Renormalization-group studies of antiferromagnetic chains. I. Nearest-neighbor interactions

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The real-space renormalization-group method introduced by workers at the Stanford Linear Accelerator Center (SLAC) is used to study one-dimensional antiferromagnetic chains at zero temperature. Calculations using three-site blocks (for the Heisenberg-Ising model) and two-site blocks (for the isotropic Heisenberg model) are compared with exact results. In connection with the two-site calculation, a duality transformation is introduced under which the isotropic Heisenberg model is self-dual. Such duality transformations can be defined for models other than those considered here, and may be useful in various block-spin calculations.

I. INTRODUCTION

During the past few years the real-space renormalization-group (RG) technique introduced by workers at the Stanford Linear Accelerator Center (SLAC) has been successfully applied to several lattice models of field theories and spin systems.[1–6] It has been shown to yield accurate results for correlation functions and low-lying energy levels, and to locate phase transitions reliably. Furthermore, calculations using this technique can be systematically improved to provide arbitrary accuracy.[4]

This is the first of two papers in which the RG technique is applied to an antiferromagnetic Heisenberg spin system with long-range interactions on a one-dimensional lattice at zero temperature:

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

where $\vec{S}(i)$ denotes a spin-$\frac{1}{2}$ operator acting on the ith lattice site. This model is of interest in view of rigorous theorems proved by Dyson and Ruelle for the Ising model analogous to Eq. (1.1).[7] According to these theorems, the Ising model is disordered at all finite temperatures if $p>2$, while for $p<2$ there is order at sufficiently low temperatures. One would like to know whether the model (1.1) also has different phases as p is varied, even at zero temperature. Further motivation for studying the model comes from the fact that the power-law interaction of Eq. (1.1) also appears in lattice field theories when the lattice gradient is defined according to the SLAC prescription.[1] In this paper various block-spin methods will be tested on the nearest-neighbor Heisenberg model which is the $p\to\infty$ limit of Eq. (1.1), reserving the case of general p for subsequent work. In particular it will be shown that a three-site blocking procedure is much more suitable for studying the model (1.1) than a two-site calculation.

This paper is organized as follows: In Sec. II the three-site blocking procedure is described and applied to the nearest-neighbor spin chain *with anisotropy* (Heisenberg-Ising model). This is done to facilitate comparison with the calculation of Sec. III: it will be useful to have studied the isotropic model of interest as an unstable fixed point (in the RG sense) of a more general model. It is shown that the three-site calculation correctly reproduces the qualitative physics of the model and gives the ground-state energy density to within 12%. Section III describes a two-site blocking procedure for the isotropic nearest-neighbor model. After the first blocking the model has been embedded as an unstable fixed point in a more general model of integer-spin particles. It is shown that a naive application of the blocking procedure leads to entirely incorrect physics for the isotropic model, and that this is due to the instability of the fixed point and the approximate nature of the calculation. Although the problem is easily understood in this context, it makes the two-site calculation too unreliable to use for general p. The situation is further clarified by introducing a duality transformation for the integer-spin model. It is suggested that such duality transformations may have applications beyond this particular model. Section IV describes ways to improve the three-site calculation of Sec. II. In particular, an approximate calculation on a nine-site block is discussed. Section V contains some concluding remarks.

II. NEAREST-NEIGHBOR HEISENBERG-ISING ANTIFERROMAGNET

In this section the three-site blocking algorithm is described and applied to the nearest-neighbor model

with Hamiltonian

$$H=\sum_{i=1}^{N-1}[S_x(i)S_x(i+1)+S_y(i)S_y(i+1)+\gamma S_z(i)S_z(i+1)]\ ,\quad \gamma\geq 0\ , \tag{2.1}$$

where the infinite-volume limit $N\to\infty$ will generally be assumed. The lattice sites may be grouped into blocks of three and labeled by ordered pairs (k,a) where $k=1,2,\ldots,\frac{1}{3}N$ specifies the block and $a=1,2,3$ labels sites within that block. Thus the ith lattice site may be relabeled (k,a) where $i=3k-3+a$. Three-site blocks are convenient because the block states will have half-integer spin as do the original degrees of freedom. The Hamiltonian may now be decomposed into two pieces, H_{in} and H_{out}, where H_{in} couples sites within a single block and H_{out} couples sites in adjacent blocks:

$$\begin{aligned}H&=H_{\text{in}}+H_{\text{out}}\ ,\\ H_{\text{in}}&=\sum_k[S_x(k,1)S_x(k,2)+S_x(k,2)S_x(k,3)\\ &\quad+S_y(k,1)S_y(k,2)+S_y(k,2)S_y(k,3)\\ &\quad+\gamma S_z(k,1)S_z(k,2)+\gamma S_z(k,2)S_z(k,3)]\ ,\\ H_{\text{out}}&=\sum_k[S_x(k,3)S_x(k+1,1)+S_y(k,3)S_y(k+1,1)\\ &\quad+\gamma S_z(k,3)S_z(k+1,1)]\ .\end{aligned} \tag{2.2}$$

To diagonalize H_{in}, it suffices to consider a single block

$$\begin{aligned}H_{\text{in}}&=\sum_k H_{\text{block}}(k)\ ,\\ H_{\text{block}}&=\vec{S}(1)\cdot\vec{S}(2)+\vec{S}(2)\cdot\vec{S}(3)\\ &\quad+\epsilon[S_z(1)S_z(2)+S_z(2)S_z(3)]\\ &=\tfrac{1}{2}\{[\vec{S}(1)+\vec{S}(2)+\vec{S}(3)]^2\\ &\quad-[\vec{S}(1)+\vec{S}(3)]^2-\tfrac{3}{4}\}\\ &\quad+\epsilon[S_z(1)S_z(2)+S_z(2)S_z(3)]\ ,\end{aligned} \tag{2.3}$$

where $\epsilon=\gamma-1$.

For $\epsilon=0$, H_{block} is rotationally invariant, and its eigenstates are found by combining $\vec{S}(1)$ and $\vec{S}(3)$ to give a total spin 0 or 1, which is then coupled to $\vec{S}(2)$. These states form a spin-$\frac{3}{2}$ multiplet and two spin-$\frac{1}{2}$ doublets and are (notation is $|S,S_z\rangle$)

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

$$|\tfrac{1}{2},\tfrac{1}{2}\rangle_0=\frac{1}{\sqrt{2}}(|\uparrow\uparrow\downarrow\rangle-|\downarrow\uparrow\uparrow\rangle),\qquad E=0\ , \tag{2.4}$$

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

plus the four corresponding states with all spins flipped and negative total S_z, where E is the energy.

For $\epsilon\neq 0$, H_{block} is invariant only under rotations about the z axis (plus the discrete symmetry $z\to -z$ which keeps the energy independent of the sign of S_z) so that states of different total spin but equal S_z can mix. One finds that $|\frac{3}{2},\frac{3}{2}\rangle$ is still an eigenstate, with energy $\frac{1}{2}\gamma$, $|\frac{1}{2},\frac{1}{2}\rangle_0$ is still an eigenstate with energy 0, but that $|\frac{3}{2},\frac{1}{2}\rangle$ and $|\frac{1}{2},\frac{1}{2}\rangle_1$ do mix. By diagonalizing a 2×2 matrix, one finds that the lowest-energy eigenstate is

$$\begin{aligned}|+\tfrac{1}{2}\rangle&\equiv(1+2x^2)^{-1/2}(|\tfrac{1}{2},\tfrac{1}{2}\rangle_1+\sqrt{2}x|\tfrac{3}{2},\tfrac{1}{2}\rangle)\ ,\\ E&=-\tfrac{1}{4}[\gamma+(\gamma^2+8)^{1/2}]\ ,\\ x&\equiv 2(\gamma-1)[8+\gamma+3(\gamma^2+8)^{1/2}]^{-1}\ .\end{aligned} \tag{2.5}$$

Thus far the state of the lattice has been described in terms of the state—spin up or spin down—of the spin-$\frac{1}{2}$ particle at each site. Since the eight eigenstates of H_{block} form a complete set, an equally good description (corresponding to a different basis in the Hilbert space of states) is obtained by specifying the eigenstate of each block. However, it is physically reasonable to expect the low-lying states of the lattice to be predominantly formed from the low-lying eigenstates of H_{block}. I therefore make the approximation of restricting attention to the sector of states built from the block states $|+\frac{1}{2}\rangle$ and $|-\frac{1}{2}\rangle$ only, $|-\frac{1}{2}\rangle$ being obtained from $|+\frac{1}{2}\rangle$ under $z\to -z$. The next step is to write an effective Hamiltonian which has the same matrix elements as the original Hamiltonian within this sector of states.

