SLAC-PUB-2439 (Rev.)
December 1979
April 1980 (Rev.)
(M)

RENORMALIZATION GROUP STUDIES OF ANTIFERROMAGNETIC CHAINS II. LONG-RANGE INTERACTIONS*

Jeffrey M. Rabin
Stanford Linear Accelerator Center
Stanford University, Stanford, California 94305

Abstract

A real-space, zero-temperature renormalization group method is used to study a Heisenberg antiferromagnetic spin chain with long-range interactions varying as (distance)$^{-p}$. Simple renormalization group equations are obtained and studied analytically, and the results are checked against a more accurate numerical calculation. The calculations provide evidence for a phase transition at $p \approx 1.85$ characterized by a change in the behavior of zero-temperature correlation functions. For $p \gtrsim 1.85$ the large-distance physics is that of the nearest-neighbor antiferromagnet, while there is a line of fixed points for $p \lesssim 1.85$. I conjecture that $p \approx 1.85$ also marks an order-disorder transition at finite temperature such as occurs in the Ising model with power-law interactions.

Submitted to Physical Review B

---

* Work supported in part by the Department of Energy under contract DE-AC03-76SF00515 and in part by a National Science Foundation Fellowship.

I. Introduction

This is the second of two papers[1] in which real-space renormalization group (RG) methods[2-8] are used to study the one-dimensional Heisenberg antiferromagnetic chain with long-range interactions,

$$H = \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} (-1)^{i-j+1} \frac{1}{|i-j|^p} \vec{S}(i) \cdot \vec{S}(j) \quad , \tag{1.1}$$

at zero temperature. The infinite-volume limit $N \to \infty$ will generally be assumed. Paper I was concerned with the nearest-neighbor limit $p \to \infty$, while this paper investigates the phases of the model as a function of p. Although little is known about the model, Dyson and Ruelle have proven[9] that the analogous Ising model,

$$H' = \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} (-1)^{i-j+1} \frac{1}{|i-j|^p} S_z(i) S_z(j) \quad , \tag{1.2}$$

is disordered at all finite temperatures if $p > 2$, while order persists at low temperatures if $p < 2$. The $(-1)^{i-j+1}$ sign factor is of course irrelevant in (1.2), and Dyson conjectured that the Ising results hold for the Heisenberg ferromagnet [Eq. (1.1) without the sign factor] as well. This paper will suggest that the results hold in the antiferromagnetic case also. In particular, evidence will be presented that the zero-temperature properties of the model (1.1) differ sharply according as $p \gtrsim 1.85$ or $p \lesssim 1.85$.

The model (1.1) is also of interest in lattice field theory since antiferromagnetic power-law interactions of precisely this form appear when the continuum field theory gradient is transcribed onto a lattice

using the SLAC prescription.[2,3] Indeed, the model (1.1) is equivalent to the strong coupling lattice Thirring ($p = 2$) and Schwinger ($p = 3$) models restricted to particular sectors of states.[3]

The paper is organized as follows. Section II presents some exact results for the cases $p = 0$ and $p \to \infty$. Section III reviews the simple three-site blocking calculation used in paper I and applies it to the model (1.1). Renormalization group equations are derived which are sufficiently simple to be studied analytically. In particular, it can be seen explicitly how the non-nearest-neighbor interactions in (1.1) disappear as the RG equations are iterated when p exceeds a certain critical value. Section IV shows that the results of the three-site calculation do not change qualitatively when one goes to a more accurate calculation using nine-site blocks. The latter calculation, unfortunately, must be carried out numerically. Section V contains the conclusions.

II. Exact Results

Although very little is known about the model (1.1) some rigorous results can be obtained by considering the limiting cases $p \to \infty$ and $p = 0$.

For $p \to \infty$ the model becomes the Heisenberg antiferromagnet with nearest-neighbor interactions which was discussed by block-spin methods in paper I. This model is exactly soluble[10] and for the present work its relevant properties are as follows. The ground state energy density is -0.4431 and the low-lying excitations are massless spin waves. The end-to-end order $\langle \vec{S}(1) \cdot \vec{S}(N) \rangle$ vanishes in the infinite-volume limit and the cluster property

$$\lim_{N\to\infty}\left[\langle\vec{S}(1)\cdot\vec{S}(N)\rangle - \langle\vec{S}(1)\rangle\cdot\langle\vec{S}(N)\rangle\right] = 0$$

is satisfied.

For $p = 0$ the Hamiltonian (1.1) becomes:

$$H = \frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}(-1)^{i-j+1}\,\vec{S}(i)\cdot\vec{S}(j) \quad . \tag{2.1}$$

All spins interact with equal strength and the fact that they form a linear chain becomes irrelevant. This Hamiltonian can also be solved exactly, by introducing the two sublattices containing respectively only even-numbered sites and only odd-numbered sites. N is assumed to be even so that each sublattice contains $\frac{1}{2}N$ sites. The Hamiltonian (2.1) may be rewritten as:

$$H = \sum_{\substack{i\ \text{even}\\ j\ \text{odd}}}\vec{S}(i)\cdot\vec{S}(j) - \frac{1}{2}\sum_{\substack{i,j\ \text{even}\\ i\neq j}}\vec{S}(i)\cdot\vec{S}(j) - \frac{1}{2}\sum_{\substack{i,j\ \text{odd}\\ i\neq j}}\vec{S}(i)\cdot\vec{S}(j)$$

$$= \sum_{i\ \text{even}}\vec{S}(i)\cdot\sum_{j\ \text{odd}}\vec{S}(j) - \frac{1}{2}\left[\sum_{i\ \text{even}}\vec{S}(i)\right]^2 - \frac{1}{2}\left[\sum_{i\ \text{odd}}\vec{S}(i)\right]^2 + \frac{3}{8}N$$

