Linear Antiferromagnetic Chain with Anisotropic Coupling*

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The exact solution is given for a linear chain of N atoms of spin $\frac{1}{2}$ coupled together by the anisotropic Hamiltonian

$$\mathcal{H}=2J\sum_{i=1}^{N}[S_i^zS_{i+1}^z+(1-\alpha)(S_i^xS_{i+1}^x+S_i^yS_{i+1}^y)].$$

The energy of the antiferromagnetic ground state is computed and comparison is made with a variational method. The parameter α is allowed to vary between 0 and 1, regulating the relative amount of Ising anisotropy. The short-range order, $\Sigma_i S_i^zS_{i+1}^z$, is calculated exactly from the variation of the ground-state energy with α. It is shown that a kink in the short-range order curve calculated using the variational method is fictitious, and the associated discontinuity in $\partial^2E/\partial\alpha^2$ is nonexistent. A discussion is given of long-range order and criticisms are presented regarding the predictions of the variational method.

I. INTRODUCTION

THE problem of a linear chain of N spin-$\frac{1}{2}$ atoms coupled together with the Heisenberg exchange interaction is one of the few many-body problems in magnetics which has been solved exactly. The solution has led to fruitful concepts which have been generalized to higher dimensional systems. One such concept was the spin wave originally put forward by Bloch[1] as a solution of the secular equation of Slater.[2] Bloch's solution was only approximate for more than one reversed spin. Bethe[3] calculated the exact interaction between spin waves on a chain for an arbitrary number of reversed spins. Hulthén,[4] using Bethe's solutions, calculated the exact ground-state energy of the antiferromagnetic linear chain ($J>0$). There followed a number of papers by different authors who attempted to generalize the treatment to two and three dimensions.[5]

Hulthén[4] also proposed a variational technique which he applied to the linear chain in order to calculate the short-range order and energy. This procedure was improved upon by Kasteleijn,[6] who solved the problem of the linear chain with both the Heisenberg isotropic interaction and the anisotropic Ising interaction present. Marshall[7] extended the isotropic calculation to two and three dimensions by use of the Bethe-Peierls approximation in addition to the variational technique, and Taketa and Nakamura[8] calculated the ground-state energy of the anisotropic coupled lattice in two and three dimensions.

Kasteleijn[6] found that by increasing the relative amount of Ising interaction, the long-range order remained zero until a critical value. As the anisotropy increased beyond this point, the long-range order rose rapidly to a maximum of perfect order at the Ising limit. Figure 5 shows the variational approach used by Kasteleijn and Marshall gives rise to a discontinuity in the second derivative of the energy E with respect to the parameter α, α being a measure of the amount of Ising interaction present. The discontinuity in $\partial^2E/\partial\alpha^2$ implies a kink in the short-range order at the critical value of α. In our exact treatment, $\partial^2E/\partial\alpha^2$ is continuous and no such effect is found.

The purpose of this investigation is to calculate exactly the solution of the linear chain of N atoms of spin $\frac{1}{2}$ coupled together with a combination of the Heisenberg and Ising interactions; and then, by means of the Feynman[9] theorem, to compute the short-range order exactly. The importance of such a calculation lies in the repeated use of the variational technique in problems of this sort. Our calculation allows comparison of the predictions derived from the variational approach for both the ground-state energy and the short-range order with their exact solution counterparts. From this comparison, a discussion of long-range order is given as well as a criticism of the variational scheme for the computation of such a function.

II. DERIVATION OF THE SECULAR EQUATION

We take the Hamiltonian for N atoms of spin $\frac{1}{2}$ on a ring to be

$$\mathcal{H}=2J\sum_i[S_i^zS_{i+1}^z+(1-\alpha)(S_i^xS_{i+1}^x+S_i^yS_{i+1}^y)], \quad (1)$$

where i goes from 1 to N, S_{N+1} being defined as S_1. For $\alpha=0$, we have the isotropic Heisenberg interaction; for $\alpha=1$, we have the pure Ising interaction. It should be noted that $S^z=\sum_i S_i^z$ commutes with $\mathcal{H}$ and is a good

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quantum number, but $S^2=(\sum_i S_i)^2=\sum_i S_i^2+\sum_{i,j}\mathbf{S}_i\cdot\mathbf{S}_j$ commutes with $\mathcal{H}$ only if $\alpha=0$. For a finite Ising anisotropy, S^2 is no longer a good quantum number. We are able to label our states by the number of up and down spins because there are no matrix elements between states of different values of S^z.

We call the state with $S^z=-NS$ the state with no spins reversed. Denoting the first reversed spin by n_1, the second reversed spin by n_2, etc., our wave function is taken as

$$\Psi=\sum_{n_1\cdots n_r} a_{n_1\cdots n_r}\Phi_{n_1\cdots n_r}, \tag{2}$$

where there are r reversed spins on the chain, and the sum goes over all $\binom{N}{r}$ distributions of r reversed spins among N spins on the chain. Because the reversed spins are identical with one another, their interchange does not affect the problem. Hence, the following order will be taken:

$$n_1<n_2<\cdots n_{r-1}<n_r.$$

$\Phi_{n_1\cdots n_r}$ is the product wave function

$$\beta_1\beta_2\cdots\beta_{n_1-1}\alpha_{n_1}\beta_{n_1+1}\cdots\beta_{n_r-1}\alpha_{n_r}\beta_{n_r+1}\cdots\beta_N,$$

