boundary and isotope scattering. The predicted variation of thermal conductivity with sample diameter was found. From 300°K to 1020°K a radial heat flow method was used which reduced the problem of heat transport by spurious thermal radiation to negligible values. At 940°K an abrupt rise in the thermal conductivity was observed. This rise may be due to bipolar diffusion, but the agreement between experiment and theory is only qualitative.

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New Method for Treating the Antiferromagnetic Ground State*

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A perturbation expansion for the ground-state energy of an antiferromagnetic spin system is obtained in terms of a linked-spin-cluster expansion similar to Goldstone's linked-Feynman-diagram expansion for the interacting Fermion system. From the energy perturbation series, perturbation series for the long- and short-range order may be obtained. Using these perturbation series, the ground-state properties are calculated through seventh order and compared with the results obtained by other investigators. In all cases, the values obtained here for the ground-state energy are lower than those which have been obtained by purely variational means. The results for the long-range order are radically different from the variational results but agree qualitatively with those obtained by spin-wave theory; however, the method is free of the usual objections which are voiced to spin-wave treatments of antiferromagnetism. The present work is incomplete in that limits on the error introduced by using only a finite number of terms of the perturbation series to calculate the physical properties are not obtained. But the author feels that the merit of the present work is in the method rather than the results since it provides a consistent framework both to settle the convergence question and to treat the antiferromagnetic spin system at finite temperatures.

I. INTRODUCTION

RECENTLY Orbach[1] has examined the ground state of a linear chain of spins one-half coupled together with a combination of the Heisenberg and Ising antiferromagnetic interactions. He was able to obtain exact values for the energy and short-range order of such a spin system by use of an iteration procedure on an IBM 701 computer. By such a method, he showed the variational predictions of Kasteleijn[2] were in error. That is, Orbach showed that the kink in the curve of short-range order versus relative Ising anisotropy predicted by Kasteleijn was nonexistent. Kasteleijn also predicted the long-range order of such a linear spin system was zero until the relative amount of Ising anisotropy reached the value at which the kink existed in the short-range order curve; thereafter, with an increase of anisotropy, the long-range order was found to rise rapidly to perfect order as the interaction approached the limit of pure Ising coupling. Though Orbach was unable to calculate the long-range order by his exact method, he did point out the dangers of relying on approximate methods, such as Kasteleijn's, for predicting the long-range order behavior of antiferromagnetic spin systems.

For the two- and three-dimensional antiferromagnetic spin systems, no exact treatment for any of the physical properties of the ground state exists except for the trivial case of the pure Ising interaction. Anderson[3] has given an approximate semiclassical spin-wave treatment which predicts an ordered ground state for two- and three-dimensional antiferromagnetic spin systems when the spins are coupled by pure nearest-neighbor isotropic exchange interactions.[4] Using a hybrid spin-wave variational method, Kubo[5] has obtained nonzero long-range order predictions for the ground state of one-, two-, and three-dimensional lattices when the spins are coupled by nearest-neighbor isotropic antiferromagnetic exchange interactions. Kubo's prediction of an ordered ground state for the linear chain, as he himself pointed out, cast unfavorable light on his approximation, since Anderson[3] had predicted disorder for the linear chain under the same circumstances. However, as has been pointed out by Orbach,[1] the

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[1] R. Orbach, Phys. Rev. **112**, 309 (1958).
[2] P. W. Kasteleijn, Physica **18**, 104 (1952).
[3] P. W. Anderson, Phys. Rev. **86**, 694 (1952).
[4] To be precise, Anderson predicts an ordered ground state when an infinitesimal anisotropy of axial symmetry is present. In the remainder of this paper it is to be understood, when we refer to the isotropic exchange interaction, that an axially symmetric infinitesimal anisotropy is assumed. Such an anisotropy is merely to make the z axis the preferred spatial direction.
[5] R. Kubo, Revs. Modern Phys. **25**, 344 (1953).

question of the long-range order of the linear chain with or without anisotropy is an unanswered one in this field except for the pure Ising interaction; thus, the contradiction between the results of Anderson and Kubo must be regarded as a deficiency of the present state of the theory rather than giving preference to one over the other.

In contradiction to the two- and three-dimensional work of Anderson and Kubo, Marshall,[6] by use of the Bethe-Peierls approximation in addition to a variational method, has predicted zero long-range order for two- and three-dimensional spin one-half systems coupled by nearest-neighbor isotropic antiferromagnetic exchange interactions. Marshall's results on long-range order are in complete agreement with those of Taketa and Nakamura[7] who generalized Kasteleijn's method to two- and three-dimensional spin one-half systems. Their results were similar to Kasteleijn's in that they predicted zero long-range order for the anisotropy below a critical value (depending on the lattice) and thereafter rising rapidly to perfect order as the anisotropy approached the Ising limit.

It is seen that there is no agreement in the existing literature, even in a qualitative sense, concerning the long-range order of the ground state of the antiferromagnetic spin system. With such disagreement existing, the theoretical status of antiferromagnetism is far from satisfactory. The purpose of the present investigation is to introduce still another method for treating the antiferromagnetic ground state, whereby it may be ultimately possible to settle rigorously the long-range order question.

The present work has been motivated by the recent successes of linked-cluster expansions in the treatment of N-body systems. Using a linked-cluster expansion, it is possible to obtain a perturbation series for the ground-state energy of the antiferromagnetic spin system; and then, by means of the Feynman theorem,[8] obtain perturbation series for the long- and short-range order of the ground state. The only question then remaining is the determination of the error introduced by using a finite number of terms of the perturbation expansions to calculate the physical properties of the ground state. The present work will be incomplete in that this question of convergence is not settled. However, the author feels that the merit of the present work lies in the method rather than in the results, since the application of the methods presented herein could eventually lead to a consistent low-temperature description of the antiferromagnetic spin system.

II. THE SPIN SYSTEM

In this paper, only those antiferromagnetics of the two-sublattice type will be treated, i.e., we assume that the physical lattice of the spin system can be divided into two sublattices, A and B say, such that all the nearest neighbors of a spin on sublattice A are on sublattice B, and vice versa. A spin operator corresponding to a spin on the A sublattice will be denoted by $\mathbf{R}_j$, while a spin operator of a spin on the B sublattice will be denoted by $\mathbf{S}_k$. The number of spins on each of the sublattices is fixed at N.

The dynamical properties of the spin system under consideration are described by the anisotropic exchange Hamiltonian

$$H=2J\sum_{\langle jk\rangle}[R_j^zS_k^z+(1-a)(R_j^xS_k^x+R_j^yS_k^y)], \quad (1)$$

where the notation $\langle jk\rangle$ implies a sum over pairs of nearest neighbors only. Herein, we treat only the case $J>0$, i.e., antiferromagnetic coupling between the spins. When $a=0$, the Hamiltonian (1) describes nearest-neighbor isotropic exchange coupling between the spins; for $a=1$, it represents a pure Ising interaction between the spins. Furthermore, we assume periodic boundary conditions; such boundary conditions allow surface effects to be neglected, since it is assumed that the lattice is periodically repeated throughout space.

When $|\mathbf{R}_j|=|\mathbf{S}_k|=\frac{1}{2}$, the Hamiltonian (1) is identical with the Hamiltonian treated by Kasteleijn,[2] Taketa and Nakamura,[7] and Orbach.[1] Since allowing $|\mathbf{R}_j|$ and $|\mathbf{S}_k|$ to be greater than one-half introduces no new difficulties into our treatment, we will carry through the formalism for an arbitrary value of spin per lattice site. Even the case for all $|\mathbf{R}_j|$ equal and all $|\mathbf{S}_k|$ equal but $|\mathbf{R}_j|\neq|\mathbf{S}_k|$ is included in our formalism, i.e., a treatment of the ground state of a ferrimagnetic model. However, such a model for ferrimagnetism would be quite naive since actual ferrimagnetic materials involve more complicated geometries than those of the two-sublattice types; also, due to the geometries of the actual ferrimagnetic crystals, more than just nearest-neighbor interactions are important.

III. THE METHOD

Essentially, the determination of the ground state of the Hamiltonian (1) is that of the determination of the ground state of an N-body problem. Naively, it might be thought that perturbation theory could be directly applied to the magnetic N-body problem described by the Hamiltonian (1); thus, one would be able to calculate, in principle, the energy and wave function of any given state of the system to high precision. Unfortunately, this is not true, since the energy correction, for a given state, obtained from perturbation theory contains terms which diverge more strongly than N as $N\rightarrow\infty$, i.e., the energy correction contains terms proportional to N^2, N^3, N^4, $\cdots$. However, one expects on physical grounds, that the energy correction for the ground state is proportional to N; hence, the terms

[6] W. Marshall, Proc. Roy. Soc. (London) **A232**, 48 (1955).
[7] H. Taketa and T. Nakamura, J. Phys. Soc. Japan **11**, 919 (1956).
[8] R. Feynman, Phys. Rev. **56**, 340 (1939).

proportional to N^2, N^3, N^4, $\cdots$ must cancel. But it is highly important that this cancellation be handled in a consistent fashion or part of the energy correction could be lost in the process. Fortunately, a perturbation method, based on the adiabatic theorem, is available which provides a consistent method for dealing with the cancellation of those terms proportional to N^2, N^3, N^4, $\cdots$, thus leaving only an energy correction, for the ground state, which is proportional to N.