$$= \vec{S}_{\text{even}}\cdot\vec{S}_{\text{odd}} - \frac{1}{2}S^2_{\text{even}} - \frac{1}{2}S^2_{\text{odd}} + \frac{3}{8}N$$

$$= \frac{1}{2}S^2_{\text{total}} - S^2_{\text{even}} - S^2_{\text{odd}} + \frac{3}{8}N \quad , \tag{2.2}$$

where I have introduced the total spins on the entire lattice and on the even and odd sublattices. The ground state evidently has $S_{\text{total}} = 0$, $S_{\text{even}} = S_{\text{odd}} = \frac{1}{4}N$, and an energy given by

$$E_o = -\frac{N^2 + N}{8} \quad . \tag{2.3}$$

The energy density diverges linearly with N and the infinite-volume limit of the theory does not exist. The first excited state has $S_{total} = 1$, $S_{even} = S_{odd} = \frac{1}{4}N$, and the excitation energy is 1. This contrasts with the massless excitations in the $p \to \infty$ theory. The end-to-end order $\langle \Phi_o | \vec{S}(1) \cdot \vec{S}(N) | \Phi_o \rangle$ in the ground state $|\Phi_o\rangle$ can be obtained as follows. The fact that all spins on a single sublattice are equivalent implies that $\langle \vec{S}(i) \cdot \vec{S}(j) \rangle$ depends only on the parities of i and j. Therefore,

$$\begin{aligned} \langle \vec{S}(1) \cdot \vec{S}(N) \rangle &= \frac{4}{N^2} \sum_{\substack{i \text{ odd} \\ j \text{ even}}} \langle \vec{S}(i) \cdot \vec{S}(j) \rangle \\ &= \frac{4}{N^2} \langle \vec{S}_{odd} \cdot \vec{S}_{even} \rangle \\ &= \frac{2}{N^2} \langle S^2_{total} - S^2_{even} - S^2_{odd} \rangle \\ &= -\frac{1}{4} - \frac{1}{N} \quad , \end{aligned} \tag{2.4}$$

which explicitly shows the breakdown of clustering due to the long-range interactions.

Additional information can be obtained by using the $p = 0$ ground state $|\Phi_o\rangle$ as a variational trial state to study the full theory (1.1). The variational energy obtained in this way is

$$\langle \Phi_o | H | \Phi_o \rangle = \frac{1}{2} \sum_{i \neq j} (-1)^{i-j+1} \frac{1}{|i-j|^p} \langle \Phi_o | \vec{S}(i) \cdot \vec{S}(j) | \Phi_o \rangle \quad . \tag{2.5}$$

It follows from Eq. (2.4) and the sublattice structure that

$$\langle \Phi_o | \vec{S}(i) \cdot \vec{S}(j) | \Phi_o \rangle = (-1)^{i-j} \left(\frac{1}{4} + \frac{1}{N} \right) \quad .$$

Therefore,

$$\langle \Phi_o | H | \Phi_o \rangle = -\left(\frac{1}{8} + \frac{1}{2N}\right) \sum_{i \neq j} \frac{1}{|i-j|^p}$$

$$= -\left(\frac{1}{4} + \frac{1}{N}\right)\left[(N-1)\,\frac{1}{1^p} + (N-2)\,\frac{1}{2^p} + \ldots + \frac{1}{(N-1)^p}\right]$$

$$= -\left(\frac{1}{4} + \frac{1}{N}\right)\left(N \sum_{k=1}^{N-1} \frac{1}{k^p} - \sum_{k=1}^{N-1} \frac{1}{k^{p-1}}\right) \quad . \qquad (2.6)$$

The exact ground state energy density is therefore bounded above by

$$\frac{E_o}{N} \leq -\left(\frac{1}{4} + \frac{1}{N}\right)\left(\sum_{k=1}^{N-1} \frac{1}{k^p} - \frac{1}{N} \sum_{k=1}^{N-1} \frac{1}{k^{p-1}}\right) \quad . \qquad (2.7)$$

This shows that the infinite-volume limit does not exist for $p \leq 1$. Since the spin operators in H have bounded matrix elements there can be no divergence in E_o/N for $p > 1$, so the theory does exist in this region.

In view of the radically different properties of the theory at $p \to \infty$ and $p = 0$, two possibilities exist. Either the theory remains in the $p = \infty$ phase all the way down to $p = 1$ where the infinite-volume limit ceases to exist, or a phase transition occurs for some $p > 1$. In the remainder of this paper block-spin techniques are applied to resolve this question.

III. Simple Calculation Using Three-Site Blocks

A. Derivation of RG Equations

This section reviews the three-site blocking algorithm used in paper I and applies it to the model (1.1), which is conveniently rewritten in the form:

$$H = \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} (-1)^{i-j+1} F(i-j) \vec{S}(i) \cdot \vec{S}(j) \quad ,$$

$$F(i-j) \equiv \frac{1}{|i-j|^p} \quad . \tag{3.1}$$

One begins by dividing the lattice into three-site blocks and relabelling each lattice site with an ordered pair (k,a), where k = 1,2,..., N/3 labels the blocks and a = 1,2,3 labels the sites within a block. The Hamiltonian is separated into the piece H_{in} which only couples sites in the same block, and the remainder H_{out}:

$$\begin{aligned} H &= H_{in} + H_{out} \quad , \\ H_{in} &= \frac{1}{2} \sum_{k} \sum_{a,a'} (-1)^{a-a'+1} F(a-a') \vec{S}(k,a) \cdot \vec{S}(k,a') \quad , \\ H_{out} &= \frac{1}{2} \sum_{k \neq k'} \sum_{a,a'} (-1)^{k-k'+a-a'+1} F\left[3(k-k') + a-a'\right] \vec{S}(k,a) \cdot \vec{S}(k',a') \quad . \end{aligned} \tag{3.2}$$