where α_i and β_i are the eigenvectors of S_i^z corresponding to the eigenvalues $+\frac{1}{2}$ and $-\frac{1}{2}$, respectively. We act on Ψ with $\mathcal{H}$ and set $\mathcal{H}\Psi=E\Psi$. We have

$$2J(1/4)(N_{\text{par}}-N_{\text{antipar}})a_{n_1\cdots n_r}+(1-\alpha)J\sum_{n_1'\cdots n_r'}a_{n_1'\cdots n_r'}=Ea_{n_1\cdots n_r}, \tag{3}$$

where the sum goes over all the N_{antipar} arrangements $n_1'\cdots n_r'$ differing from $n_1\cdots n_r$ by the interchange of two neighboring antiparallel spins. N_{par} is the number of neighboring parallel spin pairs and N_{antipar} the number of neighboring antiparallel spin pairs in the function Φ. We rewrite (3) as

$$\sum_{n_1'\cdots n_r'}[(1-\alpha)a_{n_1'\cdots n_r'}-a_{n_1\cdots n_r}]=\frac{E-\frac{1}{2}JN}{J}a_{n_1\cdots n_r}. \tag{4}$$

Defining

$$\frac{E-\frac{1}{2}JN}{J}=-2\epsilon, \tag{5}$$

then

$$2\epsilon a_{n_1\cdots n_r}=\sum_{n_1'\cdots n_r'}[a_{n_1\cdots n_r}-(1-\alpha)a_{n_1'\cdots n_r'}]. \tag{6}$$

If $\alpha=0$, we have the secular equation treated by Bloch.[1]

We impose the condition upon the solutions that the chain be a ring of N atoms such that $S_{N+1}=S_1$, which is equivalent to demanding periodic boundary conditions. It must also make no difference which reversed spin we start with in our counting process. For these reasons,

$$a_{n_1\cdots n_r}=a_{n_2\cdots n_r n_1+N}. \tag{7}$$

III. SOLUTIONS OF THE SECULAR EQUATION FOR ONE AND TWO REVERSED SPINS

In this section we shall examine in detail the case of one and two reversed spins. Our method of approach will generally follow that of Bethe[3] for the isotropic ($\alpha=0$) Hamiltonian. We examine first the solution for one reversed spin. The secular equation (6) becomes

$$2\epsilon a_n=2a_n-(1-\alpha)a_{n-1}-(1-\alpha)a_{n+1}. \tag{8}$$

This equation is satisfied by

$$a_n=e^{ikn}, \tag{9}$$

giving for ϵ the value

$$\epsilon=1-(1-\alpha)\cos k. \tag{10}$$

The periodicity condition (7) gives

$$k=2\pi\lambda/N,\qquad \lambda=0,1,2,\cdots,N-1. \tag{11}$$

The case of two reversed spins is considerably more complicated. If we assume the two reversed spins are not neighboring, the secular equation (6) becomes

$$2\epsilon a_{n_1n_2}=4a_{n_1n_2}-(1-\alpha)a_{n_1+1,n_2}-(1-\alpha)a_{n_1-1,n_2}-(1-\alpha)a_{n_1,n_2+1}-(1-\alpha)a_{n_1,n_2-1}. \tag{12}$$

If we set

$$a_{n_1n_2}=c_1e^{i(k_1n_1+k_2n_2)}+c_2e^{i(k_2n_1+k_1n_2)}, \tag{13}$$

and demand (12) for all n_1 and n_2, we have

$$\epsilon=1-(1-\alpha)\cos k_1+1-(1-\alpha)\cos k_2. \tag{14}$$

We ask for the solution if $n_2=n_1+1$. Our secular equation would have the form:

$$2\epsilon a_{n_1,n+1}=2a_{n_1,n_1+1}-(1-\alpha)a_{n_1-1,n_1+1}-(1-\alpha)a_{n_1,n_1+2}. \tag{15}$$

In order that our first secular equation (12) be valid for all distributions, it is clear that if we set

$$0=2a_{n_1,n_1+1}-(1-\alpha)a_{n_1,n_1}-(1-\alpha)a_{n_1+1,n_1+1}, \tag{16}$$

and add this to our original equation, (12), we shall generate the proper secular equation (15) if the two reversed spins are neighboring. Hence, we may look on (12) as valid for all distributions of spins subject to the subsidiary condition (16). As $S=\frac{1}{2}$, it is clear that a_{n_1,n_1} and a_{n_1+1,n_1+1} make no sense physically. If we continue our definition (13) for $a_{n_1n_2}$ to these cases, we may consider them as defined. We shall see it is condition (16) which correctly treats the interaction between spin waves.[10]

If we set

$$c_1=e^{i\varphi/2};\qquad c_2=e^{-i\varphi/2}; \tag{17}$$

and insert (13) into (16), we get

$$e^{i\varphi/2}[2e^{ik_2}-(1-\alpha)-(1-\alpha)e^{i(k_1+k_2)}]+e^{-i\varphi/2}[2e^{ik_1}-(1-\alpha)-(1-\alpha)e^{i(k_1+k_2)}]=0, \tag{18}$$

[10] This concept was presented by Bethe, reference 3.

or

$$\cot(\varphi/2) = \frac{\sin[(k_1-k_2)/2]}{(1-\alpha)\cos[(k_1+k_2)/2]-\cos[(k_1-k_2)/2]}. \quad (19)$$

If $\alpha=0$, we have Bethe's result:

$$2\cot(\varphi/2)=\cot(k_1/2)-\cot(k_2/2). \quad (20)$$

It should be noted that φ is still an odd function of k_1 and k_2 for $\alpha\neq 0$, as in the case which Bethe treated. However, an important difference between this treatment and Bethe's is that for $k_1=0$ and $k_2=0$, $\cot(\varphi/2)=0$ for $\alpha\neq 0$ whereas $\cot(\varphi/2)$ is indeterminate for $\alpha=0$.