Before the systematics of this method are applied specifically to the determination of the ground-state properties of the Hamiltonian (1), it is worth while to outline the method to be used. Let the dynamical properties of an N-body system be described by the general Hamiltonian

$$H=H_0+H_1, \tag{2}$$

where H_0 is the zeroth-order Hamiltonian which describes free "particles,"[9] while H_1 is the interaction between these particles. A perturbation method may be developed from (2) by using the adiabatic theorem. The interaction, H_1, is to be slowly switched on between $t=-\infty$ and $t=0$; then a system which at $t=-\infty$ is in an eigenstate of H_0 will slowly change into an eigenstate of the total Hamiltonian, H, between $t=-\infty$ and $t=0$. Such a result has been proved by Gell-Mann and Low[10] in essentially the form given below.

Given that $|m\rangle$ is an eigenstate of H_0,

$$H_0|m\rangle=E_m|m\rangle, \tag{3}$$

then

$$\psi_m=\lim_{\alpha\to+0}\frac{S_\alpha|m\rangle}{\langle m|S_\alpha|m\rangle} \tag{4}$$

will be an eigenstate of the total Hamiltonian, H. Further, the energy corresponding to the state ψ_m is

$$E_m+\Delta E_m=E_m+\lim_{\alpha\to+0}\frac{\langle m|H_1S_\alpha|m\rangle}{\langle m|S_\alpha|m\rangle}. \tag{5}$$

The quantity S_α in the above equations is

$$S_\alpha=1+\sum_{n=1}^{\infty}(n!)^{-1}(i\hbar)^{-n}\int_{-\infty}^{0}dt_1\int_{-\infty}^{0}dt_2\cdots\int_{-\infty}^{0}dt_n \times P[H_\alpha(t_1)H_\alpha(t_2)\cdots H_\alpha(t_n)], \tag{6}$$

where P is Dyson's[11] time ordering operator and

$$H_\alpha(t)=\exp[itH_0/\hbar]H_1\exp[-itH_0/\hbar]e^{\alpha t}. \tag{7}$$

The parameter α governs the rate of switching on the interaction; the limit $\alpha\to+0$ means that the interaction is switched on infinitely slowly, the condition for the exactness of the adiabatic theorem.

The insertion of (6) into (4) and (5) gives a perturbation method for solution of the Hamiltonian (2). Even this perturbation series for the energy [(5) after insertion of (6)] contains terms which diverge more strongly than N as $N\to\infty$. This difficulty is overcome by a linked-cluster expansion. The linked-cluster expansion was first suggested by Brueckner[12] in his treatment of infinite nuclear matter and has been proved by Goldstone[13] for this case.[14] We shall see that a linked-cluster expansion is possible for the magnetic N-body system described by the Hamiltonian (1). Such a linked-cluster expansion will enable the physical properties of the ground state of (1) to be calculated by perturbation expansions.

Before proceeding to the proof of the existence of a linked-spin-cluster expansion for the antiferromagnetic model, the essence of the proof will be discussed. It will be shown for the Hamiltonian (1) that

$$S_\alpha|0\rangle=\exp[S_{\alpha(1)}+S_{\alpha(2)}]|0\rangle, \tag{8}$$

where $|0\rangle$ is the ground state of H_0 (yet to be specified for our case), $S_{\alpha(1)}$ is a c number which is an infinite series involving linked spin clusters analogous to vacuum-vacuum Feynman diagrams, and $S_{\alpha(2)}$ is an operator which is an infinite series containing all other possible linked spin clusters. The definition of a linked spin cluster will be postponed until later. Substitution of (8) into the energy correction, ΔE_0, and dividing out the c number $\exp[S_{\alpha(1)}]$ gives

$$\Delta E_0=\lim_{\alpha\to+0}\langle 0|H_1\exp[S_{\alpha(2)}]|0\rangle. \tag{9}$$

This expression for the energy correction contains, as will be seen, only terms proportional to N. Thus, the essence of the proof is to show that $S_\alpha|0\rangle$ factors as indicated, from which it follows that the energy correction terms proportional to N^2, N^3, N^4, $\cdots$ can be divided out.

IV. TRANSFORMATION TO BOSE OPERATORS

Before the proof of (8) can be given, it is necessary to express (1) in terms of operators other than the spin operators $\mathbf{R}_j$, $\mathbf{S}_k$; this is necessary in order to obtain

[9] Let the ground state of H_0 be $|0\rangle$ and let b_i^+ represent a series of operators which generate the excited states of H_0 by operating on $|0\rangle$:

$$H_0|0\rangle=E_0|0\rangle,$$
$$H_0b_i^+|0\rangle=(E_0+E_i)b_i^+|0\rangle.$$

By H_0 corresponding to free "particles," we mean that

$$(H_0-E_0)b_1^+b_2^+\cdots b_n^+|0\rangle=(E_1+E_2+\cdots+E_n)b_1^+b_2^+\cdots b_n^+|0\rangle$$

is satisfied for all values of n. Though this requirement may appear trivial, difficulties can arise in the present problem unless the Hamiltonian (1) is split in such a manner that it is satisfied.

[10] M. Gell-Mann and F. Low, Phys. Rev. 84, 350 (1951).

[11] F. J. Dyson, Phys. Rev. **75**, 1736 (1949).

[12] K. A. Brueckner, Phys. Rev. **100**, 36 (1955).

[13] J. Goldstone, Proc. Roy. Soc. (London) **A239**, 267 (1957).

[14] Considerable interest has been shown in the applicability of linked-cluster expansions to various systems. Due to the rapidity of appearance of papers in this field, a listing of references would be incomplete; for this reason, the author has chosen to refer to only the beginning work in this field and those papers which have been explicitly used in the present investigation.

an H_0 which will correspond to free "particles."[9] First, by introducing angular momentum raising and lowering operators

$$R_j^{\pm}=R_j^x\pm iR_j^y, \tag{10a}$$

$$S_k^{\pm}=S_k^x\pm iS_k^y, \tag{10b}$$

the Hamiltonian (1) is expressed in a more convenient form:

$$H=2J\sum_{\langle jk\rangle}R_j^zS_k^z+(1-a)J\sum_{\langle jk\rangle}(R_j^+S_k^-+R_j^+S_k^-). \tag{11}$$

The Hamiltonian as expressed in (11) has a major drawback inasmuch as it seems *too* immediately obvious what portion of it should be used as an unperturbed Hamiltonian. The usual procedure in applying a perturbation treatment to magnetic systems would be to take the portion of H containing the z components of the spin operators as the unperturbed Hamiltonian. Then a set of eigenfunctions for the unperturbed Hamiltonian would be a set of product functions where each factor in a given product function was an eigenfunction of the total angular momentum and its z component for each of the spins of the lattice. However, such a choice, for our purposes, would introduce considerable difficulties; the major difficulty being that the unperturbed Hamiltonian would not describe free "particles." Since we eventually desire to reduce the nth order term of $S_\alpha|0\rangle$, Wick's theorem[15] would be exceedingly valuable for this reduction. The application of Wick's theorem would require that one have a free-particle zero-order Hamiltonian. Furthermore, the use of Wick's theorem would also require that the commutator of R_j^+ (annihilation operator) and $R_{j'}^-$ (creation operator) be a c number, likewise for the commutator of S_k^- and $S_{k'}^+$; but such is not the case.

The difficulties involved in splitting the Hamiltonian as described above may be overcome by the introduction of a new set of operators. Schwinger[16] has shown that a set of spin operators may be replaced by two sets of Bose operators. Such a replacement will enable the eventual use of Wick's theorem in the reduction of $S_\alpha|0\rangle$. Hence, following Schwinger, we introduce the transformations

$$R_j^+=u_j^+v_j, \tag{12a}$$

$$R_j^-=v_j^+u_j, \tag{12b}$$

$$R_j^z=(1/2)(u_j^+u_j-v_j^+v_j), \tag{12c}$$

$$S_k^+=x_k^+y_k, \tag{12d}$$

$$S_k^-=y_k^+x_k, \tag{12e}$$

$$S_k^z=(1/2)(x_k^+x_k-y_k^+y_k). \tag{12f}$$

By requiring these new operators to obey the commutation relations

$$[u_j,u_{j'}^+]=[v_j,v_{j'}^+]=\delta_{jj'}, \tag{13a}$$

$$[x_k,x_{k'}^+]=[y_k,y_{k'}^+]=\delta_{\kappa k'}, \tag{13b}$$

$$[u_j,v_{j'}]=[u_j,v_{j'}^+]=[x_k,y_{k'}]=[x_k,y_{k'}^+]=0, \tag{13c}$$

the commutation relations for the $\mathbf{R}_j$ and $\mathbf{S}_k$ operators follow. Hence, the replacement (12) with the requirement (13) is valid.