Singling out a particular block for attention, I write:

$$\begin{aligned} H_{in} &= \sum_{k} H_{block}(k) \quad , \\ H_{block} &= F(1)\left[\vec{S}(1) \cdot \vec{S}(2) + \vec{S}(2) \cdot \vec{S}(3)\right] - F(2)\vec{S}(1) \cdot \vec{S}(3) \\ &= \frac{1}{2} F(1) \left\{ \left[\vec{S}(1) + \vec{S}(2) + \vec{S}(3)\right]^2 - \left[\vec{S}(1) + \vec{S}(3)\right]^2 - \frac{3}{4} \right\} \\ &\quad - \frac{1}{2} F(2) \left\{ \left[\vec{S}(1) + \vec{S}(3)\right]^2 - \frac{3}{2} \right\} \quad . \end{aligned} \tag{3.3}$$

This shows that the eigenstates of H_{block} are just the simultaneous eigenstates of the total spin on a block and $\left[\vec{S}(1) + \vec{S}(3)\right]^2$. These states are [notation is $|S,S_z\rangle$; the subscript, when present, gives the value of

the spin $\vec{S}(1) + \vec{S}(3)\big]$:

$$\left.\begin{aligned} |\tfrac{3}{2},\tfrac{3}{2}\rangle &= |\uparrow\uparrow\uparrow\rangle \\ |\tfrac{3}{2},\tfrac{1}{2}\rangle &= \frac{1}{\sqrt{3}}\left(|\uparrow\uparrow\downarrow\rangle + |\downarrow\uparrow\uparrow\rangle + |\uparrow\downarrow\uparrow\rangle\right) \end{aligned}\right\} \text{ energy } = \tfrac{1}{2}F(1) - \tfrac{1}{4}F(2) \ ,$$

$$|\tfrac{1}{2},\tfrac{1}{2}\rangle_0 = \frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\downarrow\rangle - |\downarrow\uparrow\uparrow\rangle\right) \ , \ \text{energy } = \tfrac{3}{4}F(2) \ ,$$

$$|\tfrac{1}{2},\tfrac{1}{2}\rangle_1 = \frac{1}{\sqrt{6}}\left(2|\uparrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\rangle - |\uparrow\uparrow\downarrow\rangle\right) \ , \ \text{energy } = -F(1) - \tfrac{1}{4}F(2) \ , \tag{3.4}$$

plus the four corresponding states with all spins flipped and negative total S_z. It can be seen that $|\frac{1}{2},\pm\frac{1}{2}\rangle_1$ have the lowest energy regardless of the value of p. One then hopes to get a reasonable picture of the low-lying states of the lattice by restricting attention to those lattice states which are built from the block states $|\frac{1}{2},\pm\frac{1}{2}\rangle_1$ only. The next step is to write an effective Hamiltonian which has the same matrix elements as the original Hamiltonian within this sector of states. For this purpose I introduce new spin operators $\vec{S}'$ which act on the states $|\frac{1}{2},\pm\frac{1}{2}\rangle_1$ in the usual manner: ${}_1\langle\tfrac{1}{2},\tfrac{1}{2}|\, S'_z \,|\tfrac{1}{2},\tfrac{1}{2}\rangle_1 = \tfrac{1}{2}$, etc. $\vec{S}'$ is in fact just the total block spin, and the Wigner-Eckart theorem gives:

$$\langle \vec{S}(k,a) \rangle = u_a \langle \vec{S}'(k) \rangle \ ,$$

$$u_1 = u_3 = \frac{2}{3} \ , \quad u_2 = -\frac{1}{3} \ , \tag{3.5}$$

where the notation $\langle\ \rangle$ indicates any one of the four matrix elements involving the states $|\frac{1}{2},\pm\frac{1}{2}\rangle_1$. Using (3.5) to express H_{out} in terms of the block spin operators $\vec{S}'$ and observing that H_{in} is diagonal in

the sector of states of interest produces the effective Hamiltonian:

$$H^{(1)} = \sum_k \left[- F(1) - \frac{1}{4} F(2) \right] + \frac{1}{2} \sum_{k \neq k'} (-1)^{k-k'+1} \sum_{a,a'} (-1)^{a-a'}$$

$$\times u_a u_{a'} F\left[3(k-k') + a - a'\right] \vec{S}'(k) \cdot \vec{S}'(k')$$

$$\equiv \sum_k E_1 + \frac{1}{2} \sum_{k \neq k'} (-1)^{k-k'+1} F_1(k-k') \vec{S}'(k) \cdot \vec{S}'(k') \quad . \qquad (3.6)$$

Since this Hamiltonian has the same form as the original one, apart from the overall energy shift E_1, the blocks of the original lattice may be viewed as sites of a new lattice and the whole blocking procedure iterated. This generates a sequence $H^{(m)}$ of effective Hamiltonians obeying the RG equations:

$$H^{(m)} = \sum_{k=1}^{N/3^m} E_m + \frac{1}{2} \sum_{\substack{k,k'=1 \\ k \neq k'}}^{N/3^m} (-1)^{k-k'+1} F_m(k-k') \vec{S}(k) \cdot \vec{S}(k') \ , \qquad (3.7a)$$

$$E_{m+1} = 3E_m - F_m(1) - \frac{1}{4} F_m(2) \quad , \quad E_o = 0 \quad , \qquad (3.7b)$$

$$F_{m+1}(j) = \sum_{a,a'=1}^{3} (-1)^{a-a'} u_a u_{a'} F_m(3j + a - a') \ , \ F_o(j) = F(j) \ , \qquad (3.7c)$$

