0.88629)J - \frac{1}{4}J\|\alpha\|$.<br>$F(\alpha, J) \leq -\frac{1}{4}J - \frac{1}{4}\|\alpha\|J$. |

neighbors and $N$ even. Using the completely symmetric state, we get an upper bound immediately for any $J$ and $\alpha$:

$$NzF^s(\alpha, J) \leq \tfrac{1}{2}J \cdot \tfrac{1}{2}Nz + \tfrac{1}{2}J\alpha \cdot \tfrac{1}{2}Nz$$

or

$$F^s(\alpha, J) \leq \tfrac{1}{4}J(1+\alpha). \tag{47}$$

For $J < 0$, $\alpha > 0$, the lower bound is easily obtained:

$$\begin{aligned} NzF^s(\alpha, -|J|) &\geq \langle -\tfrac{1}{2}|\,J\,|\textstyle\sum \boldsymbol{\sigma}\cdot\boldsymbol{\sigma}'\rangle_{\text{g.s.}} \\ &\quad + \langle -\tfrac{1}{2}\alpha|\,J\,|\textstyle\sum' \boldsymbol{\sigma}\cdot\boldsymbol{\sigma}'\rangle_{\text{g.s.}} \\ &= -\tfrac{1}{2}|J|\,\tfrac{1}{2}Nz - \tfrac{1}{2}\alpha\,|J|\,\tfrac{1}{2}Nz \end{aligned}$$

or

$$F^s(\alpha, -|J|) \geq -\tfrac{1}{4}|J|(1+\alpha), \tag{48}$$

so that we have an exact solution as before.

For $J > 0$, Yang and Yang give a lower bound to the ground-state energy of $\frac{1}{2}J\sum \boldsymbol{\sigma}\cdot\boldsymbol{\sigma}'$, for any fixed magnetization. It follows from the Lieb–Mattis theorem that the ground state has spin zero and no magnetization. So we obtain the inequality

$$\langle \tfrac{1}{2}|\,J\,|\textstyle\sum \boldsymbol{\sigma}\cdot\boldsymbol{\sigma}'\rangle_{\text{g.s.}} \geq \tfrac{3}{4}|J|\,Nz. \tag{49}$$

Now consider the lower bound for $J < 0$, $\alpha < 0$:

$$\begin{aligned} NzF^s(-|\alpha|, -|J|) &\geq \langle -\tfrac{1}{2}|\,J\,|\textstyle\sum \boldsymbol{\sigma}\cdot\boldsymbol{\sigma}'\rangle_{\text{g.s.}} \\ &\quad + \langle \tfrac{1}{2}\,|\alpha|\,|\,J\,|\textstyle\sum' \boldsymbol{\sigma}\cdot\boldsymbol{\sigma}'\rangle_{\text{g.s.}} \\ &\geq -\tfrac{1}{4}|J|\,Nz - \tfrac{3}{4}|\alpha|\,|J|\,Nz \end{aligned}$$

or

$$F^s(-|\alpha|, -|J|) \geq -\tfrac{1}{4}|J| - \tfrac{3}{4}|J|\,|\alpha|. \tag{50}$$

For $J > 0$, $\alpha < 0$, we have

$$\begin{aligned} NzF^s(-|\alpha|, J) &\geq \langle \tfrac{1}{2}J\textstyle\sum \boldsymbol{\sigma}\cdot\boldsymbol{\sigma}'\rangle_{\text{g.s.}} \\ &\quad + \langle -\tfrac{1}{2}J|\,\alpha\,|\textstyle\sum' \boldsymbol{\sigma}\cdot\boldsymbol{\sigma}'\rangle_{\text{g.s.}} \\ &\geq -\tfrac{3}{4}JNz - \tfrac{1}{4}|\alpha|\,JNz \end{aligned}$$

or

$$F^s(-|\alpha|, J) \geq -\tfrac{3}{4}J - \tfrac{1}{4}J\,|\alpha|. \tag{51}$$

For $J > 0$, $\alpha > 0$, we have

$$NzF^s(|\alpha|, |J|) \geq -\tfrac{3}{4}JNz - \tfrac{3}{4}J\alpha Nz$$

or

$$F^s(|\alpha|, |J|) \geq -\tfrac{3}{4}J(1+\alpha). \tag{52}$$

By using a variational function which has all spins up in one sublattice and all spins down in the other, we can improve the upper bound in the case $J > 0$ to get

$$F^s(\alpha, |J|) \leq -\tfrac{1}{4}J + \tfrac{1}{4}J\alpha. \tag{53}$$

Finally, using the Yang and Yang result for one dimension, we obtain lower bounds for the linear chain, which are naturally not as good as those using the exact result:

$$\begin{aligned} F(|\alpha|, |J|) &\geq -\tfrac{3}{4}J(1+\alpha) = -0.75J(1+\alpha), \\ F(-|\alpha|, -|J|) &\geq -\tfrac{1}{4}|J| - \tfrac{3}{4}|J|\,|\alpha| \\ &= -0.25\,|J| - 0.75\,|J|\,|\alpha|, \\ F(-|\alpha|, |J|) &\geq -\tfrac{3}{4}|J| - \tfrac{1}{4}|J|\,|\alpha| \\ &= -0.75\,|J| - 0.25\,|J|\,|\alpha|. \end{aligned} \tag{54}$$

