Linear Antiferromagnetic Chain

SERGIO RODRIGUEZ*
Scientific Laboratory, Ford Motor Company, Dearborn, Michigan
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It is shown that a linear chain consisting of a large number of atoms of spin $\frac{1}{2}$ with nearest neighbor ferromagnetic or antiferromagnetic interactions is mathematically equivalent to a one-dimensional Fermi gas with two-body forces. This equivalence is used to construct a wave function for which the expectation value of the energy lies between the two approximations obtained by Hulthén. Also, a perturbation treatment is given which permits, in principle, to obtain the exact antiferromagnetic ground state.

I. INTRODUCTION

THE ground state of a linear chain of atoms of spin $\frac{1}{2}$ with ferromagnetic or antiferromagnetic interactions between nearest neighbors is known.[1,2] However, the problem is still of some interest, especially for the antiferromagnetic lattice. In this case the nature of the ground-state wave function is not completely understood, particularly in regards to its long-range order.

The analysis of this problem is carried out on the basis of the Heisenberg model,[3] the dynamical properties of which are described by the Hamiltonian operator

$$H=2J\sum_j(\mathbf{S}_j\cdot\mathbf{S}_{j+1}-\tfrac{1}{4}). \tag{1}$$

Here $\mathbf{S}_j$ is the (vector) spin operator associated with the atom in the jth position of the chain and J is the exchange integral. It will be assumed that the atoms in the system are numbered consecutively in the order they appear from left to right. The sum in (1) extends over the N atoms constituting the chain with the understanding that $\mathbf{S}_{N+1}$ is to be identified with $\mathbf{S}_1$.

At this point it is convenient to establish the notation that will be used in this paper. We choose an arbitrary set of orthogonal cartesian coordinates x, y, z. The components of $\mathbf{S}_j$ along these directions will be denoted by $S_j^{(x)}$, $S_j^{(y)}$, and $S_j^{(z)}$, and the raising and lowering operators $S_j^{(\pm)}$ are defined by the relation

$$S_j^{(\pm)}=S_j^{(x)}\pm iS_j^{(y)}. \tag{2}$$

The spin operators have the well-known properties that any two components of $\mathbf{S}_j$ anticommute while the square of a particular component is $\frac{1}{4}$ times the identity operator. Also, they verify the equation

$$\mathbf{S}_j\times\mathbf{S}_j=i\mathbf{S}_j. \tag{3}$$

The eigenvectors of $\mathbf{S}_j^{(z)}$ are designated by the symbols α_j and β_j; the corresponding eigenvalues are $\frac{1}{2}$ and $-\frac{1}{2}$.

A complete set of states suitable for the description of the sytem at hand can be specified by giving the z component of spin for each atom. One such state is

$$|0\rangle=\beta_1\beta_2\cdots\beta_N, \tag{4}$$

where all spins point in the negative z direction. All other states are obtained from $|0\rangle$ by application of the raising operators defined in (2). For example, the state with reversed spins (i.e., spins pointing in the positive z direction) at the positions j_1, j_2, $\cdots j_r$ is

$$\Phi_{j_1j_2\cdots j_r}=S_{j_1}^{(+)}S_{j_2}^{(+)}\cdots S_{j_r}^{(+)}|0\rangle. \tag{5}$$

An estimate of the ground-state energy and wave function can be obtained by means of a variational procedure which consists in choosing an appropriate trial wave function and forming the expectation value of H. This expectation value is an upper bound for the ground-state energy.

The trial wave function that is immediately suggested by analogy with the ferromagnetic problem is the Néel state

$$\Phi_n=\alpha_1\beta_2\alpha_3\beta_4\cdots. \tag{6}$$

The expectation value of the energy for this state is

$$\langle\Phi_n|H|\Phi_n\rangle=-JN. \tag{7}$$

It is a simple matter to form a state having a lower energy, for example, if we consider[4]

$$\Phi_s=2^{-N/2}\prod_{j=1,3,5,\cdots}(\alpha_j\beta_{j+1}-\beta_j\alpha_{j+1}), \tag{8}$$

it turns out that

$$\langle\Phi_s|H|\Phi_s\rangle=-1.25JN, \tag{9}$$

which is considerably lower than (6). Neither Φ_n nor Φ_s is an eigenstate of the Hamiltonian H.