In terms of these new operators, the Hamiltonian (11) is written

$$H=2J\sum_{\langle jk\rangle}(1/4)(u_j^+u_j-v_j^+v_j)(x_k^+x_k-y_k^+y_k)$$
$$+(1-a)J\sum_{\langle jk\rangle}(u_j^+y_k^+v_jx_k+v_j^+x_k^+u_jy_k). \tag{14}$$

It is still not evident how to split the Hamiltonian into unperturbed and perturbing parts. We will now show how a substitution may be made whereby it is possible to define an unperturbed Hamiltonian corresponding to free "particles." A basis for the entire spin system is given by

$$\Pi_j\Pi_k[(R+m_j')!(R-m_j')!(S+n_k')!(S-n_k')!]^{-\frac{1}{2}}$$
$$\times(u_j^+)^{R+m_j'}(v_j^+)^{R-m_j'}(x_k^+)^{S+n_k'}(y_k^+)^{S-n_k'}|0), \tag{15}$$

where the m_j' are any set of N integers or half-integers (depending on whether R is integral or half-integral) satisfying $-R\leq m_j'\leq R$, while the n_k' are any set of N integers or half-integers satisfying $-S\leq n_k'\leq S$. The function $|0)$ in (15) is defined such that

$$u_j|0)=v_j|0)=x_k|0)=y_k|0)=0. \tag{16}$$

Within the basis (15), the replacements

$$R=(1/2)(u_j^+u_j+v_j^+v_j), \tag{17a}$$

and

$$S=(1/2)(x_k^+x_k+y_k^+y_k), \tag{17b}$$

are valid. The replacements given in Eqs. (17) will reduce the Hamiltonian to a desired form. Making such replacements will be equivalent to introducing two sets of spin-deviation operators. In fact, as will be seen in Sec. VI, the introduction of spin-deviation operators will be convenient when making explicit calculations.

Using Eqs. (17), the Hamiltonian (14) may be written[17]

$$H=H_0+H_1, \tag{18}$$

[15] G. C. Wick, Phys. Rev. **80**, 268 (1950).

[16] J. Schwinger, Atomic Energy Commission Report NYO-3071, 1952 (unpublished).

[17] Of course, there are four possible substitutions that could be made using Eqs. (17). Two of these substitutions will result in a zeroth-order Hamiltonian which has a perfect ordered antiferromagnetic state for its ground state; we have chosen that substitution which results in having a ground state of H_0 corresponding to the spins on sublattice A oriented in the $+z$ direction and those on sublattice B in the $-z$ direction. The other two possible substitutions are irrelevant here but would be of value if one chose to treat the ferromagnetic problem by using the Bose operators.

where

$$H_0=E_0+2zJS\sum_{j=1}^{N} v_j^+v_j+2zJR\sum_{k=1}^{N} x_k^+x_k, \tag{19a}$$

$$H_1=\sum_{\langle jk\rangle}[J'(u_j^+y_k^+v_jx_k+v_j^+x_k^+u_jy_k)-2Jv_j^+v_jx_k^+x_k], \tag{19b}$$

and

$$E_0=-2JNzRS, \tag{20a}$$

$$J'=(1-a)J. \tag{20b}$$

In the above, z denotes the number of nearest neighbors for each spin.

From the basis of the spin system as expressed by (15), the ground state of H_0 is

$$|0\rangle=\prod_j\prod_k[(2R)!(2S)!]^{-\frac{1}{2}}(u_j^+)^{2R}(y_k^+)^{2S}|0). \tag{21}$$

The excited states of H_0, which are of interest in the reduction of $S_\alpha|0\rangle$, are obtained from $|0\rangle$ by the repeated operation of factors $v_j^+u_jx_k^+y_k$ upon this ground state. Such excited states will now be analogous to free-particle states as can be seen from the fact that H_0 is a linear combination of number operators.

Insertion of H_1, as given by (19b), into (6) gives

$$S_\alpha|0\rangle=\Big(1+\sum_{n=1}^{\infty}(i\hbar)^{-n}(n!)^{-1}\sum_{\langle 1,\cdots,n\rangle}\int_{-\infty}^{0}dt_1\int_{-\infty}^{0}dt_2\cdots\int_{-\infty}^{0}dt_n\, e^{\alpha t_1}\cdots e^{\alpha t_n}$$

$$\times P\{[J'(U_{j1}^+Y_{k1}^+V_{j1}X_{k1}+V_{j1}^+X_{k1}^+U_{j1}Y_{k1})-2JV_{j1}^+V_{j1}X_{k1}^+X_{k1}]\times\cdots$$

$$\times[J'(U_{jn}^+Y_{kn}^+V_{jn}X_{kn}+V_{jn}^+X_{kn}^+U_{jn}Y_{kn})-2JV_{jn}^+V_{jn}X_{kn}^+X_{kn}]\}\Big)|0\rangle, \tag{22}$$

where the notation $\langle 1,\cdots,n\rangle$ means the sum is over n neighboring pairs of indices $\mathbf{j}$ and $\mathbf{k}$, while

$$U_{ja}=\exp[(2izJSt_a)/(2\hbar)]u_{ja}, \tag{23a}$$

$$V_{ja}=\exp[-(2izJSt_a)/(2\hbar)]v_{ja}, \tag{23b}$$

$$X_{ka}=\exp[-(2izJRt_a)/(2\hbar)]x_{ka}, \tag{23c}$$

$$Y_{ka}=\exp[(2izJRt_a)/(2\hbar)]y_{ka}. \tag{23d}$$

V. PROOF OF THE LINKED-SPIN-CLUSTER EXPANSION

We are now in a position to perform the reduction of $S_\alpha|0\rangle$ to a linked-spin-cluster expansion. Before the reduction of the nth order term is presented, it is best to perform the reduction for the first few orders. In this way, the proof of the nth order reduction will be more readily understood; also, since a diagrammatic analysis will not be used,[18] the definition of a linked spin cluster will be more easily presented by using examples from the first few orders. Superscripts on S_α will designate the various orders of (22), e.g., $S_\alpha^{(1)}|0\rangle$ designates the term for $n=1$ in the summation of (22).

The reduction of the first order gives

$$S_\alpha^{(1)}|0\rangle=-J'(\epsilon-\beta)^{-1}\sum_{\langle 1\rangle}v_{j1}^+x_{k1}^+u_{j1}y_{k1}|0\rangle$$

$$=-J'(\epsilon-\beta)^{-1}\sum_{\langle 1\rangle}R_{j1}^-S_{k1}^+|0\rangle, \tag{24}$$

where

$$\epsilon=2zJ(R+S), \tag{25a}$$

$$\beta=i\hbar\alpha. \tag{25b}$$

The second-order terms of (22) are

$$(2!)^{-1}(J')^2(\epsilon-\beta)^{-2}\sum_{\langle 1,2\rangle}R_{j1}^-S_{k1}^+R_{j2}^-S_{k2}^+|0\rangle, \tag{26a}$$

$$S_2'|0\rangle=-(J')^2(\epsilon-\beta)^{-1}\times[(4RS)/(2\beta)]\sum_{\langle 1,2\rangle}\Delta(1,2)|0\rangle, \tag{26b}$$

$$(J')(-2J)(\epsilon-\beta)^{-1}(\epsilon-2\beta)^{-1}\times\sum_{\langle 1,2\rangle}\Delta(1,2)R_{j2}^-S_{k2}^+|0\rangle. \tag{26c}$$

For the purpose of later reference, we have defined the quantity (26b) by the symbol $S_2'|0\rangle$ and the following notation has been introduced:

$$\Delta(1,2)=\delta_j(1,2)\delta_k(1,2)=\delta_{j1j2}\delta_{k1k2}, \tag{27}$$

δ_{j1j2} and δ_{k1k2} being the usual Kronecker deltas.

To further illustrate the reduction of $S_\alpha|0\rangle$, a term of $S_\alpha^{(3)}|0\rangle$ will be evaluated. After use of the linearity of the P operator, permuting some of the Bose operators under the P operation, and applying Wick's theorem, one nonzero term of $S_\alpha^{(3)}|0\rangle$ is

$$(3!)^{-1}(i\hbar)^{-3}\sum_{\langle 1,2,3\rangle}\int_{-\infty}^{0}dt_1\int_{-\infty}^{0}dt_2\int_{-\infty}^{0}dt_3\, e^{\alpha t_1}e^{\alpha t_2}e^{\alpha t_3}\binom{3}{2}(J')^3$$

$$\times(2V_{j1}\cdot V_{j2}^+\cdot X_{k1}\cdot\cdot X_{k2}^+\cdot\cdot V_{j3}^+X_{k3}^+U_{j1}^+Y_{k1}^+U_{j2}Y_{k2}U_{j3}Y_{k3})|0\rangle, \tag{28}$$

[18] Granted, the reduction of $S_\alpha|0\rangle$, as given by (22), is amenable to a diagrammatic analysis; however, the author feels that a diagrammatic analysis of S_α is unnecessary for the purposes of this paper.