## VI. DISCUSSION

The general trend of the results shows the usual nonmagnetic character of the ground states except when all interactions are ferromagnetic. The most interesting case is $J < 0$, $\alpha < 0$. Considering the limit $\alpha \to -\infty$ and applying the Lieb–Mattis theorem, we may easily see that, for sufficiently large and negative $\alpha$, the ground state must belong to spin zero. The interesting trend of the results on short chains indicates that the ferromagnetic state becomes unstable with respect to a spin-zero state for the smallest absolute value of $\alpha$. It is, of course, easy to show that the ferromagnetic state is unstable with respect to spin waves for $\alpha < -\frac{1}{4}$, but spin waves have very high spin, $S = \frac{1}{2}N - 1$. The indications are that the spin-zero state crosses the ferromagnetic state at a very small value of $\alpha$ for large $N$. Quite possibly $\alpha = 0$ itself is a critical value; this situation is probably characteristic of one-dimensional system and is almost certainly untrue in three dimensions. Nevertheless, it emphasizes the rather tenuous nature of the ferromagnetic states.

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## APPENDIX

We give here the character tables of $D_4$, $D_6$, $D_8$, and $D_5$ for convenient reference.

$D_4$

| Class | $E$ | $C_2$ | $C_4$ | $C_2$ | $C_2'$ |
|---|---|---|---|---|---|
| Order of class | 1 | 1 | 2 | 2 | 2 |
| $A_1$ | 1 | 1 | 1 | 1 | 1 |
| $A_2$ | 1 | 1 | 1 | −1 | −1 |
| $B_1$ | 1 | 1 | −1 | 1 | −1 |
| $B_2$ | 1 | 1 | −1 | −1 | 1 |
| $E$ | 2 | −2 | 0 | 0 | 0 |

$D_6$

| Class | $E$ | $C_6$ | $C_6^2$ | $C_6^3$ | $C_2$ | $C_2'$ |
|---|---|---|---|---|---|---|
| Order of class | 1 | 2 | 2 | 1 | 3 | 3 |
| $A_1'$ | 1 | 1 | 1 | 1 | 1 | 1 |
| $A_2'$ | 1 | 1 | 1 | 1 | −1 | −1 |
| $A_1''$ | 1 | −1 | 1 | −1 | −1 | −1 |
| $A_2''$ | 1 | −1 | 1 | −1 | 1 | −1 |
| $E'$ | 2 | −1 | −1 | 2 | 0 | 0 |
| $E''$ | 2 | 1 | −1 | −2 | 0 | 0 |

$D_8$

| Class | $E$ | $C_8$ | $C_8^2$ | $C_8^3$ | $C_8^4$ | $C_2$ | $C_2'$ |
|---|---|---|---|---|---|---|---|
| Order of class | 1 | 2 | 2 | 2 | 1 | 4 | 4 |
| $A_1$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| $A_2$ | 1 | 1 | 1 | 1 | 1 | −1 | −1 |
| $B_1$ | 1 | −1 | 1 | −1 | 1 | 1 | −1 |
| $B_2$ | 1 | −1 | 1 | −1 | 1 | −1 | 1 |
| $E_1$ | 2 | 1 | 0 | −1 | −2 | 0 | 0 |
| $E_2$ | 2 | −1 | 0 | 1 | −2 | 0 | 0 |
| $E_3$ | 2 | 0 | −2 | 0 | 2 | 0 | 0 |

$D_5$

| Class | $E$ | $C_5$ | $C_5^2$ | $C_2$ |
|---|---|---|---|---|
| Order of class | 1 | 2 | 2 | 5 |
| $A_1$ | 1 | 1 | 1 | 1 |
| $A_2$ | 1 | 1 | 1 | −1 |
| $E_1$ | 2 | $\frac{1}{2}(\sqrt{5} - 1)$ | $-\frac{1}{2}(\sqrt{5} + 1)$ | 0 |
| $E_2$ | 2 | $-\frac{1}{2}(\sqrt{5} + 1)$ | $\frac{1}{2}(\sqrt{5} - 1)$ | 0 |