i.e.,

$$F_{m+1}(j) = F_m(3j) + \frac{4}{9}\left[F_m(3j-2) + F_m(3j-1) + F_m(3j+1) + F_m(3j+2)\right], \qquad (3.7d)$$

where the primes on the spin operators have been dropped for convenience. Note that the formula (3.7d) preserves the symmetry property $F_m(j) = F_m(-j)$ which was assumed in writing Eqs. (3.3) and (3.4). After roughly $m = \log_3 N$ iterations of the blocking procedure the entire lattice will be

reduced to a single block of energy E_m. The energy per original lattice site is therefore $\mathscr{E}_m \equiv E_m/3^m$. In the infinite-volume limit the energy density is given by $\mathscr{E}_\infty$, with $\mathscr{E}_m$ satisfying

$$\mathscr{E}_{m+1} = \mathscr{E}_m - \frac{1}{3^{m+1}}\left[F_m(1) + \frac{1}{4}F_m(2)\right] \quad , \quad \mathscr{E}_o = 0 \quad . \qquad (3.7e)$$

This will always be a variational upper bound on the exact ground state energy density. The problem now is to iterate the RG equations many times to find the Hamiltonian which describes the physics at very large length scales.

B. Analysis of RG Equations

A procedure for numerically iterating RG equations like (3.7) has been given by Drell, Svetitsky, and Weinstein.[5] At each iteration a finite set of function values, say $F_m(1),\ldots,F_m(100)$, are explicitly computed and stored in an array. For $|j| > 100$, $F_m(j)$ is parametrized as $F_m(j) = \frac{1}{|j|^p}\left(A_m + \frac{B_m}{j^2} + \frac{C_m}{j^4} + \frac{D_m}{j^6}\right)$, with only even order terms being required due to $F_m(j) = F_m(-j)$. The initial conditions are $A_o = 1$, $B_o = C_o = D_o = 0$, and substituting this form for F_m into (3.7d) and applying the binomial theorem produces formulas from which A_m — D_m can be computed recursively. The error introduced by using this asymptotic form for F_m is comparable to the inherent roundoff error in double precision computer arithmetic. I have performed the numerical calculation using this procedure, but due to the simplicity of Eq. (3.7d) all the important results can be obtained by an analytic study of the RG equations. This is done by considering Eq. (3.7d) in the limit of very large j where it simplifies considerably. Physically this corresponds to looking at the interaction between very distant spins. Since the RG equations by definition relate the physics of different length scales

they can be used to extend conclusions valid at large j to smaller and smaller values of j, as will now be shown.

When j is large, F(j) is sufficiently slowly varying that $F(3j \pm 1)$ and $F(3j \pm 2)$ can be approximated by F(3j). Then the first (m = 0) iteration of Eq. (3.7d) becomes

$$F_1(j) = \frac{25}{9} F_o(3j) = \frac{1}{3^p} \frac{25}{9} F_o(j) \equiv C F_o(j) \quad , \text{ for j sufficiently large.} \tag{3.8}$$

To extend this to smaller values of j assume now that j is not "sufficiently large" but that 3j-2 is, so that $F_1(3j-2) = CF_o(3j-2)$. Then the next iteration of Eq. (3.7d) looks like this:

$$\begin{aligned} F_2(j) &= F_1(3j) + \frac{4}{9}\left[F_1(3j-2) + F_1(3j-1) + F_1(3j+1) + F_1(3j+2)\right] \\ &= C\left\{F_o(3j) + \frac{4}{9}\left[F_o(3j-2) + F_o(3j-1) + F_o(3j+1) + F_o(3j+2)\right]\right\} \\ &= C F_1(j) \quad , \end{aligned} \tag{3.9}$$

and this is valid for values of j roughly 1/3 as large as those for which Eq. (3.8) was valid. Continuing to iterate Eq. (3.7d) produces equations analogous to (3.9) holding for smaller and smaller values of j until ultimately one obtains simply

$$F_{m+1}(j) = CF_m(j) \quad \text{for all } j > 1 \text{ and all sufficiently large m.} \tag{3.10}$$

The restriction to $j \neq 1$ comes about because according to Eq. (3.7d), $F_{m+1}(1)$ depends on $F_m(1)$; in fact,

$$F_{m+1}(1) = F_m(3) + \frac{4}{9}\left[F_m(1) + F_m(2) + F_m(4) + F_m(5)\right] \quad . \tag{3.11}$$

The reasoning leading to Eq. (3.10) assumed that the smallest argument

appearing on the right side of Eq. (3.7d), namely 3j-2, was greater than j, and this is only true if $j > 1$. This fact is crucial physically, since it means that the nearest-neighbor coupling $F_m(1)$ may behave differently under renormalization group transformations than the longer-range couplings. The results (3.10) and (3.11) are sufficient to reveal the physical content of the RG equations.

Proceeding with the analysis, the definition $C = 25/3^{p+2}$ shows that $C > 1$ for $p < \log_3 25 - 2 \approx 0.93$, and $C < 1$ for $p > 0.93$. By Eq. (3.10) this implies that

$$\lim_{m\to\infty} F_m(j) = \begin{cases} 0 & \text{if } p > 0.93 \\ \infty & \text{if } p < 0.93 \end{cases} . \qquad (3.12)$$

Actually this follows from Eq. (3.10) only for $j > 1$, but it holds for $j = 1$ as well: Eq. (3.11) shows that it is not possible to have $F_m(j) \to 0$ or ∞ for all $j > 1$ without having $F_m(1) \to 0$ or ∞ (respectively) also. The value $p = 0.93$ is strikingly close to the anticipated $p = 1$; unfortunately, $p = 0.93$ is <u>not</u> to be identified as the point at which the energy density diverges and the theory ceases to exist. It is clear from Eq. (3.7e) that the divergence of $F_m(j)$ is not sufficient to produce a divergence in $\mathcal{E}_m$ unless $F_m(j)$ grows by a factor of at least 3 at each iteration. This happens for $C \geq 3$, so that $p \leq -0.07$ is needed before this block-spin approximation can detect the divergence in $\mathcal{E}_m$. The significance of $p = 0.93$ is that for $p > 0.93$ this approximate calculation predicts that the theory has a massless spectrum: any mass gap, if present, must vanish along with the couplings $F_m(j)$ as $m \to \infty$. For $p < 0.93$ no statement can be made without actually solving the theory: Eq. (3.12) does not imply an infinite mass gap because a massless theory remains massless even when multiplied by a large scale factor.