More explicitly, the lowest-lying states of H_{block} are

$$\begin{aligned}|+\tfrac{1}{2}\rangle&=(1+2x^2)^{-1/2}\frac{1}{\sqrt{6}}[|\uparrow\downarrow\uparrow\rangle(2x+2)+|\uparrow\uparrow\downarrow\rangle(2x-1)+|\downarrow\uparrow\uparrow\rangle(2x-1)]\ ,\\ |-\tfrac{1}{2}\rangle&=-(1+2x^2)^{-1/2}\frac{1}{\sqrt{6}}[|\downarrow\uparrow\downarrow\rangle(2x+2)+|\downarrow\downarrow\uparrow\rangle(2x-1)+|\uparrow\downarrow\downarrow\rangle(2x-1)]\ .\end{aligned} \tag{2.6}$$

The overall sign difference between the states reflects Condon-Shortley phase conventions. The effective Hamiltonian is constructed from new spin operators $\vec{S}'$ defined by $\langle +\frac{1}{2}|S_z'|+\frac{1}{2}\rangle = \frac{1}{2}$, $\langle -\frac{1}{2}|S_z'|-\frac{1}{2}\rangle = -\frac{1}{2}$, etc. With this definition it is easy to check that in each block

$$\langle S_x(1)\rangle = \langle S_x(3)\rangle = \frac{2(1+x)(1-2x)}{3(1+2x^2)}\langle S_x'\rangle \ ,$$

$$\langle S_y(1)\rangle = \langle S_y(3)\rangle = \frac{2(1+x)(1-2x)}{3(1+2x^2)}\langle S_y'\rangle \ , \quad (2.7)$$

$$\langle S_z(1)\rangle = \langle S_z(3)\rangle = \frac{2(1+x)^2}{3(1+2x^2)}\langle S_z'\rangle \ ,$$

where the notation $\langle\ \rangle$ indicates any one of the four matrix elements involving the states $|\pm\frac{1}{2}\rangle$, and the equality $\langle\vec{S}(1)\rangle = \langle\vec{S}(3)\rangle$ follows from the even parity of these states. Using the relations (2.7) to eliminate the $\vec{S}$ operators from H_{out}, and remembering that H_{in} has been diagonalized, the effective Hamiltonian can be written

$$H^{(1)} = \sum_{k=1}^{N/3} a_1 + \sum_{k=1}^{(N/3)-1} b_1[S_x'(k)S_x'(k+1) + S_y'(k)S_y'(k+1) + \gamma_1 S_z'(k)S_z'(k+1)] \ , \quad (2.8)$$

$$a_1 = -\tfrac{1}{4}[\gamma + (\gamma^2+8)^{1/2}] \ ,$$

$$b_1 = \left[\frac{2(1+x)(1-2x)}{3(1+2x^2)}\right]^2 \ ,$$

$$\gamma_1 = \left[\frac{1+x}{1-2x}\right]^2\gamma \ .$$

Because this Hamiltonian has the same form as the original one, apart from the energy shift a_1 and the scale factor b_1, the blocks of the original lattice may be viewed as sites of a new lattice and an identical blocking procedure applied to $H^{(1)}$. In this way one generates a sequence of Hamiltonians $H^{(m)}$ describing the physics of ever larger length scales (block sizes) and obeying the following *renormalization-group equations:*

$$H^{(m)} = \sum_{k=1}^{N/3^m} a_m + \sum_{k=1}^{(N/3^m)-1} b_m[S_x(k)S_x(k+1) + S_y(k)S_y(k+1) + \gamma_m S_z(k)S_z(k+1)] \ ,$$

$$a_{m+1} = 3a_m - \tfrac{1}{4}b_m[\gamma_m + (\gamma_m^2+8)^{1/2}] \ ,$$

$$b_{m+1} = b_m\left[\frac{2(1+x_m)(1-2x_m)}{3(1+2x_m^2)}\right]^2 \ , \quad (2.9)$$