We now require that φ be single-valued:

$$-\pi\leqq\varphi\leqq\pi. \quad (21)$$

The periodicity condition (7) is

$$a_{n_1n_2}=a_{n_2,n_1+N}. \quad (22)$$

We insert (13) and (17) into (22) and give rise to the set of equations:

$$\left.\begin{aligned} Nk_1-\varphi&=2\pi\lambda_1 \quad (23a)\\ Nk_2+\varphi&=2\pi\lambda_2 \quad (23b)\end{aligned}\right\}\ \lambda_1,\lambda_2=0,1,2,\cdots,N-1.$$

Because λ_1 and λ_2 may be interchanged without affecting our solutions, we make the restriction $\lambda_1\leqq\lambda_2$. Our solutions are now completely determined for given λ_1 and λ_2 by the set of Eqs. (19), (23a), and (23b).

We consider the dependence of the wave numbers k_1 and k_2 on λ_1 and λ_2. There exist three categories of solutions to our problem. We define each category as follows:

Category I $\lambda_2-\lambda_1\geqq 2$,
Category II $\lambda_2+\lambda_2=\lambda$, $\lambda_1=\lambda_2$ (λ even),
Category III $\lambda_1+\lambda_2=\lambda$, $\lambda_1=\lambda_2-1$ (λ odd).

Corresponding to Category I we shall find solutions with real wave numbers only. In Category II there exist solely complex solutions for k_1 and k_2, and in Category III there exist complex solutions for k_1 and k_2 for $\mathrm{Re}\,k_2=\mathrm{Re}k_1>k_{\min}(\alpha)$ and real wave numbers for $k_2,k_1<k_{\min}(\alpha)$. We investigate each category separately.

Category I.—Here we have $\lambda_2-\lambda_1\geqq 2$. Given the value λ_2, λ_1 may take on the values:

$$\lambda_1=0,1,2,\cdots,\lambda_2-2. \quad (24)$$

The total number of solutions in Category I are

$$\sum_{\lambda_2=2}^{N-1}(\lambda_2-1)=\binom{N-1}{2}, \quad (25)$$

as in Bethe's solution. All the wave vectors are real, and given λ_1 and λ_2; k_1, k_2, and φ are determined uniquely from (19), (23a, b). The energy and wave function are determined from (13), (14), and (17). We denote the energy eigenvalue of Category I by ϵ_1.

Category II.—Following Bethe, we set $\lambda_1+\lambda_2=\lambda$ and hold λ even. The only allowable values for λ_1 and λ_2 (not already included in Category I) are $\lambda_1=\lambda_2=\lambda/2$. Equations (23a) and (23b) become

$$Nk_1-\varphi=\pi\lambda, \quad (26a)$$

$$Nk_2+\varphi=\pi\lambda. \quad (26b)$$

We look for solutions of the form

$$k_1=u+iv; \quad (27a)$$

$$k_2=u-iv; \quad (27b)$$

$$\varphi=\psi+i\chi. \quad (27c)$$

We find, upon subtraction of (26b) from (26a) and use of (27a, b, c), $\psi=0$; $\chi=Nv$. Then,

$$\cot(\varphi/2)=\cot\left(\frac{\psi+i\chi}{2}\right)=\cot\left(\frac{iNv}{2}\right)$$
$$=i\frac{e^{-Nv}+1}{e^{-Nv}-1}\approx -i(1+2e^{-Nv}), \quad (28)$$

where we have neglected terms of order $(e^{-Nv})^2$ and higher. From (19) and (27a, b), we have

$$\cot(\varphi/2)=\frac{i\sinh v}{(1-\alpha)\cos u-\cosh v}. \quad (29)$$

For a first approximation, we set (28) equal to $-i$. Using (28), (29), and solving for v, we find

$$e^{-v}=(1-\alpha)\cos u. \quad (30)$$

From (14), (27), and (30), we obtain

$$\epsilon_{II}=1-(1-\alpha)^2\cos^2 u. \quad (31)$$

Adding (26a) and (26b) yields $u=\pi\lambda/N$. We define $k=k_1+k_2=2u$ in order to compare ϵ_I with ϵ_{II} for the same value of k. We look for the maximum of ϵ_{II}/ϵ_I. Minimizing ϵ_I by setting

$$\partial\epsilon_I/\partial k_1=(1-\alpha)\sin k_1+(1-\alpha)\sin(k-k_1)=0,$$

we find the solution $k/2=k_1$ and $k/2=k_2$. Then

$$\epsilon_1{}^{\min}=2-2(1-\alpha)\cos(k/2). \quad (32)$$

Setting $u=k/2$ in ϵ_{II}, we find

$$\epsilon_{II}/\epsilon_I{}^{\min}=\frac{1-(1-\alpha)^2\cos^2(k/2)}{2[1-(1-\alpha)\cos(k/2)]}$$
$$=\tfrac{1}{2}[1+(1-\alpha)\cos(k/2)]\leqq 1. \quad (33)$$