$\binom{3}{2}$ being the usual binomial coefficient and the same number of superscript dots on two operators stands for the contraction of the two operators, e.g.,

$$V_{j1}\cdot V_{j2}{}^{+}\cdot = P(V_{j1}V_{j2}{}^{+}) - V_{j2}{}^{+}V_{j1}$$
$$= 0 \quad \text{if} \quad t_2 > t_1$$
$$= V_{j1}V_{j2}{}^{+} - V_{j2}{}^{+}V_{j1} \quad \text{if} \quad t_1 > t_2.$$

We rewrite (28):

$$(J')^3(i\hbar)^{-3} \sum_{\langle 1,2,3\rangle} \Delta(1,2) \times \int_{-\infty}^{0} dt_3 \int_{-\infty}^{0} dt_1 \int_{-\infty}^{t_1} dt_2 \exp[(\alpha + i\epsilon/\hbar)t_3] \times \exp[(\alpha - i\epsilon/\hbar)t_1] \exp[(\alpha + i\epsilon/\hbar)t_2] \times (u_{j1}{}^{+}u_{j2})(y_{k1}{}^{+}y_{k2})v_{j3}{}^{+}x_{k3}{}^{+}u_{j3}y_{k3}|0\rangle; \quad (29)$$

the factor $\Delta(1,2)$ and the upper limit on the t_2 integration arise from the two contractions.

We note:

$$\Delta(1,2)u_{j1}{}^{+}u_{j2}u_{j3}|0\rangle = \Delta(1,2)[2R - \delta_j(1,3)]u_{j3}|0\rangle, \quad (30a)$$

$$\Delta(1,2)y_{k1}{}^{+}y_{k2}y_{k3}|0\rangle = \Delta(1,2)[2S - \delta_k(1,3)]y_{k3}|0\rangle. \quad (30b)$$

Equations (30) are the essence of the desired illustration and the reason for explicitly considering an evaluation of a term of $S_\alpha{}^{(3)}|0\rangle$. The desired point is that, in the reduction of higher orders of $S_\alpha|0\rangle$, any $u_j{}^{+}$ operator, occurring after the application of Wick's theorem, can be paired with a $u_{j'}$ operator such that $\mathbf{j}=\mathbf{j}'$ by virtue of the multiplying contractions; the resulting number operator can then be replaced by its corresponding c-number value as has been done on the right-hand side of Eq. (30a). Similarly for any $y_k{}^{+}$ operator occurring after applying Wick's theorem.

Substituting Eqs. (30) into (29) gives, after performing the integration, the following four third-order terms:

$$(J')^3(\epsilon-\beta)^{-2}[(4RS)/(2\beta)] \sum_{\langle 1,2,3\rangle} \Delta(1,2)R_{j3}{}^{-}S_{k3}{}^{+}|0\rangle \quad (31a)$$

$$-(J')^3(\epsilon-\beta)^{-2}[(2S)/(2\beta)] \sum_{\langle 1,2,3\rangle} \Delta(1,2)\delta_j(1,3)R_{j3}{}^{-}S_{k3}{}^{+}|0\rangle \quad (31b)$$

$$-(J')^3(\epsilon-\beta)^{-2}[(2R)/(2\beta)] \sum_{\langle 1,2,3\rangle} \Delta(1,2)\delta_k(1,3)R_{j3}{}^{-}S_{k3}{}^{+}|0\rangle \quad (31c)$$

$$(J')^3(\epsilon-\beta)^{-2}(2\beta)^{-1} \sum_{\langle 1,2,3\rangle} \Delta(1,2,3)R_{j3}{}^{-}S_{k3}{}^{+}|0\rangle. \quad (31d)$$

In (31d),

$$\Delta(1,2,3) = \Delta(1,2)\Delta(1,3). \quad (32)$$

A precise definition of a "linked spin cluster" will now be given. First, with each neighboring pair of $\mathbf{j}_i$, $\mathbf{k}_i$ indices is associated a line within the physical lattice of the spin system under consideration. This line is to connect the two lattice points represented by the $\mathbf{j}_i$, $\mathbf{k}_i$ pair indices of a given neighboring pair of spins; furthermore, this line has a length equal to the lattice distance between neighboring lattice points. Then, for an nth order term of $S_\alpha|0\rangle$ there are associated with it n such lines in the physical lattice of the spin system. In general, these n lines may or may not share common lattice points as terminals; in fact, it is possible for two or more lines to have both terminal lattice points in common. An nth order linked spin cluster is then defined as a mathematical term occurring in nth order of $S_\alpha|0\rangle$ such that each of the n associated lattice lines is physically connected to all other $(n-1)$ lattice lines. That is, given any two of the n lines, these two lines are connected, either by having one or both terminal lattice points in common, or through intermediate lines (these intermediate lines being in the original n lines) by these intermediate lines sharing terminal lattice points among themselves and the given two lines. A term is not to be considered linked *unless* the connection of the associated lattice lines *is required* by the existence of Kronecker delta factors in the term. That is, a term is not linked if the connection of the associated lattice points is accidental, being due to only letting the summation on the pair indices cover their full range and not required by Kronecker deltas in the term under consideration. Furthermore, the above definition is such that when the linked spin cluster represents a term which is merely a c number operating on $|0\rangle$, the summation may be performed and the resulting term is proportional to N; this fact will be important when the energy correction due to the perturbation is calculated.[19] Terms not satisfying the above definition will be referred to as "unlinked."

Examples of the above definition of linked spin clusters are (24), (26b), (26c), (31b), (31c), and (31d). Terms (26a) and (31a) are unlinked; however, it is seen that (26a) is $(1/2!)[S_\alpha{}^{(1)}]^2|0\rangle$ and (31a) is $[S_2'][S_\alpha{}^{(1)}]|0\rangle$ which begins to suggest the factorization of $S_\alpha|0\rangle$ as stated in (8). To prove (8), it is necessary to consider the nth order of $S_\alpha|0\rangle$.

[19] Regardless of how one chooses to define linkedness of terms, the important thing is that a c-number linked term is proportional to N when considering a ground-state problem. In fact, an nth order linked term (ground-state problem) could be defined as a term which is proportional to N when the summation, neglecting operators occurring in the term for this purpose, over the n pairs of $\mathbf{j}_i$, $\mathbf{k}_i$ indices is performed.

Since the P operator is linear and the Bose operators can be permuted at will under the P operation, (22) may be rewritten

$$S_\alpha|0\rangle=\Big\{1+\sum_{n=1}^{\infty}(i\hbar)^{-n}(n!)^{-1}\sum_{\langle 1,\cdots,n\rangle}\int_{-\infty}^{0}dt_1\int_{-\infty}^{0}dt_2\cdots\int_{-\infty}^{0}dt_n e^{\alpha t_1}e^{\alpha t_2}\cdots e^{\alpha t_n}\sum_{r=0}^{n}\sum_{s=0}^{(n-r)}\binom{n}{r}\binom{n-r}{s-r}(J')^s(-2J)^{n-s}$$
$$\times P[(U_{j_1}{}^{+}Y_{k_1}{}^{+}V_{j_1}X_{k_1})\cdots(U_{j_r}{}^{+}Y_{k_r}{}^{+}V_{j_r}X_{k_r})(V_{j_{r+1}}{}^{+}X_{k_{r+1}}{}^{+}U_{j_{r+1}}Y_{k_{r+1}})\cdots(V_{j_s}{}^{+}X_{k_s}{}^{+}U_{j_s}Y_{k_s})$$
$$\times(V_{j_{s+1}}{}^{+}V_{j_{s+1}}X_{k_{s+1}}{}^{+}X_{k_{s+1}})\cdots(V_{j_n}{}^{+}V_{j_n}X_{k_n}{}^{+}X_{k_n})]\Big\}|0\rangle, \quad (33)$$

where

$$\binom{n}{r} \quad \text{and} \quad \binom{n-r}{s-r}$$

are binomial coefficients.