$$\gamma_{m+1} = \gamma_m\left[\frac{1+x_m}{1-2x_m}\right]^2 \ ,$$

$$a_0 = 0, \quad b_0 = 1, \quad \gamma_0 = \gamma \ ,$$

where

$$x_m \equiv 2(\gamma_m - 1)[8 + \gamma_m + 3(\gamma_m^2+8)^{1/2}]^{-1} \ .$$

(The primes on the block spin operators in $H^{(m)}$ have been dropped for simplicity.) Here a_m is a c-number contribution to the energy which after sufficiently many iterations of the blocking procedure becomes the dominant contribution. In fact, on the finite lattice of length N, after roughly $m = \log_3 N$ iterations the whole lattice has been reduced to a single block and a_m is the *only* contribution to the energy. Since at each iteration the number of lattice sites drops by a factor $\frac{1}{3}$, the energy per original lattice site is to be computed as $a_m/3^m \equiv \mathcal{E}_m$. Returning to an infinite lattice by letting $N \to \infty$, one obtains an energy density given by $\lim_{m\to\infty}\mathcal{E}_m$, where $\mathcal{E}_m$ satisfies

$$\mathcal{E}_{m+1} = \mathcal{E}_m - \frac{1}{12(3^m)}b_m[\gamma_m + (\gamma_m^2+8)^{1/2}] \ ,$$
$$\mathcal{E}_0 = 0 \ . \quad (2.10)$$

Since the whole RG procedure may be viewed as a variational calculation in which the set of variational trial states is "thinned out" or "truncated" with each iteration, the energy density computed from Eq. (2.10) will always be an upper bound on the true energy density.

The RG equations have three fixed points in the region $\gamma \geq 0$: $\gamma = 0$ (isotropic XY model), $\gamma = 1$ (isotropic Heisenberg model), and $\gamma = \infty$ (Ising model). I now proceed to discuss them.

a. $\gamma = 0$. Near this point the RG equations become

$$\gamma_{m+1} = \tfrac{1}{2}\gamma_m \ , \quad (2.11a)$$

$$b_{m+1} = [\tfrac{1}{2} + O(\gamma_m)]b_m \ , \quad (2.11b)$$

$$\mathcal{E}_{m+1} = \mathcal{E}_m - \frac{1}{12(3^m)}b_m(2\sqrt{2} + \gamma_m) \ . \quad (2.11c)$$

Equation (2.11a) implies that if $|\gamma|$ is small the system will be driven to the isotropic XY form: the $\gamma = 0$ fixed point is *stable*. According to Eq. (2.11b), $\lim_{m\to\infty} b_m = 0$, which implies that the isotropic XY model is a massless theory: after sufficiently many iterations it is possible to construct variational trial states with arbitrarily small excitation energy. It is also possible to compute the energy density at the point $\gamma = 0$: Eqs. (2.11b) and (2.11c) imply $\mathcal{E}_{m+1} = \mathcal{E}_m - (\sqrt{2}/6^{m+1})$. This leads to a geometric series for $\mathcal{E}_\infty$ whose sum is $\mathcal{E}_\infty = -\frac{1}{5}\sqrt{2} = -0.2828$, to be compared with the exact result[8] $\mathcal{E} = -1/\pi = -0.3183$. The error is 11%.

b. $\gamma = 1$. Near this point $\gamma = 1 + \epsilon$ with $|\epsilon| \ll 1$,

and the RG equations become

$$\epsilon_{m+1} = \tfrac{5}{3}\epsilon_m \ , \tag{2.12a}$$

$$b_{m+1} = \tfrac{4}{9} b_m (1 - \tfrac{2}{9}\epsilon_m) \ , \tag{2.12b}$$

$$\mathcal{E}_{m+1} = \mathcal{E}_m - \frac{b_m}{3^{m+1}}(1+\epsilon_m) \ . \tag{2.12c}$$

