fluctuations from low-frequency noise measurements. The frequency of the lower limit of the $\frac{3}{2}$ power law is given by Lax as $2L^2/\tau_0^2 D$ which, using the data of Table III results in values of 80, 70 and 17 cps. These are sufficiently far above the lower turnover frequency due to τ_0 to justify the procedure. Unfortunately, the experimental data are not sufficiently extensive in this region to allow an experimental estimate of these frequencies for comparison. However, the spectra are not inconsistent with these values.

VII. ACKNOWLEDGMENT

The author has benefited considerably by the opportunity to discuss much of this work with Robert J. Robinson whose continued enthusiasm is sincerely appreciated.

PHYSICAL REVIEW VOLUME 119, NUMBER 2 JULY 15, 1960

Linear Antiferromagnetic Chain*

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(Received February 16, 1960)

The properties of the low-lying states of the antiferromagnetic chain are studies by means of a variational method. A trial wave function is exhibited which has an energy very close to that of the correct ground state and which displays a long-range order.

I. INTRODUCTION

WE are concerned, in the present work, with a system of N atoms of spin $\frac{1}{2}$ arranged on a line and coupled together by an interaction described by the Hamiltonian operator

$$H=\tfrac{1}{2}J\sum_j(\boldsymbol{\sigma}_j\cdot\boldsymbol{\sigma}_{j+1}-1). \tag{1}$$

The quantity J is the exchange integral and is positive for an antiferromagnetic lattice. The operator $\boldsymbol{\sigma}_j$ is the Pauli spin operator associated with the jth atom in the line. The sum over j extends over all the atoms in the system.

Several authors[1–4] have examined this problem by a method that consists in writing the Hamiltonian (1) in terms of anticommuting operators. The expression (1) can be written in the form

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

where

$$H_0=\sum_k \epsilon(k)\eta^*(k)\eta(k), \tag{3}$$

and

$$H_1=2JN^{-1}\sum_{k_1k_2k_3k_4} v(k_1k_2k_3k_4)\eta^*(k_1)\eta(k_2)\eta^*(k_3)\eta(k_4), \tag{4}$$

with

$$\epsilon(k)=-2J(1-\cos k), \tag{5}$$

and

$$v(k_1k_2k_3k_4)=\exp[i(k_1-k_2)]\bar{\Delta}(k_1-k_2+k_3-k_4). \tag{6}$$

The wave number k takes the values $2\pi n/N$, in which n is an integer and where two wave numbers k and k' differing by an integral multiple of 2π are to be considered identical. The symbol $\bar{\Delta}(k)$ is unity when k is zero or an integral multiple of 2π, and zero otherwise. The operators $\eta^*(k)$ and $\eta(k)$ satisfy the anticommutation relations characteristic of operators representing the creation and destruction of Fermi particles, i.e., we have

$$\{\eta^*(k),\eta^*(k')\}=\{\eta(k),\eta(k')\}=0, \tag{7}$$

and

$$\{\eta^*(k),\eta(k')\}=\bar{\Delta}(k-k'). \tag{8}$$

The operator (2) has been discussed in more detail elsewhere.[4] It will be sufficient here to remark that, as the ground state is a singlet,[5] we need only consider states in which there are $N/2$ Fermi particles present. This is immediately understood by looking at the identity

$$\sum_k \eta^*(k)\eta(k)=\tfrac{1}{2}N+\tfrac{1}{2}\sum_j \sigma_j^{(z)}. \tag{9}$$

The ground-state energy of (1) has been calculated exactly by Hulthén[6] using a method invented by Bethe.[7] Approximations to the ground-state wave function, using the variational principle have been given by