By application of Wick's theorem,

$$P[(U_{j_1}{}^{+}Y_{k_1}{}^{+}V_{j_1}X_{k_1})\cdots(V_{j_n}{}^{+}V_{j_n}X_{k_n}{}^{+}X_{k_n})]$$

may be replaced by a sum of normal products which contains all possible contractions within the sum. This sum is then to act on the state $|0\rangle$. For a term of the sum to give a nonzero contribution to (33), the normal product cannot contain any V_j or X_k operators, since these acting on $|0\rangle$ would give zero by (16) and (21); thus, each term of interest in the sum contains products of contractions such that all the V_j and X_k operators have been contracted and the product is multiplied by a normal product of $U_j{}^{+}$, U_j, $Y_k{}^{+}$, Y_k, $V_j{}^{+}$, $X_k{}^{+}$ operators. Each of the $U_j{}^{+}$ and $Y_k{}^{+}$ operators, occurring in the normal product, will be able to be paired with a $U_{j'}$ or $Y_{k'}$ operator to form a number operator by virtue of the multiplying contractions. To the right of these number operators is essentially a product of $u_{j''}$ and $y_{k''}$ operators acting on $|0\rangle$; thus, these operators may be replaced by c numbers in a manner similar to Eqs. (30). Hence, (33) is reduced by Wick's theorem to a sum of terms; each term is a product of contractions, factors of the types $[2R-\delta_j(n,m_1)-\cdots-\delta_j(n,m_i)]$ and $[2S-\delta_k(p,q_1)-\cdots-\delta_k(p,q_j)]$, and a normal product of U_j, Y_k, $V_j{}^{+}$, $X_k{}^{+}$ operators acting on $|0\rangle$. For each term, the multiplication of the $[2R-\delta_j(n,m_1)-\cdots-\delta_j(n,m_i)]$ and $[2S-\delta_k(p,q_1)-\cdots-\delta_k(p,q_j)]$ factors may be explicitly carried out, giving a sum of subterms (the individual terms remaining after this multiplication is performed will be referred to as *subterms*) for each term originally arising from application of Wick's theorem. Since the U_j, Y_k, $V_j{}^{+}$, $X_k{}^{+}$ all commute, the factors in each subterm can be rearranged at will. We choose to rearrange each subterm into linked factors such that each linked factor is linked within itself and unlinked with all other factors of the subterm. Some of the subterms of a given order will give identical contributions to (33). Two subterms will be called *identical* if one is obtained from the other by a permutation of pair indices; two subterms which do not satisfy this definition will be called *distinct.*

For ease of notation in what follows, a $(U_j{}^{+}Y_k{}^{+}V_jX_k)$ factor of (33) will be called an "A," a $(V_j{}^{+}X_k{}^{+}U_jY_k)$ factor of "B," and a $(V_j{}^{+}V_jX_k{}^{+}X_k)$ factor a "C." Each linked factor of a given subterm may then be thought of as consisting of a given number of A's, B's, and C's linked together by contractions between pairs of their operators and Kronecker deltas arising by replacement of number operators by c numbers; also present in each linked factor will be the U_j, Y_k, $V_j{}^{+}$, $X_k{}^{+}$ operators, from the same A's, B's, and C's, left after the contractions and number operators have been considered. Thus, (33) may be written schematically as follows:

$$S_\alpha|0\rangle=\Big\{1+\sum_{n=1}^{\infty}\sum_{\text{subterms}}[r!(s-r)!(n-s)!]^{-1}$$
$$\times\Big[\begin{matrix}f_1\ A\text{'s},\ g_1\ B\text{'s},\ h_1\ C\text{'s}\\ \text{linked together}\end{matrix}\Big]\cdots\Big[\begin{matrix}f_1\ A\text{'s},\ g_1\ B\text{'s},\ h_1\ C\text{'s}\\ \text{linked together}\end{matrix}\Big]\Big[\begin{matrix}f_2\ A\text{'s},\ g_2\ B\text{'s},\ h_2\ C\text{'s}\\ \text{linked together}\end{matrix}\Big]\cdots\Big[\begin{matrix}f_2\ A\text{'s},\ g_2\ B\text{'s},\ h_2\ C\text{'s}\\ \text{linked together}\end{matrix}\Big]$$
$$\times\cdots\Big[\begin{matrix}f_m\ A\text{'s},\ g_m\ B\text{'s},\ h_m\ C\text{'s}\\ \text{linked together}\end{matrix}\Big]\cdots\Big[\begin{matrix}f_m\ A\text{'s},\ g_m\ B\text{'s},\ h_m\ C\text{'s}\\ \text{linked together}\end{matrix}\Big]\Big\}|0\rangle, \quad (34)$$

where the integration signs, summations, $(1/i\hbar)$, J', and $(-2J)$ factors have been considered as an integral part of the individual linked factors. In (34), we have schematically written a general subterm which contains p_1 factors wherein f_1 A's, g_1 B's, and h_1 C's are linked together in an identical fashion, the only difference being that each of the p_1 linked factors contains different pair indices; p_2 factors wherein f_2 A's, g_2 B's, and h_2 C's are linked together in an identical fashion; $\cdots$; p_m factors wherein f_m A's, g_m B's, and h_m C's are linked together in an identical fashion.

The number of identical subterms generated in the

nth order term having r A's, $(s-r)$ B's, and $(n-s)$ C's is [considering the general subterm which has been schematically written in (34)] $r!(s-r)!(n-s)!\times(p_1!p_2!\cdots p_m!)^{-1}$. The factor $(p_1!p_2!\cdots p_m!)^{-1}$ is necessary to divide out the number of permutations corresponding to the interchange of *all* the indices of one linked factor with all the indices of another linked factor of the same type, i.e., a permutation of linked factors; such permutations do not contribute to the number of identical subterms, since they correspond to identical contractions in the reduction of (33) by Wick's theorem. Thus, (34) becomes

$$S_\alpha|0\rangle=\Big\{1+\sum_{n=1}^{\infty}\sum_{\text{distinct subterms}}(p_1!p_2!\cdots p_m!)^{-1}\Big[\begin{matrix}f_1\ A\text{'s},\ g_1\ B\text{'s},\ h_1\ C\text{'s}\\ \text{linked together}\end{matrix}\Big]^{p_1}\Big[\begin{matrix}f_2\ A\text{'s},\ g_2\ B\text{'s},\ h_2\ C\text{'s}\\ \text{linked together}\end{matrix}\Big]^{p_2}\times\cdots\Big[\begin{matrix}f_m\ A\text{'s},\ g_m\ B\text{'s},\ h_m\ C\text{'s}\\ \text{linked together}\end{matrix}\Big]^{p_m}\Big\}|0\rangle. \quad (35)$$

From (35), it is seen that

$$S_\alpha|0\rangle=\exp[\text{sum of linked subterms}]|0\rangle, \quad (36)$$

which shows that $S_\alpha|0\rangle$ may be factored as indicated by (8).

VI. GROUND-STATE ENERGY

The ground-state energy could be calculated by using (5); however, it is more convenient to use another expression given by Gell-Mann and Low.[10] This expression for the energy of the ground state is

$$E=E_0+\lim_{\alpha\to+0}\beta\lambda\frac{\partial}{\partial\lambda}[\ln\langle 0|S_\alpha|0\rangle], \quad (37)$$

where λ is the coupling constant of the interaction. Only those terms of S_α which are c numbers will contribute to the expectations value in (37); these terms are analogous to terms corresponding to "vacuum-vacuum" Feynman diagrams in quantum electrodynamics. Henceforth, terms which have a nonzero expectation value in the state $|0\rangle$ will be referred to as "ground-state terms." Using the notation of Eq. (8) and the result of Eq. (36), the ground-state energy is

$$E=E_0+\lim_{\alpha\to+0}\beta\lambda\frac{\partial}{\partial\lambda}[S_{\alpha(1)}]. \quad (38)$$

This relation, instead of (5), will be used in calculating the ground-state energy.

Although the Bose operators introduced in Sec. IV were convenient for showing the existence of a linked-spin-cluster expansion, they are not the best choice for explicit calculations. By defining spin-deviation operators m_j and n_k,

$$m_j=R-R_j^z, \quad (39a)$$

$$n_k=S+S_k^z, \quad (39b)$$

the Hamiltonian (11) becomes

$$H=H_0+H_1, \quad (40)$$

where

$$H_0=E_0+2zJS\sum_{j=1}^{N}m_j+2zJR\sum_{k=1}^{N}n_k, \quad (41a)$$

$$H_1=\sum_{\langle jk\rangle}[J'(R_j^+S_j^-+R_j^-S_k^+)-2Jm_jn_k]. \quad (41b)$$

This separation of the Hamiltonian is identical with the separation expressed by Eqs. (18) and (19).

Since the separation of the Hamiltonian is the same in (18) as in (40), the results of the calculation of $S_\alpha|0\rangle$ by use of either Eqs. (19) or Eqs. (41) will eventually reduce, order for order, to identical forms; thus, the same final separation of $S_\alpha|0\rangle$ into linked and unlinked terms will be obtained regardless of the operators used in the calculation. It is easier to perform the explicit calculation of $S_\alpha|0\rangle$ using Eqs. (41) since the Hamiltonian is expressed in terms of a smaller number of operators than when the Bose operators are used; thus, fewer operations are required to obtain a given order of $S_\alpha|0\rangle$. The only purpose in introducing the auxiliary Bose operators was to prove the validity of the linked-spin-cluster expansion; at the present time, the author knows no way to prove the validity of the linked-spin-cluster expansion using the Hamiltonian as expressed in Eqs. (41).