We see that $\epsilon_{II}<\epsilon_I{}^{\min}$ for $k\neq 0$ and $\alpha=0$, and $\epsilon_{II}<\epsilon_I{}^{\min}$ for all k if $\alpha\neq 0$. This result is similar to Bethe's except

that the equivalence of $\epsilon_{\mathrm{I}}{}^{\min}$ and ϵ_{II} at $k=0$ is no longer true for $\alpha\neq 0$. From (5), $E=JN/2-2J\epsilon$. If $J<0$ (ferromagnetic case), the lowest lying states are in Category II. If $J>0$ (antiferromagnetic case), the lowest lying states are in Category I. It is precisely this division which makes possible the calculation of the antiferromagnetic ground state.[11]

It is now convenient to examine the form of the wave function in Categories I and II. In Category I, k_1 and k_2 are real and related only by the three conditions (19), (23a), and (23b). The form of the wave function is given by (13) and (17). These eigenstates can be classified as unbound in the same sense as two interacting particles scattering from one another.

In Category II, however, we have $k_1=u+iv$ and $k_2=u-iv$ where u and v are related by (30). From (13), (17), and (27), we obtain

$$a_{n_1n_2}=2e^{iu(n_1+n_2)}\cosh[v(\tfrac{1}{2}N-(n_2-n_1))].$$

If we normalize these states we see that the two reversed spins tend to be localized to nearest neighbor positions. That is, $|a_{n_1n_2}|$ is a maximum for $n_2=n_1+1$ and dies off exponentially as n_2 leaves this value. v is a measure of the width of the complex, and u is a measure of the velocity of motion of the center of gravity of the complex around the chain. The solutions of Category II represent the bound states of the problem.

Category III.—In this category, Eqs. (23a) and (23b) become

$$Nk_1-\varphi=\pi(\lambda-1), \tag{34a}$$

$$Nk_2+\varphi=\pi(\lambda+1), \tag{34b}$$

where we have set $\lambda_1=(\lambda-1)/2$ and $\lambda_2=(\lambda+1)/2$. A solution of this set which satisfies (19) is $k_1=k_2$ and $\varphi=\pi$. This solution destroys the wave function Ψ for, if we set $k_1=k_2=k/2$ and $\varphi=\pi$, then

$$\Psi=\sum_{n_1n_2} e^{(ik/2)(n_1+n_2)}(e^{i\pi/2}+e^{-i\pi/2})\Phi_{n_1n_2}\equiv 0.$$

We look for other types of solutions. We try the complex solutions of Category II. Using (27a, b) and (34a, b) we find $\psi=\pi$ and $\chi=Nv$. Then,

$$\cot(\varphi/2)=\cot(\pi/2+iNv/2)$$
$$=-\tan(iNv/2)\approx -i(1-2\epsilon^{-Nv}), \tag{35}$$

to the same approximation as before. Demanding (19), in the first approximation we have the same relation between u and v as in Category II, *viz.*, (30). To examine the situation more closely, we set $v=v_0+\delta$ where $(1-\alpha)\cos u=e^{-v_0}$ exactly, and solve for δ using (19) and (35). It turns out that δ is very small (on the order of $1/N$) for both Category II and Category III, and $\cdot>0$ for Category II but <0 for Category III. This difference would normally be unimportant because of the relative size of v_0. But v_0 gets smaller as u becomes smaller, as can be seen from (30), and there may exist a point at which $\delta\approx v_0$, in which case, for Category III, $v<0$. Such a situation destroys the entire procedure as our calculation diverges, and no complex solutions exist for k in such a region.

We find the value of k such that v is negative and then state the solutions for such a region. As Bethe has shown, such a region may be found by examining the slope of $Nk_1-\varphi\equiv F$ as a function of k_1. For small k_1, F can decrease with increasing k_1. Such a region is where the solutions of Category III of the complex type fail. We set $k_1+k_2=k$ and hold k fixed. Then,

$$\frac{\partial F}{\partial k_1}=N-\frac{\partial}{\partial k_1}2\operatorname{arc\,cot}\times\left[\frac{\sin[(2k_1-k)/2]}{(1-\alpha)\cos(k/2)-\cos[(2k_1-k)/2]}\right]$$
$$=N=\frac{2}{1-(1-\alpha)\cos(k/2)}, \tag{36}$$

where we have set $k_1=k_2=k/2$ for convenience. Demanding $\partial F/\partial k_1<0$ results in

$$\cos(k/2)\geqq\frac{1}{(1-\alpha)}(1-2/N). \tag{37}$$

We see that the complex solutions of Category III are always valid for $\alpha>2/N$ but are not allowed for $\alpha<2/N$ and k such that (37) holds. We expand the cosine term in (37) and find

$$\frac{k^2}{8}\leqq\frac{(2/N)-\alpha}{1-\alpha} \tag{38}$$

as the condition on k such that the complex solutions are no longer valid. If k satisfies (38) we find, with Bethe, the solutions are of the type