* Supported in part by the U. S. Atomic Energy Commission.
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several authors.[8] These states are constructed in order to ascertain whether or not there is a long-range order in the low-lying states of the antiferromagnetic chain. Of particular interest to us is the work of Kasteleijn.[8] He constructed a wave function for which the expectation value of

$$H_\alpha=\tfrac{1}{2}J\sum_j[\sigma_j^{(z)}\sigma_{j+1}^{(z)}-1]+\tfrac{1}{2}J(1-\alpha)\sum_j[\sigma_j^{(x)}\sigma_{j+1}^{(x)}+\sigma_j^{(y)}\sigma_{j+1}^{(y)}], \quad (10)$$

is rather low for all values of α in the range $0\leqslant\alpha\leqslant 1$. Here α is an anisotropy parameter. When $\alpha=0$, H_α reduces to (1). The axes x, y, and z are three orthogonal directions. Examination of Kasteleijn's state reveals that the long-range order is zero for α less than a critical value α_0 and then increases rapidly beyond this value. Also, it is found that there is a discontinuity in the derivative of the short-range order with respect to the anisotropy parameter. Orbach[9] re-examined the work of Kasteleijn and showed that the latter behavior is spurious, thereby casting doubt on the validity of Kasteleijn's conclusion in regard to the behavior of the long-range order.

The purpose of this paper is to exhibit a trial wave function for (1) for which the energy is very close to the correct ground state. It will be proved that this state displays a long-range order suggesting (in contradiction to Kasteleijn's work) that the ground state probably is an ordered state.

II. THE WAVE FUNCTION

In this section we shall construct, by a variational procedure, a low-lying wave function for the operator (2). In order to do this we introduce new creation and destruction operators as follows:

$$\xi^*(k)=\cos[\tfrac{1}{2}\phi(k)]\eta^*(k)+\sin[\tfrac{1}{2}\phi(k)]\eta^*(k+\pi), \quad (11)$$

where $\phi(k)$ is a real function of k satisfying the condition

$$\phi(k+\pi)=-\phi(k). \quad (12)$$

From (11), (12), (7), and (8) it follows that the operators $\xi^*(k)$ and $\xi(k)$ also satisfy anticommutation relations. The function $\phi(k)$ will remain arbitrary subject to the constraint (12). The transformation (11) is analogous to the transition from plane wave states to Bloch waves in the electron theory of metals. If $\phi(k)\equiv 0$, $\xi^*(k)$ and $\eta^*(k)$ are identical. Equation (11) can be inverted to give

$$\eta^*(k)=\cos[\tfrac{1}{2}\phi(k)]\xi^*(k)-\sin[\tfrac{1}{2}\phi(k)]\xi^*(k+\pi). \quad (13)$$

We now construct our trial wave function

$$\varphi(\phi)=\prod_m\xi^*(m)|0\rangle. \quad (14)$$

Here m takes all the values of the wave vector k in the interval $\pi/2<m<3\pi/2$ and $|0>$ is the vacuum state [i.e., the state for which $\eta^*(k)\eta(k)|0\rangle=0$ for all k]. The reason for the choice of interval given above is that the state (14) gives the lowest unperturbed energy H_0. The expectation value of H for this state is obtained after some tedious but straightforward computation. The result is

$$E(\phi)=\langle\varphi(\phi)|H|\varphi(\phi)\rangle=-NJ\left[\frac{1}{2}+\frac{2}{\pi}p_N(\phi)+\frac{2}{\pi^2}q_N^2(\phi)+\frac{2}{\pi^2}p_N^2(\phi)\right], \quad (15)$$

with

$$p_N(\phi)=-\pi N^{-1}\sum_m\cos m\cos\phi(m), \quad (16)$$

and

$$q_N(\phi)=\pi N^{-1}\sum_m\sin\phi(m). \quad (17)$$

If we let N approach infinity

$$p_N(\phi)\to p(\phi)=-\frac{1}{2}\int_{\pi/2}^{3\pi/2}\cos m\cos\phi(m)dm, \quad (18)$$

and

$$q_N(\phi)\to q(\phi)=\frac{1}{2}\int_{\pi/2}^{3\pi/2}\sin\phi(m)dm. \quad (19)$$

If $\phi\equiv 0$, then[3,4]

$$\lim_{N\to\infty}\frac{E(\phi)}{NJ}=-\left(\frac{1}{2}+\frac{2}{\pi}+\frac{2}{\pi^2}\right)=-1.3393. \quad (20)$$