After expressing $S_\alpha|0\rangle$ in a slightly different form than (6), the explicit calculation of this quantity may be performed, giving a method whereby the ground-state energy of our antiferromagnetic model may be calculated to any desired degree of precision. From (6) it is seen that

$$S_\alpha|0\rangle=\Big\{1+\sum_{n=1}^{\infty}(i\hbar)^{-n}\int_{\infty}^{0}dt_n\int_{-\infty}^{0}dt_{n-1}\cdots\int_{-\infty}^{0}dt_1\times\exp[i(H_0-E_0)t_n/\hbar+n\alpha t_n]H_1\times\exp[i(H_0-E_0)t_{n-1}/\hbar+(n-1)\alpha t_{n-1}]H_1\times\cdots\exp[i(H_0-E_0)t_1/\hbar+\alpha t_1]H_1\Big\}|0\rangle. \quad (42)$$

Thus, from (42), it is seen that given $S_\alpha{}^{(n-1)}|0\rangle$, $S_\alpha{}^{(n)}|0\rangle$

is obtained from

$$S_\alpha^{(n)}|0\rangle = (i\hbar)^{-1}\int_{-\infty}^{0} dt_n \exp[i(H_0-E_0)t_n/\hbar+n\alpha t_n] \times \sum_{\langle n\rangle}[J'(R_{j_n}{}^+S_{k_n}{}^- + R_{j_n}{}^-S_{k_n}{}^+) - 2Jm_{j_n}n_{k_n}] \times S_\alpha^{(n-1)}|0\rangle. \quad (43)$$

As remarked earlier, in the application of (38) to the calculation of the ground-state energy, only linked ground-state terms need be considered. It is seen from (43) that a linked ground-state term in nth order will never generate a linked ground-state term in any higher order. Also, it is obvious from (42) that an nth-order linked ground-state term will contain a factor $(1/n\beta)$ and β will occur elsewhere in this term in energy denominators of the form $(c\epsilon-d\beta)$ with $c\neq 0$. For the application of (38), it is possible to insert a factor λ (which is to be set equal to unity later) in the perturbing Hamiltonian (41b); then an nth order linked term would contain a factor $(\lambda)^n$. Thus, the energy correction due to an nth-order linked ground-state term may be schematically written

$$\{\lim_{\alpha\to+0} \beta\lambda\partial/\partial\lambda[(\lambda)^n(1/n\beta)m]\}_{\lambda=1},$$

where m contains all other factors of this linked term, including a summation over n pair indices. Performing the differentiation and taking the limit gives $(\lambda)^nM \to M$ for $\lambda=1$, where $M=\lim_{\alpha\to+0} m$, which exists since m contains β (i.e., α) only in energy denominators. Since the summation contained in M is over Kronecker deltas which serve to link all the n pair indices of the sum, the sum will be proportional to N. It is thus seen that the energy correction due to a single linked ground-state term is proportional to N; hence, the total energy correction due to the interaction (41b) will be proportional to N as desired.

If an nth-order term contributes M to the energy correction, there exists an $(n+i)$th term which contributes $(2J/\epsilon)^iM$. The occurrence of these terms is due to the $-2J\sum_{\langle jk\rangle} m_jn_k$ term of H, but by no means is this the only effect of the $-2J\sum_{\langle jk\rangle} m_jn_k$ term. It is seen from (43) that for a linked ground-state term to occur in nth order, a term of the form $\sum_{\langle 1,\cdots,n-1\rangle} D(1,2,\cdots,n-1) \times R_{j_a}{}^-S_{k_b}{}^+|0\rangle$ must occur in the $(n-1)$th order. The quantity $D(1,2,\cdots,n-1)$ is to represent schematically a product of Kronecker deltas which are linked together, while j_a could be any of the $(n-1)$ **j** indices and k_b any of the $(n-1)$ **k** indices. Then, both the terms

$$\sim[(4RS)/(n\beta)]\sum_{\langle 1,\cdots,n\rangle} D(1,2,\cdots,n-1) \times \delta_j(n,a)\delta_k(n,b)|0\rangle$$

and

$$\sim(2J)(\epsilon-n\beta)^{-1}\sum_{\langle 1,\cdots,n\rangle} D(1,2,\cdots,n-1) \times \delta_j(n,a)\delta_k(n,b)R_{j_n}{}^-S_{k_n}{}^+|0\rangle$$

occur in nth order. If the former term contributes M to the energy correction, it is seen from (43) and (38) that the latter term will generate a term in $(n+1)$th order which will contribute $(2J/\epsilon)M$. Iteration of this process shows that a term occurs in $(n+i)$th order which contributes $(2J/\epsilon)^iM$ to the energy correction. The occurrence of such terms enables a partial summation of the perturbation series for the energy to be performed since $\sum_{i=0}^{\infty}(2J/\epsilon)^iM = M\epsilon(\epsilon-2J)^{-1}$.

The energy correction due to all the linked ground-state terms of nth order, *plus* the summation of terms of the form $(2J/\epsilon)^iM$ in all higher orders, will be denoted by E_n. The E_n have been calculated through E_7 in the manner indicated by (43); they are

TABLE I. Values of the lattice sums defined by Eqs. (45).

Lattice	A	B	C
Linear chain	3	10	5
Plane square	9	100	25
Simple cubic	15	310	53
Body-centered	27	1000	125

$$E_2 = -J^2(1-a)^2z(4RS)(\epsilon-2J)^{-1}N, \quad (44a)$$

$$E_3 = 0, \quad (44b)$$

$$E_4 = J^4(1-a)^4z(4RS)N[\epsilon^2(\epsilon-2J)]^{-1}[4z(R+S)-A(4RS)-2], \quad (44c)$$

$$E_5 = 2J^5(1-a)^4z(4RS)N[\epsilon^3(\epsilon-2J)]^{-1}[12z(R+S)-3A(4RS)-z^2(4RS)-6], \quad (44d)$$

$$E_6 = 2J^6(1-a)^4z(4RS)N[\epsilon^4(\epsilon-2J)]^{-1}[56z(R+S)-7z^2(4RS)-15A(4RS)-28]+2J^6(1-a)^6z(4RS)N \times[\epsilon^4(\epsilon-2J)]^{-1}[10zA(4RS)(R+S)+26z(R+S)-20z^2(R+S)^2-B(4RS)^2-8A(4RS)-8], \quad (44e)$$

$$E_7 = 2J^7(1-a)^4z(4RS)N[\epsilon^5(\epsilon-2J)]^{-1}[240z(R+S)-33z^2(4RS)-120-71A(4RS)]+4J^7(1-a)^6z(4RS)N \times[\epsilon^5(\epsilon-2J)]^{-1}[174z(R+S)+66zA(4RS)(R+S)+4C(4RS)(R+S)+12z^3(4RS)(R+S) -140z^2(R+S)^2-2A^2(4RS)^2-3z^2A(4RS)^2-5B(4RS)^2-58A(4RS)-52]. \quad (44f)$$

TABLE II. Values for the C_i of Eq. (46) as functions of the lattice and the magnitude of the spin.

$R=S=$	$\frac{1}{2}$	1	$\frac{3}{2}$	2	$\frac{5}{2}$
Lattice			C_1		
Chain	1.0000	0.3333	0.2000	0.1429	0.1111
Plane	0.3333	0.1429	0.0909	0.0667	0.0526
sc	0.2000	0.0909	0.0588	0.0435	0.0345
bcc	0.1429	0.0667	0.0435	0.0323	0.0256
Lattice			C_2		
Chain	−0.4590	0.0292	0.0284	0.0226	0.0184
Plane	−0.0098	0.0123	0.0098	0.0078	0.0065
sc	−0.0015	0.0054	0.0045	0.0037	0.0031
bcc	0.0047	0.0050	0.0037	0.0029	0.0024
Lattice			C_3		
Chain	0.1953	−0.0058	0.0003	0.0031	0.0034
Plane	0.0046	0.0011	0.0020	0.0020	0.0018
sc	0.0011	0.0009	0.0010	0.0009	0.0008
bcc	0.0006	0.0010	0.0009	0.0008	0.0006

In Eqs. (44), z is the number of nearest neighbors, while A, B, and C are lattice sums defined by

$$A=(Nz)^{-1}\sum_{\langle 1,\cdots,4\rangle}\delta_j(2,3)\delta_k(3,1)\delta_j(1,4)\delta_k(4,2), \tag{45a}$$

$$B=(Nz)^{-1}\sum_{\langle 1,\cdots,6\rangle}\delta_j(2,3)\delta_k(3,1)\delta_j(1,5)\delta_k(5,4)\times\delta_j(4,6)\delta_k(6,2), \tag{45b}$$

$$C=(Nz)^{-1}\sum_{\langle 1,\cdots,7\rangle}\delta_j(6,4)\delta_k(4,5)\delta_j(5,3)\delta_k(3,6)\times\delta_j(6,2)\delta_k(2,1)\delta_j(1,5)\Delta(2,7). \tag{45c}$$

Explicit evaluation of A, B, and C for the lattices of interest gives Table I.

The ground-state energy of the antiferromagnetic spin system is written

$$E=-2zJNRS[1+C_1(1-a)^2+C_2(1-a)^4+C_3(1-a)^6+\cdots]. \tag{46}$$

The C_i have been evaluated, using Eqs. (44) and Table I, for the lattices of interest and values of $R=S=\frac{1}{2}$, 1, $\frac{3}{2}$, 2, $\frac{5}{2}$; the results of this evaluation are given in Table II. The C_1 listed in Table II are exact, while the C_2 and C_3 are approximate, having been only evaluated through E_7 of Eqs. (44).