Equation (2.12a) shows that this fixed point is *unstable:* however small ϵ_0 may be, after many iterations one will have $\epsilon_m \sim 1$ and Eqs. (2.12) will cease to hold. According to Eq. (2.12b), $b_m \to 0$ at $\epsilon = 0$ so that the isotropic Heisenberg model is massless. Finally, using Eqs. (2.12b) and (2.12c) to compute the energy density at $\epsilon = 0$ gives $_{m+1} = \mathcal{E}_m - \frac{1}{3}(\frac{4}{27})^m$, a geometric series whose sum is $\mathcal{E}_\infty = -\frac{9}{23} = -0.3913$. This differs by 12% from the exact result,[9] $\mathcal{E} = -0.4431$.

c. $\gamma = \infty$. In the limit $\gamma >> 1$ the RG equations become

$$x_m = \tfrac{1}{2}\left(1 - \frac{3}{\gamma_m}\right) \ , \tag{2.13a}$$

$$\gamma_{m+1} = \tfrac{1}{4}\gamma_m^3\left(1 - \frac{2}{\gamma_m}\right) \ , \tag{2.13b}$$

$$b_{m+1} = \frac{4}{\gamma_m^2} b_m \left(1 + \frac{6}{\gamma_m}\right) \ , \tag{2.13c}$$

$$\mathcal{E}_{m+1} = \mathcal{E}_m - \frac{1}{6(3^m)} b_m \gamma_m \ . \tag{2.13d}$$

Equation (2.13b) demonstrates the stability of the $\gamma = \infty$ fixed point: once γ_m becomes large, it essentially cubes itself with each iteration. Equations (2.13b) and (2.13c) imply that for γ sufficiently large,

$$b_{m+1}\gamma_{m+1} = b_m \gamma_m = b_0 \gamma_0 = \gamma \ , \tag{2.14}$$

so that Eq. (2.13d) gives the energy density as

$$\mathcal{E}_\infty = -\gamma \sum_{m=0}^{\infty}\left(\frac{1}{(6\times 3^m)}\right) = -\tfrac{1}{4}\gamma \ .$$

This is the *exact* result for the Ising model $\gamma \to \infty$, which is easily understood since the block states $|\pm\tfrac{1}{2}\rangle$ become in this limit

$$\begin{aligned} |+\tfrac{1}{2}\rangle &= |\uparrow\downarrow\uparrow\rangle - \frac{1}{\gamma}|\uparrow\uparrow\downarrow\rangle - \frac{1}{\gamma}|\downarrow\uparrow\uparrow\rangle \ , \\ |-\tfrac{1}{2}\rangle &= -|\downarrow\uparrow\downarrow\rangle + \frac{1}{\gamma}|\downarrow\downarrow\uparrow\rangle + \frac{1}{\gamma}|\uparrow\downarrow\downarrow\rangle \ , \end{aligned} \tag{2.15}$$

so that the RG algorithm constructs the exact Ising ground state. The fact that $b_m \to 0$ in this case is not sufficient to give a massless theory because $\gamma_m \to \infty$. The mass gap for any $\gamma > 1$ is in fact given by $b_\infty \gamma_\infty$, which is the gap at the stable Ising fixed point. This quantity is shown to be nonzero in the discussion of end-to-end order given below.

The picture that emerges from this analysis is that, for $0 \leq \gamma < 1$, the system is driven to the massless isotropic XY form, while for $\gamma > 1$ it is driven to the massive Ising form. The unstable fixed point $\gamma = 1$ separates the two regimes. This is precisely the known behavior of this model.[10] One might ask how this approximate calculation is able to locate the correct phase transition exactly, at $\gamma = 1$. This is guaranteed by a symmetry: at $\gamma = 1$ the system becomes rotationally invariant, and the RG transformation has been defined so as to preserve rotational invariance if it is initially present. This point will be important in Sec. III.