The really interesting question, left open by Eq. (3.12), is how $F_m(1)$ behaves relative to the other terms in the Hamiltonian. In particular, under what conditions will $F_m(1) \to \infty$ relative to the other $F_m(j)$ so that the effective Hamiltonian ultimately contains only nearest-neighbor interactions? According to Eq. (3.11), if $F_m(1)$ is much greater than the other $F_m(j)$ then $F_{m+1}(1) = \frac{4}{9}F_m(1)$. Comparing this with Eq. (3.10) requires $C < 4/9$ if the assumption $F_m(1) >> F_m(j>1)$ is to be maintained as $m \to \infty$. $C < 4/9$ corresponds to $p > \log_3 \frac{25}{4} \approx 1.67$, and it is easy to see that $p > 1.67$ is sufficient as well as necessary for $H^{(m)}$ to approach nearest-neighbor form. On the other hand, for $p < 1.67$ it is impossible to have $F_m(1) \to \infty$ relative to the other $F_m(j)$. But $F_m(1) \to 0$ relative to the other $F_m(j)$ is also impossible since by Eq. (3.11) $F_{m+1}(1) > F_m(3) = \frac{1}{C}F_{m+1}(3)$ for large m; thus $F_m(1)/F_m(3)$ is bounded below by $1/C$ as $m \to \infty$. Assuming that $H^{(m)}$ does in fact iterate to a fixed form, the only possibility for $p < 1.67$ is that all the ratios $F_m(1)/F_m(j)$ approach finite nonzero values as $m \to \infty$. The interaction thus remains long-range; furthermore, since $F_m(j) \sim 1/j^p$ for large j, the form of the interaction will be different for each p. In this sense each $p < 1.67$ is in the domain of a separate fixed point.

The energy density computed numerically from Eq. (3.7e) is displayed as the upper curve in Fig. 1. The precise location of the vertical asymptote ($p = -0.07$) is not apparent due to the limited range on the vertical axis. As discussed in paper I, the curve lies 12% above the exact answer in the nearest-neighbor limit $p \to \infty$.

C. Discussion

Several remarks are in order regarding the significance of each of the three points $p = -0.07$, 0.93 and 1.67 at which the character of the fixed-point Hamiltonian $H^{(\infty)}$ changes. (Of course, it is the change in the behavior of $H^{(\infty)}$ that is significant, rather than the precise numerical values found for the critical points. One would not expect the critical points to be very accurately located by the present crude calculation.) It should be realized at the outset that there are basically two ways to obtain information about a theory from a block-spin calculation such as this one. The first way is to solve the fixed-point Hamiltonian. In the present case this will not work for $p < 1.67$ where the fixed-point Hamiltonian contains long-range interactions and is at least as difficult to solve as the original theory. The second way is to study the lattice states iteratively constructed by the blocking procedure. This is not always practical, and in the present case it will not distinguish the phases of the theory because the same lattice states are constructed for all values of p. Therefore, the conclusions drawn from the present calculation are necessarily rather sketchy.

The present calculation does not detect the energy density divergence until $p \leq -0.07$, which compares poorly enough with the anticipated $p \leq 1$ to warrant some discussion. Recall that the ground state energy density was identified as $\lim_{m \to \infty} E_m/3^m$ on the basis of an argument which iterated the blocking procedure until the entire lattice was reduced to a single block. Suppose instead that one performs some fixed number M of iterations, then takes the infinite-volume limit and studies the resulting Hamiltonian $H^{(M)}$. The energy density may be

estimated by $3^{-M}\langle\phi|H^{(M)}|\phi\rangle$ with some variational trial state $|\phi\rangle$. In particular, since $F_M(j) \sim 1/j^p$ asymptotically, the expectation value of $H^{(M)}$ in the ordered state $|\Phi_o\rangle$ of Section II will contain a divergence at $p = 1$ coming from the operator part of $H^{(M)}$. In this way one recovers the correct result. This illustrates that it is always better, when possible, to extract information from the effective Hamiltonian than to continue iterating until the lattice is reduced to a single block. The point is simply that in any variational approximate calculation better trial states exist than the ones being used. In the present case, for p near 1 the state $|\Phi_o\rangle$ is better than the states built using the blocking procedure.

As noted above, the significance of the point $p = 0.93$ is that for $p > 0.93$ the theory is expected to be massless based on the RG equations alone, while for $p < 0.93$ the issue cannot be resolved without further study of the fixed-point Hamiltonian. The theory may be massless for $p < 0.93$ or a mass gap may exist. It might seem that the mass gap would have to be infinite if nonzero because it should diverge with the coupling function $F_m(j)$, but this is not correct. The proper conclusion is that the blocking procedure has identified a class of block states whose energies diverge with the block size when $p < 0.93$. These states certainly need not be the lowest-lying excitations in the system, although to the extent that they are not, the motivation for the blocking scheme as a probe of the low-lying spectrum is weakened. Nevertheless, the suppression of this class of excitations at finite temperature is useful thermodynamic information.