TABLE III. Ground-state energy (in units of $-JNz/2$) of the spin one-half antiferromagnetic system as a function of the anisotropy and lattice.

	Linear chain				
a	Orbach's exact	Present work	square	sc	bcc
0	(1.7726)[a]	1.7363	1.3281	1.1997	1.1481
0.1	1.6555	1.6127	1.2660	1.1616	1.1191
0.2	1.5411	1.5032	1.2105	1.1277	1.0934
0.3	1.4311	1.4028	1.1615	1.0978	1.0712
0.4	1.3279	1.3096	1.1189	1.0719	1.0521
0.5	1.2344	1.2244	1.0828	1.0499	1.0360
0.6	1.1536	1.1419	1.0531	1.0320	1.0230
0.7	1.0880	1.0864	1.0299	1.0180	1.0129
0.8	1.0396	1.0393	1.0133	1.0080	1.0057
0.9	1.0100	1.0100	1.0033	1.0020	1.0014
1.0	1.0000	1.0000	1.0000	1.0000	1.0000

[a] The exact value for the energy of the linear chain when $a=0$ has been given by L. Hulthén, Arkiv Mat. Astron. Fysik **26A**, No. 1 (1938).

For the special case of $R=S=\frac{1}{2}$, the ground-state energy as a function of the anisotropy has been calculated; the results of this calculation are given in Table III. Orbach's exact results for the linear chain have also been included in Table III for comparison with the present work. Our results for 2- and 3-dimensional spin one-half systems are compared with those of other investigators in Table IV.

VII. LONG- AND SHORT-RANGE ORDER

The long-range order parameter is defined as the absolute value of the difference between the two sublattice magnetizations, normalizing to unity for perfect order. That is, the long-range order parameter is defined as the absolute value of the expectation value of

$$\xi=\tfrac{1}{2}[(NR)^{-1}\sum_{j=1}^{N}R_j^z-(NS)^{-1}\sum_{k=1}^{N}S_k^z]. \tag{47}$$

This is, or is equivalent to, the long-range order parameter used by most other investigators. The short-range order parameter is defined as the expectation value of

$$\eta=(RSNz)^{-1}\sum_{\langle jk\rangle}R_j^zS_k^z. \tag{48}$$

For perfect antiferromagnetic order, $\bar{\eta}=-1$.

TABLE IV. Comparison of the present work with the work of other investigators for spins of magnitude one-half coupled by isotropic exchange.

	$-2E/NJz$ obtained by				
Lattice	Present work	Marshall	Taketa and Nakamura	Kubo	Anderson
Square	1.328	1.312	1.282	1.294	1.316
sc	1.200	1.203	1.181	···	1.194
bcc	1.148	1.157	1.133	1.138	···

Perturbation series for the long- and short-range order are easily obtained by using Feynman's theorem.[8] This theorem states that, for bound systems, if $H=H(\lambda_1,\lambda_2,\cdots)$, where the λ_i are parameters, then the expectation value of $\partial H/\partial\lambda_i$ in a given eigenstate is equal to $\partial E/\partial\lambda_i$, E being the energy eigenvalue of the state.

Since $R=S$, ξ is rewritten as

$$\xi=1-(2RN)^{-1}[\sum_{j=1}^{N}m_j+\sum_{k=1}^{N}n_k]. \tag{49}$$

The H_0 of Eq. (41a) can be replaced by

$$H_0=E_0+2JSz\lambda_1[\sum_{j=1}^{N}m_j+\sum_{k=1}^{N}n_k]. \tag{50}$$

Then, using Feynman's theorem, the long-range order

of the ground state is

$$|\bar{\xi}| = 1-(4RSJzN)^{-1}(\partial E/\partial\lambda_1)_{\lambda_1=1}, \quad (51)$$

with E being given by Eqs. (44) after suitable modifications are made in connection with the modification of the Hamiltonian as expressed by (50). It is easily seen that the only modification of Eqs. (44) is, in general, a change of the factor $[\epsilon^{n-2}(\epsilon-2J)]^{-1}$ in E_n to $[(\lambda_1\epsilon)^{n-2}(\lambda_1\epsilon-2J)]^{-1}$. Similarly, the short-range order of the ground state, by Feynman's theorem, is

$$\bar{\eta} = (2JRSNz)^{-1}[E+(1-a)\partial E/\partial a]. \quad (52)$$

The long-range order has been calculated using (51); the result of this calculation is

$$|\bar{\xi}| = 1-[D_1(1-a)^2+D_2(1-a)^4 + D_3(1-a)^6+\cdots], \quad (53)$$

where the D_i, through E_7, are given in Table V as functions of the magnitude of the spin for the lattices

TABLE V. Values for the D_i of Eq. (53) as functions of the lattice and the magnitude of the spin.

$R=S=$	$\frac{1}{2}$	1	$\frac{3}{2}$	2	$\frac{5}{2}$
Lattice		D_1			
Chain	1.0000	0.2222	0.1200	0.0816	0.0617
Plane	0.2222	0.0816	0.0496	0.0356	0.0277
sc	0.1200	0.0496	0.0311	0.0227	0.0178
bcc	0.0816	0.0356	0.0227	0.0166	0.0131
Lattice		D_2			
Chain	−1.1260	0.0873	0.0623	0.0443	0.0340
Plane	0.0026	0.0259	0.0180	0.0135	0.0108
sc	0.0049	0.0103	0.0078	0.0061	0.0050
bcc	0.0120	0.0089	0.0062	0.0047	0.0038
Lattice		D_3			
Chain	0.6445	−0.0183	0.0010	0.0090	0.0050
Plane	0.0115	0.0030	0.0056	0.0054	0.0051
sc	0.0026	0.0025	0.0026	0.0024	0.0021
bcc	0.0014	0.0028	0.0024	0.0020	0.0017

of interest. For the special case of spins one-half, the long-range order as a function of the anisotropy is plotted in Fig. 1 which also includes Kasteleijn's[2] results for the long-range order of the linear chain. From Eqs. (44) and (52), the short-range order of the ground state is

$$\bar{\eta} = -1+C_1(1-a)^2+3C_2(1-a)^4 + 5C_3(1-a)^6+\cdots, \quad (54)$$

where the C_i are given by Table II. The short-range order as a function of the anisotropy, for spins of magnitude one-half, is plotted in Fig. 2. It is to be emphasized that the curves of Figs. 1 and 2 have been drawn using calculations through E_7 only; this point is exceedingly important for the case of the linear chain.

VIII. DISCUSSION OF THE RESULTS

In this paper, we have applied a linked-cluster method to obtain a perturbation series for the ground-state energy of the antiferromagnetic spin systems specified by the Hamiltonian (1). From the perturbation series for the energy, perturbation series for the long- and short-range order have been obtained by using Feynman's theorem. Given one of these perturbation series, one would like to know limits on the error introduced by using only a finite number of its terms to calculate the desired physical property. Unfortunately, the present work does not answer such a question and it is necessary, at present, to revert to approximate arguments based on the relative magnitude of the various terms in the perturbation expansion. For such arguments it is necessary to list the contributions of E_7 to the energy, long-, and short-range order; such contributions, for spin one-half systems, are given in

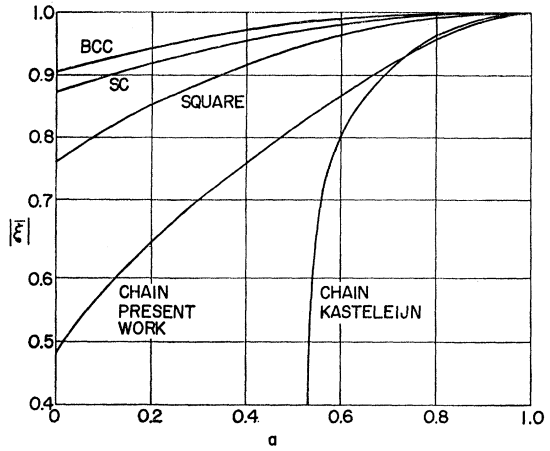

FIG. 1. The long-range order as a function of anisotropy and lattice for spin one-half systems. The curves marked "bcc," "sc," "square," and "chain present work" have been drawn using Eq. (53) through seventh order in the perturbation calculation. Kasteleijn's result for the linear chain is plotted for comparison; his curve drops to zero at $a=0.517$.

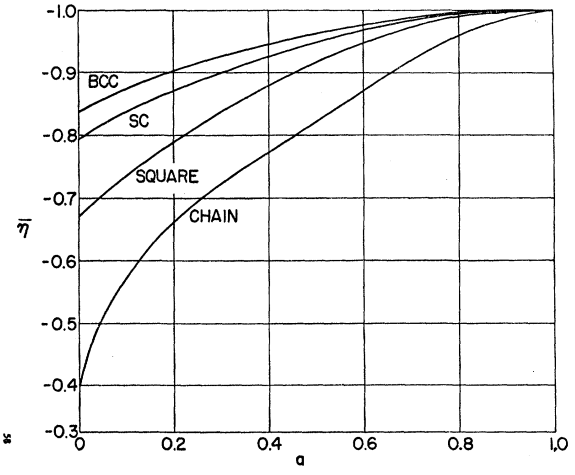

FIG. 2. The short-range order as a function of anisotropy and lattice for spin one-half systems. These curves have been drawn using Eq. (54) through seventh order in the perturbation calculation.