$$k_1=k_0-2f/N;\qquad k_2=k_0+2f/N. \tag{39}$$

From (19), noting k_0 and f/N are small, we obtain

$$\cot(\varphi/2)\approx\frac{2f}{N}\frac{1}{\alpha+(1-\alpha)k_0^2/2}.$$

We find $2\varphi=2\pi-4f$ upon subtraction of (34b) from (34a) so that $\cot(\varphi/2)=\tan f$. Then

$$\frac{\tan f}{f}=\frac{4}{N[2\alpha+(1-\alpha)k_0^2]}. \tag{40}$$

[11] A calculation by E. Ledinegg and P. Urban, Acta Phys. Austriaca 8, 167 (1953), of the susceptibility of a ferromagnetic chain at absolute zero uses solely the solutions of Category I. Although it is true that there are far fewer solutions of the type of Category II than of Category I, in a susceptibility calculation near saturation ($S^z\approx -NS$) it is the statistical distribution of states which is important and not solely the total number. As the states of Group II lie lower than those which they considered, one may question their results.

Noting $k_0=\pi\lambda/N$, we see we have determined k_1 and k_2 as a function of λ.

We now examine the significance of this division of states. We see that the complex solutions of the type of Category II are found in Category III also[12] and part of the states in Category III thereby represent the bound states of the problem. The states given by the condition (38) and the wave vectors (39) arise from the fact that the chain is finite. It must be possible in a finite chain to construct running waves of nearly equal wave numbers so that after a complete revolution of the chain the states are still approximately in phase with each other without necessitating complex wave numbers. This is possible only for a finite chain and such a condition is found in (38), because no nonzero value of k exists which will satisfy (38) in the limit of infinite N. The dependence of these states on the anisotropy α arises from the relative size of the diagonal matrix elements of $\mathfrak{IC}$ with respect to the off diagonal terms. For $\alpha=0$ we may build such states. However, as α increases, the relative size of the off diagonal terms decrease and such states are no longer possible to construct for $\alpha>2/N$. Indeed, in the opposite limit for which $\alpha<0$, these states become much more numerous corresponding to the magnitude of the off diagonal elements increasing relative to the diagonal terms.[13] The number of these states decreases with increasing α as is seen directly in (38).

We count the number of states in Categories II and III and find, exactly as in Bethe's work, that there are $N-1$ such solutions. If these are added to the $\binom{N-1}{1}$ solutions of Category I, we arrive at $\binom{N}{2}$ solutions in solutions in all which is exactly the correct number.

IV. GENERALIZATION TO r REVERSED SPINS

Our previous results go over to the case of r reversed spins in exactly the same manner as in Bethe[3] and Hulthén.[4] Our wave function is

$$\Psi=\sum_{n_1\cdots n_r} a_{n_1\cdots n_r}\Phi_{n_1\cdots n_r}, \tag{2}$$

as before. We assume s-wave numbers different from zero and look for a solution of the form

$$a_{n_1\cdots n_r}=\sum_{P_\mu}\sum_{P}\exp\{i[\sum_{j=1}^{s}k_{P_j}n_{\mu j}+\tfrac{1}{2}\sum_{j<l}\varphi_{P_jP_l}]\}, \tag{41}$$

where $\sum_P$ means the addition of all the $s!$ different permutations of the figures $k_1\cdots k_s$ among themselves. P_j is the number which, after the permutation P, follows in place of j. The sum $\sum_{P_\mu}$ goes over $\binom{r}{s}$ combinations of s figures among the r values $1, 2, \cdots r$. We set $n_{\mu 1}<n_{\mu 2}<\cdots<n_{\mu s}$ as an interchange of any two reversed spins leaves our solution invariant. We insert (41) into the secular equation (6) and find

$$\epsilon=\sum_j[1-(1-\alpha)\cos k_j], \tag{42}$$

as each term in (41) satisfies (6) and so must their sum. We insure our secular equation be valid for neighboring reversed spins by setting

$$0=2a_{n_1\cdots n_x,\ n_x+1,\ \cdots n_r}-(1-\alpha)a_{n_1\cdots n_x,\ n_x\cdots n_r}-(1-\alpha)a_{n_1\cdots n_x+1,\ n_x+1\cdots n_r}. \tag{43}$$

Inserting (41) in (43), we get

$$\cot(\varphi_{jl}/2)=\frac{\sin[(k_j-k_l)/2]}{(1-\alpha)\cos[(k_j+k_l)/2]-\cos[(k_j-k_l)/2]}. \tag{44}$$

The periodicity condition (7) leads to

$$Nk_j=2\pi\lambda_j+\sum_{l(l\neq j)}\varphi_{jl};\quad \lambda_j=0, 1, 2, \cdots, N-1. \tag{45}$$

All of these results follow in the same manner as in Bethe's[3] calculation.