It is of interest to consider the amount of long-range order in (6) and (8) as defined, for example, by

$$4N^{-1}\sum_j\langle\mathbf{S}_j\cdot\mathbf{S}_{j+\lambda}\rangle,$$

where λ is an even integer. For the Néel state this quantity is

$$4N^{-1}\sum_j\langle\Phi_n|\mathbf{S}_j\cdot\mathbf{S}_{j+\lambda}|\Phi_n\rangle=1, \tag{10}$$

for all even λ however large; for Φ_s we have

$$4N^{-1}\sum_j\langle\Phi_s|\mathbf{S}_j\cdot\mathbf{S}_{j+\lambda}|\Phi_s\rangle=0, \tag{11}$$

* Present address: Department of Physics, University of Illinois, Urbana, Illinois.

[1] E. Teller, Z. Physik **62**, 102 (1930).

[2] H. A. Bethe, Z. Physik **71**, 205 (1931); A. Sommerfeld and H. A. Bethe, *Handbuch der Physik*, edited by H. Geiger and K. Scheel (Verlag Julius Springer, Berlin, 1933), Vol. 24, Part 2, pp. 604–618.

[3] W. Heisenberg, Z. Physik **49**, 619 (1928).

[4] P. W. Anderson, Phys. Rev. **83**, 1260 (1951).

instead. Thus, Φ_n exhibits complete long-range order whereas Φ_s displays no such property.

Hulthén[5] has used the variational principle to obtain a smaller upper bound for the ground-state energy. He constructed two states. The first has the average energy $-1.3156\,JN$ while the second, which is obtained by a more complicated procedure, yields an expectation value of H equal to $-1.349\,JN$. Both results compare quite well with Bethe's exact result $-1.3863\,JN$.

The procedure of Hulthén has been generalized by Marshall[6] to the two- and three-dimensional lattices. Kasteleijn[7] has considered the situation in which the exchange coupling is anisotropic, introducing an extra admixture of Ising interaction in the Hamiltonian operator of the system. The exact solution of the latter problem has been given by Orbach.[8]

The purpose of the present paper is twofold. Firstly we shall show that it is possible to form a simple wave function that gives an upper bound to the ground-state energy equal to $-1.3393\,JN$. The wave function that we shall construct is, in a sense, a generalization of the state (8). Secondly, a perturbation expansion will be indicated that allows us, in principle, to obtain the exact ground state of the antiferromagnetic lattice. To accomplish this program we prove that the problem of finding the eigensolutions of (1) for N large is equivalent to that of a one-dimensional Fermi gas with two-body interactions. Then we show that the ground state of the fermion system, neglecting the forces between the particles, has the average energy given above. Successively better approximations can be obtained by considering the interactions of the different pseudoparticles as a perturbation. Table I gives a summary of the results of several calculations.

TABLE I. Upper bound for the ground-state energy of the linear antiferromagnetic chain according to several calculations.

Wave function	Expectation value of $-H/JN$
Néel [Eq. (6)]	1.0000
Singlet pairs [Eq. (8)]	1.2500
Hulthén (first approximation)	1.3156
Present work	1.3393
Hulthén (second approximation)	1.349
Exact solution	1.3863

[5] L. Hulthén, Arkiv Mat. Astron. Fysik **26A**, No. 1 (1938).
[6] W. Marshall, Proc. Roy. Soc. (London) **A232**, 48 (1955).
[7] P. W. Kasteleijn, Physica **18**, 104 (1952).
[8] R. Orbach, Phys. Rev. **112**, 309 (1958).

II. TRANSFORMATION OF THE HAMILTONIAN

The main purpose of this section is to transform the Hamiltonian operator H into the form

$$H=H_0+H_1, \tag{12}$$

where H_0 represents the energy of a system of non-interacting Fermi particles and H_1 describes two-body interactions among them.

Equation (1) can be rewritten in the form

$$H=-\tfrac{1}{2}JN+2J\sum_j S_j^{(z)}S_{j+1}^{(z)} +\sum_j (S_j^{(+)}S_{j+1}^{(-)}+S_j^{(-)}S_{j+1}^{(+)}), \tag{13}$$

which is more adequate for our purpose than (1). We now define the following operators

$$\mu_j^{(\pm)}=(-2)^{j-1}S_1^{(z)}S_2^{(z)}\cdots S_{j-1}^{(z)}S_j^{(\pm)}. \tag{14}$$

It is easy to see that $\mu_j^{(+)}$ and $\mu_j^{(-)}$ are each other's Hermitian conjugates. From the properties of the spin operators it is readily established that the operators $\mu_j^{(\pm)}$ satisfy the following anticommutation relations

$$\{\mu_j^{(+)},\mu_{j'}^{(+)}\}=\{\mu_j^{(-)},\mu_{j'}^{(-)}\}=0, \tag{15a}$$

and

$$\{\mu_j^{(+)},\mu_{j'}^{(-)}\}=\delta_{jj'}. \tag{15b}$$

We have used the notation

$$\{A,B\}=AB+BA; \tag{16}$$

$\delta_{jj'}$ is equal to unity if $j=j'$ and zero otherwise.