TABLE VI. The seventh-order corrections to the energy, long- and short-range order for spin one-half systems.

a	Chain	Square	sc	bcc
		$-2E_7/JNz$		
0	0.0879	0.0054	0.0007	0.0006
0.2	0.0187	0.0024	0.0004	0.0002
0.4	0.0017	0.0008	0.0002	0.0001
0.6	−0.0003	0.0002	···	···
0.8	···	···	···	···
Long-range order correction $= -(E_7/JNz)[(6z-5)/(z-1)]$				
0	0.3076	0.0169	0.0021	0.0017
0.2	0.0655	0.0075	0.0012	0.0007
0.4	0.0058	0.0025	0.0005	0.0002
0.6	−0.0009	0.0005	0.0001	···
0.8	−0.0001	···	···	···
Short-range order correction $= -(2/JNz)[E_7+(1-a)\partial E_7/\partial a]$				
0	0.4980	0.0134	0.0004	0.0016
0.2	0.1176	0.0065	0.0008	0.0007
0.4	0.0159	0.0023	0.0004	0.0002
0.6	0.0002	0.0005	0.0001	···
0.8	−0.0001	···	···	···

Table VI. In all cases, the corresponding quantities for spins of magnitude greater than one-half are less than the quantities given in Table VI.

From Table III, it is seen that our results for the ground-state energy of the linear chain are slightly higher than the exact results, differing by about 2% for $a=0$, 0.8% for $a=0.5$, and thereafter rapidly approaching the exact value as $a \rightarrow 1.0$. However, it should be pointed out that the values given in Table III for the linear chain are all lower than those obtained variationally by Kasteleijn[2] by a larger amount than they differ from the exact values. It appears from Table VI that the rapidity of convergence for the energy perturbation series increases as the number of nearest neighbors increases and/or the anisotropy increases; one would therefore expect the results given in Table III to be much more accurate for the two- and three-dimensional cases than for the one-dimensional case. In fact, as is seen from Table IV, the ground-state energies for two- and three-dimensional lattices calculated by the present method through E_7 lie below those obtained by other workers with the exception of those obtained by Marshall for the cubic lattices. By using the Bethe-Peierls approximation in addition to the variational technique, Marshall may have overshot the true value of the energy for the cubic lattices as he admits is possible in his treatment. It appears doubtful, though possible, from an inspection of Table VI, that Marshall's results for the cubic lattices would lie between the exact value and the value obtained here through E_7.

Our result, through E_7, for the short-range order of the linear chain for $a=0$ differs by about 31% from Orbach's[1] exact result. Such a large deviation could be anticipated from inspection of Table VI. However, for $a>0.2$, the short-range order for the linear chain, obtained here through E_7, does not differ by more than 5% from the exact results. It is to be expected that the curves of Fig. 2 are much more accurate for the two- and three-dimensional spin systems than for the linear chain though, as mentioned earlier, limits on the error have not been obtained.

The most controversial issue on which the present work has a bearing is concerned with the long-range order of the spin system. The results plotted in Fig. 1 are radically different from those obtained variationally by Kasteleijn,[2] Marshall,[6] and Taketa and Nakamura.[7] For example, for $a<0.517$, Kasteleijn predicted zero long-range order for the linear chain of spins one-half, while our method, through E_7, gives 0.81 when $a=0.50$. Similar disagreements exist between the curves of Fig. 1 for two- and three-dimensional lattices and the results of Taketa and Nakamura. Granted, it appears from an inspection of Table VI that the curve of Fig. 1 for the linear chain should not be taken too literally when $a<0.2$, but it also seems that for $a>0.4$ the higher-order terms of the perturbation series should not contribute enough to change the plotted results significantly. It is to be remembered that our method gives a better value for the energy; thus, one should expect the wave function, and hence the long-range order, to be better than the one obtained variationally. Also, for the linear chain in particular, states of very low excitation energy exist which have $|\xi|=0$. Since the variational method discriminates only with respect to the energy, such states will not necessarily be properly weighted by a variational treatment; however, such states only occur in very high orders of our perturbation expansion and thus have exceedingly small coefficients when the ground state is expressed as a linear combination of product functions. Furthermore, it is expected from the results of Table VI that the curves of Fig. 1 for the two- and three-dimensional lattices should be much more accurate than the one for the linear chain.

Though our results for the two- and three-dimensional lattices when $a=0$ are qualitatively the same as those obtained by Anderson[3] and Kubo,[5] the method used to obtain them is completely free of the objections to the spin-wave theory raised by Marshall.[20] Marshall particularly objected to the use of the Holstein-Primakoff[21] formalism in the spin-wave theory, since it introduces large contributions from fictitious states which have no physical existence. An interesting point in the present method is that nonphysical intermediate states do contribute to the energy perturbation series in the same way that Goldstone[13] has shown that nonphysical intermediate states which violate the Pauli exclusion principle occur in the perturbation expansion

[20] W. Marshall, Proc. Roy. Soc. (London) **A232**, 69 (1955).
[21] I. Holstein and H. Primakoff, Phys. Rev. **58**, 1098 (1940).

for the interacting fermion system. In any event, even without the convergence question being settled, the author feels that the present results are at least on a strong a footing as the variational ones. Furthermore, the merit of the present work lies in the method rather than the results for two reasons: (1) It provides a systematic way in which it should be possible to settle the long-range order question by an investigation of the convergence of the perturbation series. (2) The use of linked spin clusters could ultimately lead to a consistent treatment of the collective modes of the antiferromagnetic spin system in a manner similar to Hubbard's[22] treatment of the collective motions of the electron plasma.

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[22] J. Hubbard, Proc. Roy. Soc. (London) **A240**, 539 (1957).

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Dependence of Secondary Electron Emission from MgO Single Crystals on Angle of Incidence

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The influence of the angle of incidence of primary electrons on the energy distribution and total yield of secondary electrons from MgO cleaved single crystals has been studied. Charging effects were minimized by using single pulse techniques. The relative number of low-energy secondary electrons decreases with increasing angles of incidence. The effect appears to be most marked at primary energies in the vicinity of the maximum of the yield curve. At lower and higher primary energies the dependence on angle of incidence diminishes. Under most conditions the total yield increases with increasing angles of incidence. The magnitude of the increase is influenced by the primary electron energy. At low energies a slight decrease in total yield with increasing incidence angles has been observed. A dependence of the backscattered fraction of electrons on the angle of incidence of the primaries has been observed at several primary electron energies.

A number of maxima and minima occur superposed on the gross variation of total yield with angle of incidence. The angular positions of the maxima are insensitive to primary energy but show a dependence on the crystal orientation. Several models for accounting for the phenomena are discussed.

I. INTRODUCTION

A NUMBER of workers have investigated features of the dependence of secondary electron yield of solids on the angle of incidence of the primary electrons.[1,2] The yield is generally found to increase as the angle of incidence is increased. Qualitatively this is explained by the decreased distance to the surface that a secondary, produced at a given point along the path of a primary electron, must traverse in order to escape. Except for the work of Shatas, Marshall, and Pomerantz,[2] who have demonstrated that for very high primary energies and thin targets the yield varies according to the relationship $\delta(\theta)=\delta_0 \sec\theta$, quantitative descriptions have been inadequate due to the inability to treat properly both the processes of production and escape of the internal secondary electrons.

The purpose of this paper is to describe several experiments investigating some additional features of the dependence of secondary electron emission on angle of incidence. First the energy distribution of the emerging low-energy secondary electrons is determined as a function of the incidence angle. Secondly the change in total yield with angle of incidence is determined for insulating single crystals of MgO. Finally an unexpected dependence of the secondary electron yield on the direction of the primary electron beam with respect to certain crystallographic directions is described.[3]

II. EXPERIMENTAL PROCEDURE

The MgO single crystal[4] targets employed in this investigation were cleaved along (100) planes to about

[1] H. Bruining, *Physics and Application of Secondary Electron Emission* (Pergamon Press, Ltd., New York, 1954), p. 100. A. J. Dekker, *Solid-State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, Inc., New York, 1958), p. 297.

[2] R. A. Shatas, J. F. Marshall, and M. A. Pomerantz, Phys. Rev. **102**, 682 (1956).

[3] Preliminary accounts of these experiments were presented at the New York and Ithaca meetings of the American Physical Society, 1958 [A. B. Laponsky and N. R. Whetten, Bull. Am. Phys. Soc. **3**, 46 (1958); **4**, 265 (1958)]. Also see A. B. Laponsky and N. R. Whetten, Phys. Rev. Letters **3**, 510 (1959).

[4] The MgO crystals were obtained from Infra Red Development Company, Welwyn Garden City, Hertfordshire, England.