We may now determine the lowest eigenvalue E. We assume for simplicity that N is even and set $r=N/2$ for minimum S^z (i.e., $N/2$ spins reversed). We see that no wave numbers k_i and k_j can be equal as $\varphi_{ij}=\pm\pi$ in such a case and we may factor an $(e^{i\pi/2}+e^{-i\pi/2})$ out of Eq. (41). This occurs for $\alpha\neq 0$ even if $k_i=k_j=0$ so that we must neglect solutions for which $k_i=k_j$ for all values of k_i. For $J>0$, as in Sec. III, the lowest lying state corresponds to the real wave number solutions of Category I.[14] Thus, we hold $\lambda_{j+1}-\lambda_j\geqq 2$. Noting interchange of the λ_j's does not affect the solution we require $\lambda_1<\lambda_2<\lambda_3<\cdots<\lambda_r$ and, from (23), $0\leqq\lambda_j\leqq N-1$. Because $(N/2)\lambda_j$'s exist, as we have $N/2$ reversed spins, we must occupy the points $0, 1, 2, \cdots, N-1$ with $N/2$ objects λ, such that at every point there is at most one object and every two of the objects are separated by at least one unoccupied point. Noting the equivalence of $\lambda=0$ and $\lambda=N$, we may do this in 2 ways, *viz*:

$1, 3, 5, 7, 9, \cdots N-1$ Distribution A,
$0, 2, 4, 6, 8, \cdots N-2$ Distribution B,

where we have labelled the distributions as shown. We rewrite λ_j as

$$\lambda_j=2j-1,\quad j=1, 2, \cdots N/2 \qquad \text{Distribution } A, \tag{46}$$

$$\lambda_j=2j-2, \qquad \text{Distribution } B. \tag{47}$$

[12] Except that $a_{n_1n_2}=2e^{iu(n_1+n_2)}\sinh\{v[\frac{1}{2}N-(n_2-n_1)]\}$ because $\psi=\pi$.

[13] This interesting case was communicated to me by Dr. W. Marshall.

[14] The generalization to the case of r reversed spins follows easily from the form of ϵ_{I} and ϵ_{II}.

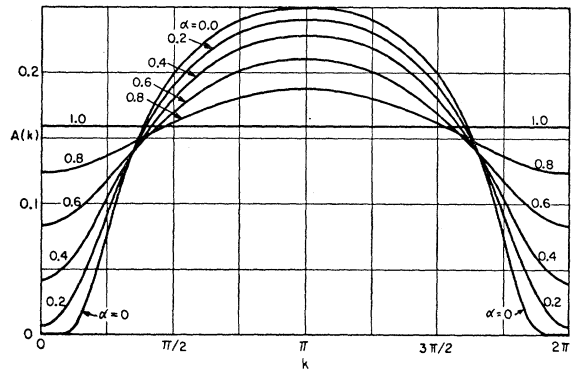

FIG. 1. $A(k)$ as a function of k for representative values of α.

The significance of these distributions arise from the displacement properties of the chain. We displace the chain by one and find our wave function (2) is multiplied by $\exp(i\sum_j k_j)$. This equals, from (45),

$$\exp\left[i\left(\frac{2\pi}{N}\sum_j \lambda_j+\frac{1}{N}\sum_{l\neq j}\varphi_{jl}\right)\right].$$

But $\sum_{l\neq j}\varphi_{jl}=0$ as φ_{jl} is odd upon interchange of j and l. Equation (2) is then multiplied by

$$\exp\left(\frac{2\pi}{i\overline{N}}\sum_j \lambda_j\right)\Bigg\}=(-1)^{N/2} \quad \text{distribution } A,$$
$$\Bigg\}=(-1)^{N/2-1} \quad \text{distribution } B,$$

using (46) and (47). That the lowest lying wave functions should have this property was first proven by Marshall.[7]

From (45) and (42), the larger the λ_j's, the lower the energy, so that we shall calculate the energy of Distribution A.[15] This distribution is the one Hulthén considered.

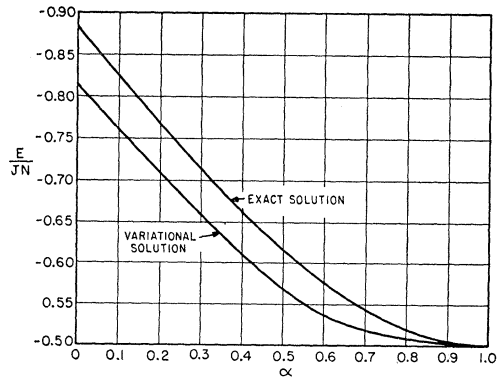

FIG. 2. The reduced energy of the linear antiferromagnetic chain, E/JN, as a function of α for the exact solution and the variational solution.

[15] Though the choice is purely academic. By ignoring terms in $1/N$ in our subsequent integral equation, we are ignoring equivalently the difference between Distribution B and Distribution A.

We pass to the limit (for large N) and introduce for the discrete variable j, the continuous variable x, defined by $j=Nx/2$. We similarly set $l=Ny/2$ and let k_j be written as $k(x)$. φ_{jl} is written as $\varphi[k(x),k(y)]$. We rewrite (45) as

$$k(x)=2\pi x+\tfrac{1}{2}\int_0^1 \varphi[k(x),k(y)]dy, \tag{48}$$

ignoring terms in $1/N$. Equation (42) becomes

$$\epsilon=(N/2)\int_0^1 [1-(1-\alpha)\cos k(x)]dx, \tag{49}$$

and (44) is written

$$\cot\left[\frac{\varphi[k(x),k(y)]}{2}\right]$$
$$=\frac{\sin\{[k(x)-k(y)]/2\}}{(1-\alpha)\cos\{[k(x)+k(y)]/2\}-\cos\{[k(x)-k(y)]/2\}}, \tag{50}$$

where $-\pi\leqq\varphi\leqq\pi$.