For example, if the Ising model of Eq. (1.2) is treated by the block-spin method of this section one finds that $\lim_{m\to\infty} F_m(j) = \infty$ for $p < 2$. The states constructed by the blocking procedure in this case are the

exact ground states plus states formed by flipping blocks of spins. The divergence of $F_m(j)$ means that at finite temperature flips of large blocks of spins are suppressed. This is responsible for the persistence of order in this model up to a finite critical temperature when $p < 2$. Based on this example one may conjecture that the Heisenberg antiferromagnet also is ordered at low temperatures in some range of p, given as $p < 0.93$ in this very crude calculation.

The point $p = 1.67$ represents the approximate location of a true phase transition, separating the "nearest-neighbor phase" $p > 1.67$ from the "long-range phase" $p < 1.67$. The phases may be distinguished, for example, by the behavior of the correlation function $\langle \vec{S}(i) \cdot \vec{S}(j) \rangle$ of very widely separated spins. The correlation function will be governed by the fixed-point Hamiltonian which is quite different in the two phases. In practice one may consider the translationally invariant correlation function $\mathcal{C}(k) = \lim_{N \to \infty} \frac{1}{N} \sum_i \langle \vec{S}(i) \cdot \vec{S}(i+k) \rangle$ so as to average out edge effects associated with the block walls in a block-spin calculation. Following the treatment of the Hamiltonian, $\vec{S}(i) \cdot \vec{S}(i+k)$ is replaced by an effective operator at each iteration, using Eq. (3.5). When the Hamiltonian achieves its fixed form the required expectation values are computed in its ground state. If the fixed-point Hamiltonian is not solvable, one has no recourse but to continue iterating until the dot products of spins are reduced to squares of single spins with expectation value 3/4. This yields much poorer results: in the present case it leads to correlation functions with no dependence on p, since the block states have none! Indeed, one may be skeptical about the results of the present calculation on the grounds that the same variational trial states are used for all values of p. This problem is corrected in the improved calculation to be discussed next.

IV. Improved Calculation Using Nine-Site Blocks

Although the three-site calculation definitely indicates the presence of a phase transition at $p \approx 1.67$, one would like some assurance that the conclusions do not change qualitatively when more accurate calculations are done. The greatest single drawback of the three-site calculation is that the block eigenstates are completely determined by the rotational invariance, rather than the detailed structure, of the interactions. The nine-site calculation to be discussed now does not suffer from this problem.

The algorithm employed here is just as in Section III. One restricts the full Hamiltonian (3.1) to a nine-site block and, by diagonalizing, determines the lowest-lying spin-1/2 doublet of eigenstates. Taking matrix elements between these states produces the relations analogous to (3.5):

$$\langle \vec{S}(k,a) \rangle = u_a \langle \vec{S}'(k) \rangle \quad , \quad a = 1,2,\ldots,9, \tag{4.1}$$

which may be used to construct the effective Hamiltonians. The u_a, however, will no longer be constants but will change with the value of p and from iteration to iteration. The RG equations will take the form:

$$H^{(m)} = \sum_{k=1}^{N/9^m} E_m + \frac{1}{2} \sum_{\substack{k,k'=1 \\ k \neq k'}}^{N/9^m} (-1)^{k-k'+1} F_m(k-k') \, \vec{S}(k) \cdot \vec{S}(k') \quad , \tag{4.2a}$$

$$F_{m+1}(j) = \sum_{a,a'=1}^{9} (-1)^{a-a'} u_a^{(m)} u_{a'}^{(m)} F_m(9j + a - a') \quad , \quad F_o(j) = F(j) \quad , \tag{4.2b}$$

$$E_{m+1} = 9E_m + e_m \quad , \quad E_o = 0 \quad , \tag{4.2c}$$

where e_m are the energies of the doublet of states constructed at

successive iterations. These RG equations must be iterated numerically using the method of Drell, Svetitsky, and Weinstein described in Section III.

Although there are 512 independent states on a nine-site block, one does not need to diagonalize 512×512 matrices to carry out the above program. It suffices to determine the $S_z = 1/2$ member of the lowest-lying spin-1/2 doublet, which will have even parity. Simple combinatorics shows that there are exactly 22 spin-1/2, $S_z = 1/2$, even parity states on a nine-site block. One of these states can be constructed by two iterations of the three-site blocking procedure [compare Eq. (3.4)]:

$$|\psi\rangle = \frac{1}{\sqrt{6}}\Big[2|\tfrac{1}{2},\tfrac{1}{2}\rangle_1\,|\tfrac{1}{2},-\tfrac{1}{2}\rangle_1\,|\tfrac{1}{2},\tfrac{1}{2}\rangle_1 - |\tfrac{1}{2},\tfrac{1}{2}\rangle_1|\tfrac{1}{2},\tfrac{1}{2}\rangle_1|\tfrac{1}{2},-\tfrac{1}{2}\rangle_1$$

$$- |\tfrac{1}{2},-\tfrac{1}{2}\rangle_1|\tfrac{1}{2},\tfrac{1}{2}\rangle_1|\tfrac{1}{2},\tfrac{1}{2}\rangle_1\Big] \quad ,$$

where $$|\tfrac{1}{2},\tfrac{1}{2}\rangle_1 = \frac{1}{\sqrt{6}}\,(2|\uparrow\downarrow\uparrow\rangle - |\uparrow\uparrow\downarrow\rangle - |\downarrow\uparrow\uparrow\rangle) \quad ,$$

and $$|\tfrac{1}{2},-\tfrac{1}{2}\rangle_1 = \frac{1}{\sqrt{6}}\,(-2|\downarrow\uparrow\downarrow\rangle + |\downarrow\downarrow\uparrow\rangle + |\uparrow\downarrow\downarrow\rangle) \quad . \qquad (4.3)$$

The next state is obtained by applying the block Hamiltonian to $|\psi\rangle$ and eliminating the component of the resulting state along $|\psi\rangle$, and the remaining 20 states are constructed by repeatedly applying the block Hamiltonian to the last state constructed and orthonormalizing the whole set. The matrix to be diagonalized is then 22×22.