We remember now that $\phi(m)$ is at our disposal. Let us consider an arbitrary variation $\delta\phi(m)$ of $\phi(m)$. The energy $E(\phi)$ will be an extremum for $\phi(m)$ if the corresponding variation δE of E vanishes. This condition leads to the integral equation

$$[\pi+2p(\phi)]\cos m\sin\phi(m)+2q(\phi)\cos\phi(m)=0. \quad (21)$$

The functions $p(\phi)$ and $q(\phi)$ are integrals that depend on ϕ. Equation (21) can be solved if we notice that the solution (in the range $\pi/2<m<3\pi/2$) must be of the form given by the equation

$$\tan\phi(m)=-\beta/\cos m, \quad (22)$$

where β is a constant to be determined later. For this function we have[10]

$$p=\gamma\int_0^{\pi/2}(1-\gamma^2\sin^2\theta)^{-\frac{1}{2}}\cos^2\theta d\theta=\gamma B(\gamma^2), \quad (23)$$

and

$$q=(1-\gamma^2)^{\frac{1}{2}}\int_0^{\pi/2}(1-\gamma^2\sin^2\theta)^{-\frac{1}{2}}d\theta=(1-\gamma^2)^{\frac{1}{2}}K(\gamma^2). \quad (24)$$

The parameter γ is defined by

$$\gamma=(1+\beta^2)^{-\frac{1}{2}}. \quad (25)$$

[8] P. W. Kasteleijn, Physica **18**, 104 (1952), see also references 4, 5, and 6.

[9] R. Orbach, Phys. Rev. **112**, 309 (1958).

[10] For the definition of the functions B, K, and D see E. Jahnke and F. Emde, *Tables of Functions* (Dover Publications, New York, 1945), pp. 73–85.

TABLE I. Expectation value of the energy and order parameters for several trial wave functions.

Wave function	$-E/JN$	ρ	ρ_1
Néel State[a]	1.0000	1	-1
Singlet pairs[a]	1.2500	0	-0.5
Hulthén (first approximation)	1.3156	...	-0.54
$\varphi(0)$	1.3393	0	-0.4052
Hulthén (second approximation)	1.349	...	...
$\varphi(\phi)$ (present work)	1.3646	0.2633	-0.59
Exact solution	1.3863	...	-0.5962

[a] For the definitions of these states see reference 4.

Substitution of (23) and (24) into (21) and (22) yields the following trascendental equation for γ

$$\gamma D(\gamma^2)=\pi/2. \tag{26}$$

Numerical solution of (26) gives $\gamma=0.9505$. The corresponding value of the energy is

$$E(\phi)=-(2NJ/\pi^2)K^2(\gamma^2)=-1.3646NJ. \tag{27}$$

In Table I a summary is given of the results of several calculations. We also give some of the order parameters defined below.

We turn out attention now to the study of the order properties of our trial wave functions. A measure of the order is, for example, the correlation of the z components of the spin of two atoms a distance λ apart. Here the z-direction is the axis of quantization. In principle, one should calculate $\langle \boldsymbol{\sigma}_j \cdot \boldsymbol{\sigma}_{j+\lambda}\rangle$ but this turns out to be extremely difficult. If we define

$$\hat{\rho}_\lambda = N^{-1}\sum_j \sigma_j^{(z)}\sigma_{j+\lambda}^{(z)}, \tag{28}$$

we obtain

$$\begin{aligned}\rho_\lambda(\phi)&=\langle\varphi(\phi)|\hat{\rho}_\lambda|\varphi(\phi)\rangle\\ &=(2/\pi)^2(1-\gamma^2)[K^2(\gamma^2)-H_\lambda^2(\gamma^2)]\\ &\qquad\qquad \text{if } \lambda \text{ is even } (\neq 0)\\ &=-(2/\pi)^2(1-\gamma^2)K^2(\gamma^2)-(\gamma^2/\pi^2)[H_{\lambda-1}(\gamma^2)\\ &\qquad +H_{\lambda+1}(\gamma^2)]^2 \quad \text{if } \lambda \text{ is odd,}\end{aligned} \tag{29}$$

where

$$H_\lambda(\gamma^2)\equiv\int_0^{\pi/2}\frac{\cos\lambda\theta d\theta}{(1-\gamma^2\sin^2\theta)^{\frac{1}{2}}}. \tag{30}$$