We see that a discontinuity exists in $\varphi[k(x),k(y)]$ at $x=y$ as φ jumps between $-\pi$ and $+\pi$. Taking note of this, we differentiate (48) with respect to $k(x)$. After combining terms,

$$1=\pi\frac{dx}{dk}+\tfrac{1}{2}\int_0^1 dk'$$
$$\times\left[\frac{[1-(1-\alpha)\cos k'](dy/dk)_{k=k'}}{1+(1-\alpha)^2\cos^2[(k+k')/2]-(1-\alpha)(\cos k+\cos k')}\right], \tag{51}$$

where we have changed variables in our integrand from y to $k(y)\equiv k'$. Now dx/dk has a simple meaning.[16] If $(N/2)A(k)dk$ is the number of those wave numbers which lie between k and $k+dk$, and $(N/2)dx$ is the number of indices between $(N/2)x$ and $(N/2)(x+dx)$, then because a wave number exists for every index the two expressions may be set equal: $A(k)=dx/dk$. Equation (49) goes into

$$\epsilon=(N/2)\int_0^{2\pi}[1-(1-\alpha)\cos k]A(k)dk, \tag{52}$$

and (51) into

$$A(k)=1/\pi-(1/2\pi)\int_0^{2\pi}dk'$$
$$\times\left[\frac{[1-(1-\alpha)\cos k']A(k')}{1+(1-\alpha)^2\cos^2[(k+k')/2]-(1-\alpha)(\cos k+\cos k')}\right]. \tag{53}$$

[16] This argument was given by Hulthén, reference 4.

We must solve the integral equation (53) for $A(k)$, and then insert $A(k)$ into (52) to compute the ground-state energy.

V. SOLUTION OF THE INTEGRAL EQUATION

It should be noted that Eq. (53) is of the simple inhomogeneous type

$$u(x)=f(x)+\int_a^b K(x,y)u(y)dy,$$

where $f(x)$ and $K(x,y)$ are known and $u(x)$ is to be found. The equation was solved by the author on the IBM 701 by the process of iteration. A first approximation for $A(k)$ was obtained by breaking up the integration into a finite sum of 40 parts, and then rewriting (53) as a series of 40 linear equations and solving the set of equations numerically.[17] This gave the function $A(k)$ at 40 points in the interval 0 to 2π. A first approximation to $A(k)$ was found by connecting the points with straight lines. The approximation was inserted into the integrand of (53), and the process of iteration begun.

TABLE I. Ground-state energy of the linear antiferromagnetic chain.

α	$-E/JN$	α	$-E/JN$	α	$-E/JN$
0.00	0.88629	0.35	0.68924	0.70	0.54399
0.05	0.85688	0.40	0.66396	0.75	0.53076
0.10	0.82774	0.45	0.63989	0.80	0.51980
0.15	0.79894	0.50	0.61722	0.85	0.51119
0.20	0.77056	0.55	0.59614	0.90	0.50499
0.25	0.74272	0.60	0.57681	0.95	0.50125
0.30	0.71556	0.65	0.55938	1.00	0.50000

Convergence was reached on the average after the fourth iteration to an accuracy of eight decimal places. The solutions for $A(k)$ were computed for 19 values of α (resp. 0.05, 0.10, 0.15, $\cdots$ 0.95, 1.00) and representative forms are shown below in Fig. 1.[18] It should be noted that $A(k)$ seems to be a very smoothly varying function of α. The energy was calculated at the 19 points and is plotted in Fig. 2. The exact values of the energy are given in Table I at each of the 19 points (and at $\alpha=0$).[19]

VI. CALCULATION OF THE SHORT-RANGE ORDER

We are able to calculate the expectation value of the short-range order

$$\sum_i S_i^z S_{i+1}^z,$$

if we know ϵ as a function of α, because of the form of the Hamiltonian. This follows because

$$\partial\mathcal{H}/\partial\alpha=-2J\sum_i (S_i^x S_{i+1}^x+S_i^y S_{i+1}^y), \qquad (54)$$

[17] On a suggestion by Dr. W. Marshall.

[18] For $\alpha=0$, we have plotted Hulthén's solution for $A(k)$ for comparison. It should be noted that $A(0)=0$ for $\alpha=0$, but, as soon as α increases from zero, $A(0)$ likewise increases from zero.

[19] Here we have used Hulthén's result for $\alpha=0$.

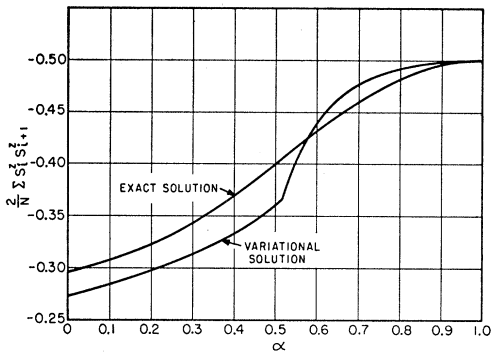

FIG. 3. The short-range order, $\Sigma_i S_i^z S_{i+1}^z$, as a function of α for the exact solution and the variational solution.

which, from the Feynman[9] theorem, has the expectation value $\partial E/\partial\alpha$. We find, using (5),

$$\sum_i S_i^z S_{i+1}^z=N/4-\epsilon-(1-\alpha)\partial\epsilon/\partial\alpha. \qquad (55)$$

This function and

$$\sum_i [S_i^z S_{i+1}^z-\tfrac{1}{2}(S_i^x S_{i+1}^x+S_i^y S_{i+1}^y)],$$

the short-range z directional preference, are plotted *versus* α in Figs. 3 and 4, respectively.