If $j_1, j_2, \cdots j_r$ are arranged in increasing order we have

$$\Phi_{j_1 j_2\cdots j_r}=\mu_{j_1}^{(+)}\mu_{j_2}^{(+)}\cdots\mu_{j_r}^{(+)}|0\rangle, \tag{17}$$

so that the use of $\mu_j^{(\pm)}$ does not, by itself, contribute to the solution of our problem. However, if we introduce

$$\eta_k^*=N^{-\frac{1}{2}}\sum_j e^{ikj}\mu_j^{(+)}, \tag{18}$$

and its Hermitian conjugate η_k we can transform H to the form (12) in a rather simple way. Here, because of the periodicity around the chain the quantity k is given by

$$k=(2\pi n)/N, \tag{19}$$

with $N=0, 1, 2, \cdots N-1$. Only these values of k need be considered as two operators η_k^* and $\eta_{k'}^*$ are identical if k and k' differ by an integral multiple of 2π. It is easy to prove from Eqs. (15), (18), and (19) that

$$\{\eta_k^*,\eta_{k'}^*\}=\{\eta_k,\eta_{k'}\}=0, \tag{20a}$$

and

$$\{\eta_k^*,\eta_{k'}\}=\bar{\Delta}(k-k'). \tag{20b}$$

The quantity $\bar{\Delta}$ is defined by

$$\begin{aligned}\bar{\Delta}(k-k')&=1 \quad \text{if } k=k'\pm 2\pi\tau;\quad \tau=0, 1, 2, \cdots\\ &=0 \quad \text{otherwise.}\end{aligned} \tag{21}$$

The operator $\eta_k^*(\eta_k)$ represents the creation (destruction) of a pseudoparticle in the state characterized by the wave number k. These elementary excitations are Fermi particles and the occupation number of a particular state k is $\eta_k^*\eta_k$. From (14) and (18) it follows that the total number operator is

$$\sigma=\sum_k \eta_k^*\eta_k=\sum_j \mu_j^{(+)}\mu_j^{(-)}=\sum_j S_j^{(+)}S_j^{(-)} =\tfrac{1}{2}N+\sum_j S_j^{(z)}. \tag{22}$$

To obtain the last equality we have made use of the identity

$$S_j^{(z)}=S_j^{(+)}S_j^{(-)}-\tfrac{1}{2}. \tag{23}$$

It is easy to show

$$S_j^{(+)}S_{j+1}^{(-)}+S_j^{(-)}S_{j+1}^{(+)}=\mu_j^{(+)}\mu_{j+1}^{(-)}+\mu_{j+1}^{(+)}\mu_j^{(-)}. \quad (24)$$

Strictly speaking Eq. (24) holds for $1\leqslant j<N$ but not for $j=N$. Nevertheless we substitute

$$J\sum_j(\mu_j^{(+)}\mu_{j+1}^{(-)}+\mu_{j+1}^{(+)}\mu_j^{(-)}),$$

for

$$J\sum_j(S_j^{(+)}S_{j+1}^{(-)}+S_j^{(-)}S_{j+1}^{(+)})$$

in (13). Of course, this substitution changes H slightly, but the eigenvalues and eigenfunctions of the new Hamiltonian will be rigorously equal to those of (13) in the limit when N becomes infinite. We also have

$$J\sum_j(\mu_j^{(+)}\mu_{j+1}^{(-)}+\mu_{j+1}^{(+)}\mu_j^{(-)})=\sum_k(2J\cos k)\eta_k^*\eta_k. \quad (25)$$

In the representation generated by the operators η_k^* the most interesting part of the Hamiltonian is the Ising interaction

$$H_I=2J\sum_j S_j^{(z)}S_{j+1}^{(z)}. \quad (26)$$

Using Eq. (23) we can rewrite the Ising Hamiltonian in the form

$$H_I=\tfrac{1}{2}JN-2J\sum_j S_j^{(+)}S_j^{(-)}+2J\sum_j S_j^{(+)}S_j^{(-)}S_{j+1}^{(+)}S_{j+1}^{(-)}. \quad (27)$$