Two quantities are of particular interest: the long-range order ρ defined as

$$\rho=\lim_{\lambda\to\infty}\rho_{2\lambda}(\phi), \tag{31}$$

and the short-range order $\rho_1(\lambda=1)$. As $H_{2\lambda}(\gamma^2)$ approaches zero as λ becomes large we have

$$\rho=(2/\pi)^2(1-\gamma^2)K^2(\gamma^2)=0.2633. \tag{32}$$

From (29) we also obtain

$$\rho_1=-0.59. \tag{33}$$

Another order parameter frequently used is the fractional number of spins pointing in the positive direction of quantization on the sublattice formed by atoms in even positions in the chain. Such an order parameter is obtained by forming the expectation value of the operator

$$\hat{f}=N^{-1}\sum_j(1+e^{i\pi j})\sigma_j^{(+)}\sigma_j^{(-)},$$

where

$$\sigma_j^{(\pm)}=\tfrac{1}{2}(\sigma_j^{(x)}\pm i\sigma_j^{(y)}). \tag{34}$$

For the state $\varphi(\phi)$ we obtain

$$\begin{aligned}f(\phi)&=\langle\varphi(\phi)|\hat{f}|\varphi(\phi)\rangle=\tfrac{1}{2}+\pi^{-1}(1-\gamma^2)^{\frac{1}{2}}K(\gamma^2)\\ &=0.7566.\end{aligned} \tag{35}$$

In the opinion of the authors, the value of $f(\phi)$ is not as faithful a measure of order as ρ. In fact, associated with $\varphi(\phi)$ there is a state vector $\varphi(-\phi)$ which gives the same expectation value of the energy of the system. Physically $\varphi(-\phi)$ is obtained from $\varphi(\phi)$ by reversing all the spins of the system in all terms constituting $\varphi(\phi)$. One can easily show that the states $\varphi(\phi)$ and $\varphi(-\phi)$ are asymptotically orthogonal, i.e., that their inner product becomes vanishingly small as N approaches infinity. Each of the state vectors

$$\psi_\pm=2^{-\frac{1}{2}}[\varphi(\phi)\pm\varphi(-\phi)] \tag{36}$$

has an expectation value of the energy $E(\psi_\pm)=E(\phi)$. For the states $\psi_\pm$ the expectation value of f is $\frac{1}{2}$, i.e., there are $N/4$ spins pointing in the upward direction in the even sublattice. It is interesting to observe that low-lying states exist for which the net magnetization of the sublattices formed by atoms in even and odd positions are nonvanishing. These considerations are enough to show that the results of Kasteleijn[8] are spurious. Incidentally, it is a very simple matter to prove that for the true ground state the expectation value of $\hat{f}$ is also $\frac{1}{2}$. In fact, the ground state can be written as a linear combination of states $|\mu\rangle$ in which each atom is in an eigenvector state of the operator $\sigma_j^{(z)}$ (the z-direction is the arbitrary direction of quantization). Only such states $|\mu\rangle$ for which the total spin in the z direction vanishes will appear with non-zero coefficients in the expression of the correct ground state. Reversal of all the spins of the system will reproduce the ground-state wave function except perhaps for a constant factor of absolute value unity. Thus the states $|\mu\rangle$ and $|\bar{\mu}\rangle$ each of which is obtained from the other by flipping all the spins have the same probability amplitude in the expansion of the ground-state wave function. Thus, it becomes obvious that, for the true ground state of the antiferromagnetic lattice $f=\frac{1}{2}$. However, if the system is known to be in a state such as $\varphi(\phi)$ at time $t=0$ it will take a time of the order of years before it will be in the state $\varphi(-\phi)$.[11] Then, if the system is in $\varphi(\phi)$ at time $t=0$ it will display a net magnetization in each of the two sublattices (formed by atoms in even and odd positions) during a rather long period of time. Nevertheless, we prefer ρ as a

[11] P. W. Anderson, Phys. Rev. **86**, 694 (1952).