VII. COMPARISON WITH THE VARIATIONAL TECHNIQUE

We may now compare our solutions with a variational calculation performed by Kasteleijn[6] for the same Hamiltonian. As indicated in the introduction and shown in Fig. 5, Kasteleijn's approximate wave function implies a discontinuity in $\partial^2 E/\partial\alpha^2$ as a function of α which results in a sharp corner in the first derivative $\partial E/\partial\alpha$, neither of which is found in the exact solution. The energy of Kasteleijn's solution is compared with the exact energy computed in Sec. V in Fig. 2. The variational short-range order is compared with the exact short-range order in Fig. 3. It should be noted that there is no kink in the exact short-range order curve. The mesh in the exact calculation was 0.05 on the α scale, so it is improbable that such a sharp bend

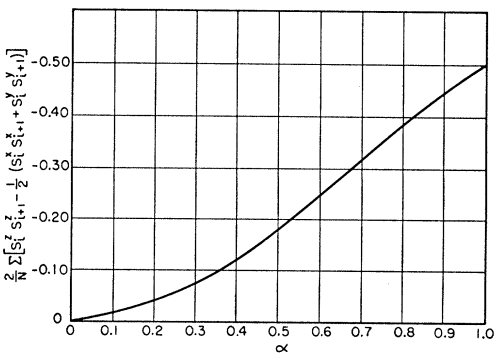

FIG. 4. The short-range z-directional preference, $\Sigma_i[S_i^z S_{i+1}^z-\frac{1}{2}(S_i^x S_{i+1}^x+S_i^y S_{i+1}^y)]$ as a function of α for the exact solution.

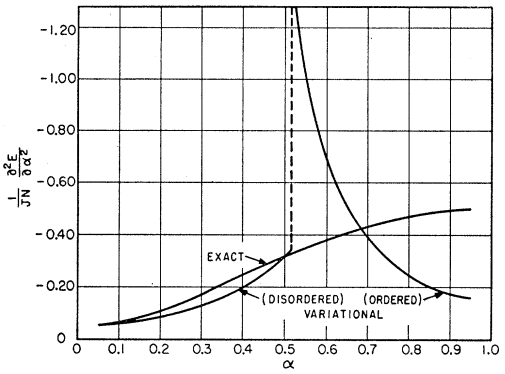

FIG. 5. $\partial^2 E/\partial\alpha^2$ as a function of α for the exact solution and the variational solution.

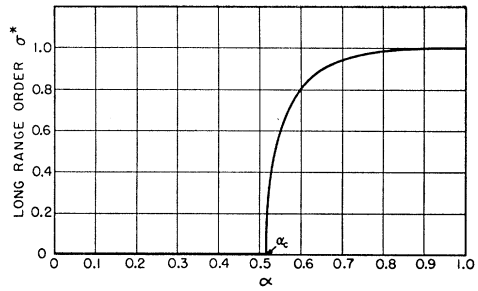

FIG. 6. The long-range order, σ^*, as a function of α for the variational calculation. $\sigma^* = (2/N)|m_1 - m_2|$, where m_1 and m_2 are the number of plus spins in even and odd places, respectively, on the chain.

could have been hidden by the coarseness of the mesh. It appears that the variational scheme used by Kasteleijn gives the approximate form of the short-range order except for the kink which is not present in the exact solution.

VIII. CONCLUSIONS

According to the variational method, the long-range order sets in as shown in Fig. 6 where α_c is at the same point as the kink in the variational short-range ordering curve. The energy expression of Kasteleijn at that point is quite smooth (as is the exact energy). One can say that the energy of the system is relatively insensitive to the long-range order, or, conversely, that the long-range order is a very sensitive function of the energy. If the ground state of a system has a given long-range order, a state lying very close to the ground state may have a very different long-range order. As shown in Fig. 2, the variational calculation results in an incorrect value for the energy of the ground state for all values of $\alpha < 1$. For these reasons, the conclusions reached from the variational treatment with regard to long-range order may be put in some doubt in the region of $\alpha < 1$. The calculation of Kasteleijn implies a sharp kink in the short-range order curve as a function of α and it should be noted that a similar kink exists in the long-range order curve of Fig. 6. The latter kink may also be fictitious, but unfortunately the long-range order cannot be calculated by the exact method utilized in this paper. One certainly cannot say that because the exact short-range order is a smoothly varying function of α, the long-range order should be a smoothly varying function too, but neither can one say the contrary—that there is any sudden discontinuity in the long-range order.

The problem of determining the ground-state long-range order of the linear chain with or without anisotropy ($\alpha < 1$) is an unanswered one in this field. The references in the literature regarding the existence or nonexistence of long-range order have either been "educated guesses" or rely on approximate calculations. The author believes that this paper has shown some of the dangers of such conclusions. Until an exact method is found, as far as the author can see, there is no dependable method as yet to determine the long-range order of the linear antiferromagnetic chain.

IX. ACKNOWLEDGMENTS

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