In paper I an alternative scheme was suggested, in which only the 2×2 matrix representing the block Hamiltonian in the subspace spanned by $|\psi\rangle$ and $H_{\text{block}}|\psi\rangle$ is diagonalized to obtain approximate nine-site eigenstates. This is based on the idea that $|\psi\rangle$ is already a reasonable approximation

to a nine-site eigenstate and in perturbation theory would mix most strongly with the state $H_{block}|\psi\rangle$. Indeed, one finds by diagonalizing the 22×22 matrices that the exact lowest-lying eigenstate typically gets about 90% of its amplitude from the two states $|\psi\rangle$ and $H_{block}|\psi\rangle$. Since the error in an energy goes as the square of the error in a state vector, energies computed by the 2×2 diagonalization typically are within 1% of the exact nine-site energies. The approximation is thus very good. For definiteness, however, the results to be reported in this section come from the exact nine-site diagonalization using the 22×22 matrices.

Numerical iteration of the RG equations (4.2) shows that there are still three critical values of p with the same qualitative properties discussed in Section III. The region in which the energy density diverges is found to be $p \lesssim 0.18$ (as compared to -0.07 from the previous, less accurate, calculation), the couplings $F_m(j)$ diverge for $p \lesssim 1.11$ (as compared to 0.93), and the transition separating the long-range and nearest-neighbor phases occurs at $p \approx 1.85 \pm 0.05$ (as compared to 1.67). This last value is hard to estimate from numerical data because as the transition point is approached from above the long-range couplings $F_m(j > 1)$ decay more and more slowly. Very near the transition it is impossible to tell whether the long-range couplings ultimately vanish or not. However, it is significant that this critical point moved <u>up</u> from 1.67. Had it moved down one might have suspected that an exact calculation would reveal <u>no</u> transition in the "physical region" $p > 1$.

The ground state energy density resulting from this calculation is given by the lower curve in Fig. 1. For $p \to \infty$ the energy density is -0.4212, 5% above the correct value.

Since the block states now depend on p, correlation functions computed using nine-site blocks will have p-dependence and will distinguish the long-range and nearest-neighbor phases. In a simple block-spin calculation of the present type (non-variational) one obtains a power-law falloff at large distances, where the exponent is a constant throughout the nearest-neighbor phase but depends on p once the long-range phase is entered. It is worth emphasizing that no evidence will be found for the violation of the cluster property known to occur at $p = 0$. The effective operator representing the end-to-end order after m iterations satisfies the RG equation:

$$\left[\vec{S}(1) \cdot \vec{S}(N)\right]_{Eff}^{(m+1)} = u_1^{(m)} u_9^{(m)} \left[\vec{S}(1) \cdot \vec{S}(N)\right]_{Eff}^{(m)} , \qquad (4.4)$$

and since $u_1^{(m)}, u_9^{(m)} < 1$ [this follows from Eq. (4.1) and the fact that the magnitude of the expectation value of S_z in a non-eigenstate is less than 1/2] one has $\lim_{N \to \infty} \langle \vec{S}(1) \cdot \vec{S}(N) \rangle = 0$. This is because a cluster property is really built into block-spin calculations: at any iteration correlations between spins in different blocks are ignored. This is also why the calculations locate the energy density divergence poorly. The most one could hope for is that if the cluster property is violated,

then $\langle \vec{S}(1) \cdot \vec{S}(N) \rangle$ will go to zero more slowly as the accuracy of the calculation is improved.

V. Concluding Remarks

The most accurate calculation discussed in this paper indicates that the Heisenberg antiferromagnet (1.1) has a phase transition at $p \approx 1.85$. The phases can be distinguished by the form of the fixed-point Hamiltonian and the behavior of correlation functions such as $\langle \vec{S}(i) \cdot \vec{S}(j) \rangle$. The large-p phase has the physics of the nearest-neighbor antiferromagnet while for $p \lesssim 1.85$ there is a line of fixed points. The calculation predicts that the model is massless for $p \gtrsim 1.11$. More detailed statements cannot be made due to the intractability of the fixed-point Hamiltonian for $p \lesssim 1.85$.

It is interesting to speculate on how these numbers will change in more accurate calculations. As the accuracy increases, the point at which the energy density begins to diverge must approach $p = 1$. The point at which the couplings begin to diverge must be at a larger value of p, since the couplings must grow by a factor L at each iteration to get a divergent energy density, with L the number of sites per block. The calculations done here suggest that the divergent couplings and the divergent energy density are separated by about 1 unit of p. It is tempting to suppose that the onset of the divergent couplings occurs at $p \approx 2$ and coincides with the nearest-neighbor to long-range phase transition. The divergent couplings in the long-range phase then make it possible that there is long-range order at finite temperature in this phase. Thus, Dyson's conjecture for the Heisenberg ferromagnet (see the Introduction) may hold for the antiferromagnet as well.

It is difficult to recommend reliable ways to improve the present calculations. Simply going to bigger blocks soon becomes cumbersome due to the size of the matrices to be diagonalized. Another possibility is to write effective Hamiltonians valid for more block states than just the lowest pair. This method generally gives large increases in numerical accuracy because the additional states contain information on energy levels and the density of states not present in the lowest-lying pair of states alone. For example, the two-site calculation using four states per block for the nearest-neighbor Heisenberg model (paper I) gives almost the same accuracy in the energy density as the nine-site calculation discussed here. However, this method will not preserve the form of the original Hamiltonian but will embed it in a more general (and more complicated) theory after the first iteration. As discussed in paper I, it is then necessary to study the phases of the more general theory and to understand how the original theory has been embedded. Finally, variational calculations in which the block states are chosen to minimize the ground state energy after many iterations rather than to diagonalize the block Hamiltonians can give excellent results,[4] but how to choose good variational trial states is an open question.