measure of the long range as the operation of reversing all the spins of a state leaves ρ unchanged. There is another more important reason for this choice. The idea of ordering of an antiferromagnetic lattice arises mainly from the results of neutron diffraction experiments. In neutron diffraction one can show that the system will display a superlattice structure if its low-lying states have nonzero components of the tensor[12]

$$N^{-1}\sum_j \langle \sigma_j(0)\sigma_{j+\lambda}(t)\rangle, \tag{37}$$

which change sign as λ changes from even to odd values. Here $\sigma_j(t)$ is the Heisenberg operator defined as follows

$$\sigma_j(t)=\exp(itH/\hbar)\sigma_j \exp(-itH/\hbar), \tag{38}$$

and t is the time. The parameter ρ is one of the components of (37) for $t=0$.

We conclude this work with two remarks. Firstly, the transformation (11) is equivalent to introducing new one-particle wave functions for the solution of the many electron problem. It is, in this sense similar to the Hartree-Fock approximation where the best one-particle wave functions are obtained by an iteration procedure. The new states have an implicit periodicity which is twice that of the real system. From the physical point of view this periodicity is obtained if the sublattices of even and odd positions have net (opposite) magnetizations. This was also obtained by a semiphenomenological theory which led to the present work. We expect, as in the theory of metals, that this periodicity will produce a gap in the energy spectrum of the antiferromagnet and such behavior is, in fact, obtained in the present theory. The expectation value of the energy of the state

$$\xi^*(\pi/2-\epsilon)\xi(\pi/2+\epsilon)\varphi(\phi)$$

was calculated in the limit $\epsilon=+0$. A comparison with the energy of the ground state (27) gives the numerical value $\Delta E=2.07J$ for the energy gap. This should not be regarded as a proof that a gap in the spectrum of the antiferromagnetic lattice exists but rather as an indication that such a behavior is possible. A similar result has been obtained by des Cloizeaux[13] by a different method. Secondly, we remark that a measure of the accuracy of the trial wave function (14) can be obtained by calculating the function $A(k)$ as introduced by Hulthén[6] and Orbach.[9] $\frac{1}{2}NA(k)dk$ is the average number of spin-wave states in the ground state with wave numbers lying in the interval $(k, k+dk)$. For the spin waves one must take the excitations created by the operators $\eta^*(k)$ because the exact ground-state energy [see Eq. (52) in reference 9] is

$$E_0=\frac{1}{2}N\int_0^{2\pi}\epsilon(k)A(k)dk,$$

with $\epsilon(k)$ given by (5). Using (13) and (14) the function $A(k)$ for our trial wave function is

$$A(k)=\pi^{-1}\langle\eta^*(k)\eta(k)\rangle = (2\pi)^{-1}[1-\gamma\cos k(1-\gamma^2\sin^2 k)^{-\frac{1}{2}}]. \tag{39}$$

This function is plotted in Fig. 1 together with the values obtained for the exact ground state,[9] the Néel state ($\gamma=0$) and the state for which $\phi=0$, i.e., $\gamma=1$.

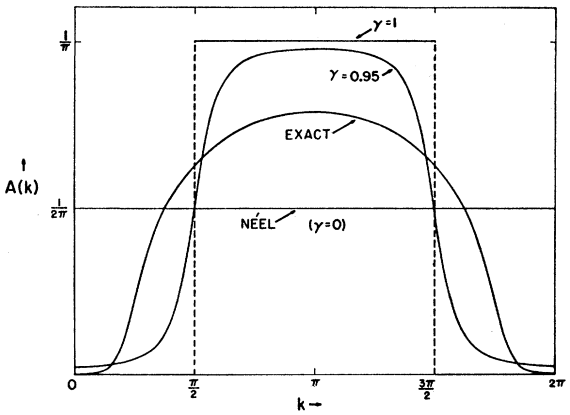

FIG. 1. $A(k)$ as a function of k for several trial wave functions and for the exact solution of the antiferromagnetic chain.

III. ACKNOWLEDGMENTS

One of the authors (S. R.) has profited from conversations with Professor T. D. Schultz. The other author (T. W. R.) is grateful for stimulating discussions with David and Harold Falk.

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