If we make use of the definitions of the operators $\mu_j^{(\pm)}$ and η_k^* we find

$$H_I=\tfrac{1}{2}JN-2J\sum_k\eta_k^*\eta_k+H_1, \quad (28)$$

where

$$H_1=2JN^{-1}\sum_{l_1l_2l_3l_4}\cos(l_1-l_4)\times\bar{\Delta}(l_1+l_2-l_3-l_4)\eta_{l_1}^*\eta_{l_2}^*\eta_{l_3}\eta_{l_4}. \quad (29)$$

Thence, we finally get

$$H=H_0+H_1, \quad (30)$$

with

$$H_0=\sum_k\epsilon(k)\eta_k^*\eta_k, \quad (31)$$

and

$$\epsilon(k)=-2J(1-\cos k). \quad (32)$$

We remark that the total number of Fermi particles present in the system need not be conserved. However, the Hamiltonian operator H commutes with the total number operator σ so that the eigenstates of the system can be chosen in such a way that they are simultaneous eigenvectors of H and σ. We see, from (22), that σ is essentially a measure of the z component of the total spin of the system. Therefore, the statement that σ is a constant of the motion is equivalent to the well-known fact that, in the Heisenberg model, $\sum_j S_j^{(z)}$ is a constant of the motion.

Marshall[6] has shown that (we assume N even) the ground state of an antiferromagnet is a singlet, i.e., a state for which $\langle S^2\rangle=0$ and $\langle\sum_j S_j^{(z)}\rangle=0$. Thus, to obtain the ground state of the antiferromagnetic line, it is enough to restrict outselves to the case in which the number of fermions present is $\frac{1}{2}N$. The ground state φ_0 of H_0 is that in which all single-particle states such that $\pi/2\leqslant k\leqslant 3\pi/2$ are occupied, while all others are empty. The unperturbed energy of this state, for large N, is

$$\epsilon_0=\frac{N}{2\pi}\int_{\pi/2}^{3\pi/2}dk\epsilon(k)=-NJ(1+2/\pi). \quad (33)$$

The state φ_0 is

$$\varphi_0=\prod_m\eta_m^*|0\rangle, \quad (34)$$

where the range of m is given by the inequality

$$\pi/2\leqslant m\leqslant 3\pi/2.$$

It is convenient, to simplify the passage to the limit $N\to\infty$, to make the following definitions

$$\sum_k f(k)=(N/2\pi)\int_k f(k), \quad (35)$$

$$\bar{\Delta}(k)=2\pi N^{-1}\Delta(k), \quad (36)$$

$$\eta_k^*=(2\pi N^{-1})^{\frac{1}{2}}\xi_k^*. \quad (37)$$

When $N\to\infty$

$$\int_k f(k)\to\int dk\, f(k), \quad (38)$$

and

$$\Delta(k)\to\sum_{\tau=-\infty}^{\infty}\delta(k-2\pi\tau). \quad (39)$$

In Eq. (39) $\delta(k)$ is the Dirac δ function. With this notation we can rewrite Eqs. (31) and (29) in the form

$$H_0=\int_k\epsilon(k)\xi_k^*\xi_k, \quad (40)$$

$$H_1=\frac{1}{4}\int_{l_1l_2l_3l_4}v(l_1l_2l_3l_4)\xi_{l_1}^*\xi_{l_2}^*\xi_{l_3}\xi_{l_4}, \quad (41)$$

where

$$v(l_1l_2l_3l_4)=(2J/\pi)[\cos(l_1-l_4)-\cos(l_1-l_3)]\times\Delta(l_1+l_2-l_3-l_4). \quad (42)$$

We now calculate the expectation value of H for the state φ_0. To obtain this quantity we need

$$\langle\varphi_0|H_1|\varphi_0\rangle=-\frac{1}{2}\int_{m_1m_2}v(m_1m_2m_1m_2), \quad (43)$$

where the sum is over those states m that are occupied in φ_0. For large N we obtain

$$\langle\varphi_0|H_1|\varphi_0\rangle=NJ(\tfrac{1}{2}-2/\pi^2), \quad (44)$$

so that

$$\langle\varphi_0|H|\varphi_0\rangle=-NJ[\tfrac{1}{2}+(2/\pi)+(2/\pi^2)]=-1.3393\,JN. \quad (45)$$

We observe that the value obtained in (45) lies between the two approximations exhibited by Hulthén.[5]