Acknowledgements

I would like to thank Helen Quinn, Ben Svetitsky, and Marvin Weinstein for many helpful conversations and for comments on the manuscript.

This work was supported in part by the Department of Energy under contract number DE-AC03-76SF00515, and in part by a National Science Foundation Fellowship.

References

1. J. M. Rabin, Phys. Rev. B21, 2027 (1980) will be referred to as paper I.
2. S. D. Drell, M. Weinstein and S. Yankielowicz, Phys. Rev. D14, 487 (1976).
3. S. D. Drell, M. Weinstein and S. Yankielowicz, Phys. Rev. D14, 1627 (1976).
4. S. D. Drell, M. Weinstein and S. Yankielowicz, Phys. Rev. D16, 1769 (1977).
5. S. D. Drell, B. Svetitsky and M. Weinstein, Phys. Rev. D17, 523 (1978).
6. S. D. Drell and M. Weinstein, Phys. Rev. D17, 3203 (1978).
7. R. Jullien, J. N. Fields and S. Doniach, Phys. Rev. B16, 4889 (1977).
8. R. Jullien and P. Pfeuty, Phys. Rev. B19, 4646 (1979).
9. D. Ruelle, Commun. Math. Phys. 9, 267 (1968); F. J. Dyson, Commun. Math. Phys. 12, 91 (1969).
10. H. Bethe, Z. Phys. 71, 205 (1931); L. Hulthén, Ark. Mat. Astron. Fys. 26A, No. 11 (1938); J. des Cloizeaux and J. J. Pearson, Phys. Rev. 128, 2131 (1962).

Figure Captions

1. Renormalization group results for the ground state energy density of the Heisenberg model with $(\text{distance})^{-p}$ interactions. The upper curve is the three-site calculation of Section III; the lower curve is the nine-site calculation of Section IV. The exact result in the limit $p \to \infty$, -0.4431, is marked.

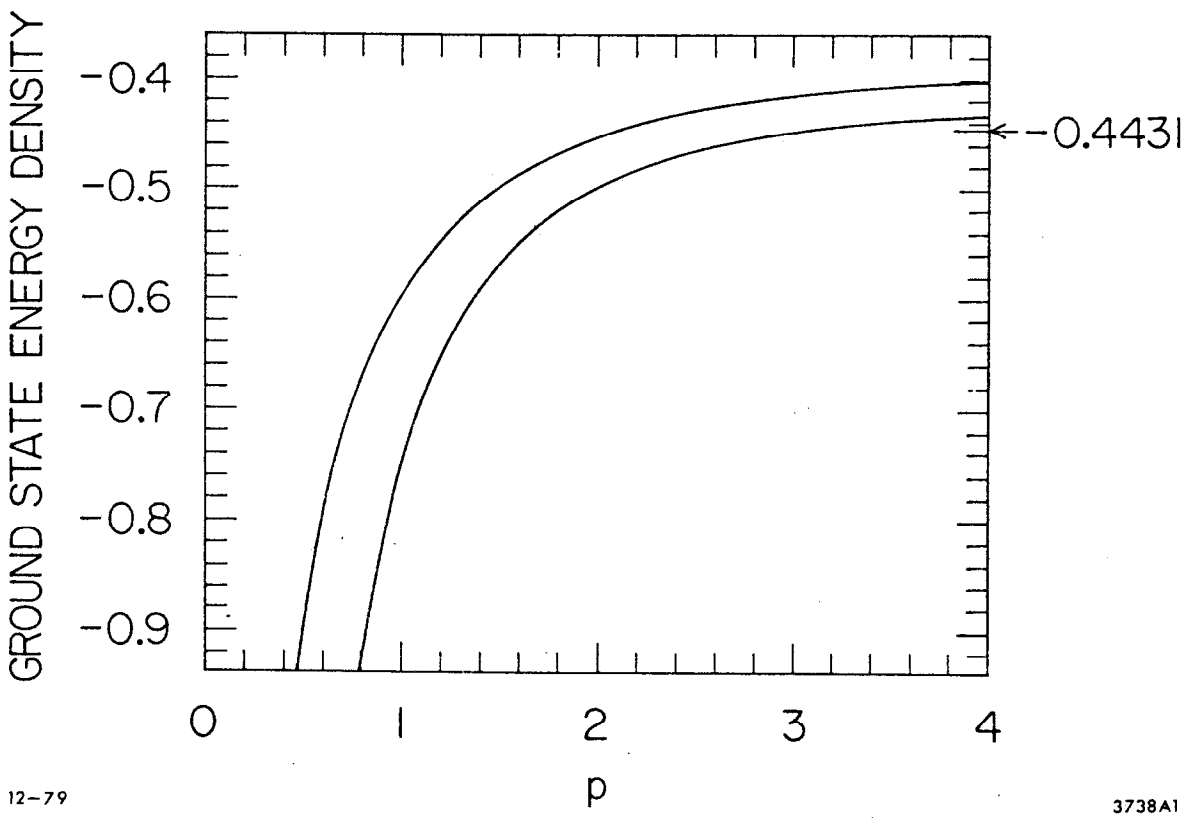
GROUND STATE ENERGY DENSITY
-0.4
-0.5
-0.6
-0.7
-0.8
-0.9
-0.4431
0
1
2
3
4
p
12-79
3738A1

Fig. 1