III. PERTURBATION ANALYSIS

A perturbation theory analysis for a Hamiltonian of the form (30) has been given in detail by Hugenholtz.[9] The procedure consists in obtaining the function

$$D(z)=\langle\varphi_0|R(z)|\varphi_0\rangle \tag{46}$$

of the complex energy parameter z. $R(z)$ is the resolvent operator

$$R(z)=(H-z)^{-1}. \tag{47}$$

The quantity $D(z)$ can be written in the form of a series expansion of matrix elements of operators containing integral powers of H_1 and $(H_0-z)^{-1}$. These matrix elements can be expressed in terms of contributions arising from different types of diagrams. In such diagrams each creation or destruction operator is represented by a line, while each interaction H_1 appears as a vertex to which four lines converge. The contributions to $D(z)$ coming from connected diagrams (i.e., diagrams which cannot be divided into two or more sub-diagrams without cutting any lines) are proportional to N, whereas the contributions due to disconnected diagrams vary as higher powers of N. It is possible to express the sum of the contributions of disconnected diagrams in terms of those arising from connected diagrams alone. We shall not give a description of the procedure but merely quote the results useful for our purpose. The ground-state energy is

$$E_0=\epsilon_0+\langle\varphi_0|[H_1-H_1(H_0-\epsilon_0)^{-1}H_1+H_1(H_0-\epsilon_0)^{-1}\times H_1(H_0-\epsilon_0)^{-1}H_1-\cdots]_c|\varphi_0\rangle, \tag{48}$$

where the subindex c means that only those contributions arising from connected diagrams are to be considered. The ground-state wave functions is

$$\psi_0=N_0^{\frac{1}{2}}[1-(H_0-\epsilon_0)^{-1}H_1+(H_0-\epsilon_0)^{-1}\times H_1(H_0-\epsilon_0)^{-1}H_1-\cdots]_L|\varphi_0\rangle. \tag{49}$$

The subindex L indicates that only contributions that come from diagrams in which each intermediate state and the final state are different from φ_0 are to be taken into account. The quantity $N_0^{\frac{1}{2}}$ is the normalization factor. Equations (48) and (49) were derived, for the first time, by Goldstone.[10]

[9] N. H. Hugenholtz, Physica **23**, 481 (1957).
[10] J. Goldstone, Proc. Roy. Soc. (London) **A239**, 267 (1957); see also C. Bloch, Nuclear Phys. **7**, 451 (1958).

As an example, we give the second order correction to the ground-state energy

$$-\langle\varphi_0|[H_1(H_0-\epsilon_0)^{-1}H_1]_c|\varphi_0\rangle=-\frac{NJ}{\pi^3}\sum_{\tau=-\infty}^{\infty}\int dk_1dk_2dm_1dm_2\times\frac{\sin^2[(k_1-k_2)/2]\sin^2[(m_1-m_2)/2]}{\cos k_1+\cos k_2-\cos m_1-\cos m_2}\times\delta(k_1+k_2-m_1-m_2+2\pi\tau). \tag{50}$$

The integrations over k are performed in the range of states which are empty in φ_0 (i.e., over the intervals $0\leqslant k\leqslant\pi/2$ and $3\pi/2\leqslant k\leqslant 2\pi$) while the integrations over m are calculated in the interval $\pi/2\leqslant m\leqslant 3\pi/2$.

IV. CONCLUDING REMARKS

Teller[1] has shown that, in the ferromagnetic case ($J<0$), the ground state of the system is $|0\rangle$ and that the corresponding eigenvalue is zero. This ground state is degenerate, the degree of degeneracy being $N+1$. To each eigenvalue of $\sum_j S_j^{(z)}$ there corresponds an eigenstate of H and the total z component of spin, which is degenerate with $|0\rangle$. We now look at this statement from the point of view of our Fermi gas. We have an energy band defined by (32) (with $J<0$) that is full when it contains N fermions. The ground state of the the system containing an arbitrary number r ($0\leqslant r\leqslant N$) of particles in the band has always a zero energy. The Hamiltonian (30) provides us with an example of a many body system in which the ground state energy is known exactly. Thus, (30) may be used as a test for the accuracy of approximate techniques for obtaining the ground-state energy of a many fermion system.

The state φ_0 is a good approximation to the antiferromagnetic ground state only for the isotropic Heisenberg Hamiltonian. It is in the case of an anisotropic coupling that the virtues of the solution given by Kasteleijn become apparent. The question of what is the long range order of the ground state and how does it vary with the anisotropy of the coupling (as defined, for example, by Orbach) cannot be answered in a simple way by the present work.

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