It is also possible to calculate the end-to-end order in the ground state, defined as $|\langle \vec{S}(1)\cdot\vec{S}(N)\rangle|$. This is done, in direct analogy to the treatment of H, by replacing the operator $\vec{S}(1)\cdot\vec{S}(N)$ with an effective operator having the same matrix elements in the sector of states retained at each iteration. Since the first and last spins on the lattice are also the first spin in the first block and the third spin in the last block, Eqs. (2.7) and (2.9) show that after m iterations the appropriate effective operator is

$$[\vec{S}(1)\cdot\vec{S}(N)]_{\text{eff}}^{(m)} = b_m\left[S_x(1)S_x\left(\frac{N}{3^m}\right) + S_y(1)S_y\left(\frac{N}{3^m}\right)\right] + \frac{1}{\gamma} b_m \gamma_m S_z(1) S_z\left(\frac{N}{3^m}\right) \ . \tag{2.16}$$

Since $b_m \to 0$ in all cases, the end-to-end order may be computed as

$$|\langle \vec{S}(1)\cdot\vec{S}(N)\rangle| = |\langle S_z(1)S_z(\text{last})\rangle|\frac{1}{\gamma} b_\infty \gamma_\infty \ , \tag{2.17}$$

where the expectation value on the right-hand side is evaluated in the ground state of the fixed-point Hamiltonian $H^{(\infty)}$. Clearly this predicts no end-to-end order for $0 \leq \gamma \leq 1$. The vanishing of the order for $\gamma = 1$ may also be obtained as a consequence of the rotational symmetry of the theory and the cluster property

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

For $\gamma > 1$ the system is driven to the Ising model for which $|\langle S_z(1)S_z(\text{last})\rangle| = \frac{1}{4}$. Using Eqs. (2.9), one has for $\gamma > 1$

$$|\langle \vec{S}(1)\cdot\vec{S}(N)\rangle| = \tfrac{1}{4}\prod_{n=0}^{\infty}\frac{4}{9}\frac{(1+x_n)^4}{(1+2x_n^2)^2} \ . \tag{2.18}$$

This infinite product is in fact convergent and nonzero. For m sufficiently large that $\gamma_m >> 1$, one finds from Eq. (2.13a) that $\frac{4}{9}[(1+x_m)^4/(1+2x_m^2)^2] = 1 - O(\gamma_m^{-2})$. The product (2.18) is finite and

nonzero if and only if the sum

$$\sum_{n>m} \ln[1-O(\gamma_n^{-2})] \cong -\sum_{n>m} O(\gamma_n^{-2})$$

converges. Since $\gamma_{n+1} \simeq \gamma_n^3$ for $n > m$, the sum is highly convergent. It is important to note that the end-to-end order depends not only on which fixed point is ultimately reached, but also on the rapidity with which it is approached.

It is also easy to obtain the limiting behavior of the end-to-end order as $\gamma \to 1+$ using Eq. (2.18). Set $\gamma = 1+\epsilon$ with $|\epsilon| \ll 1$. According to Eq. (2.12a), one iteration of the RG equations changes ϵ into $\frac{5}{3}\epsilon$. Since $x_0 \cong 0$ for $\gamma \cong 1$, it follows from Eq. (2.18) that

$$|\langle \vec{S}(1)\cdot\vec{S}(N)\rangle|(\epsilon) = \tfrac{4}{9}|\langle \vec{S}(1)\cdot\vec{S}(N)\rangle|(\tfrac{5}{3}\epsilon) \ , \tag{2.19a}$$

a functional equation which is solved by

$$|\langle \vec{S}(1)\cdot\vec{S}(N)\rangle|(\epsilon) \propto \epsilon^{1.6}, \quad 0<\epsilon \ll 1 \ ,$$

where

$$1.6 = \frac{\ln(\frac{4}{9})}{\ln(\frac{3}{5})} \ . \tag{2.19b}$$

Figures 1 and 2 show the results of numerical iteration of the RG equations. Figure 1 compares the ground-state energy density computed from Eq. (2.10) with the exact solution of Orbach,[9] while Fig. 2 displays the results of the present calculation for the end-to-end order and the mass gap. Note that the energy density and mass gap both refer to the Hamiltonian used by Orbach, which differs slightly from that used here:

$$\begin{aligned} H_{\text{Orbach}} &= \sum_i \{(1-\alpha)[S_x(i)S_x(i+1)+S_y(i)S_y(i+1)]+S_z(i)S_z(i+1)\} \\ &= \frac{1}{\gamma}\sum_i [S_x(i)S_x(i+1)+S_y(i)S_y(i+1)+\gamma S_z(i)S_z(i+1)] \ , \end{aligned} \tag{2.20}$$

with

$$\gamma = \frac{1}{1-\alpha} \ ,$$

so that the region $1 \leq \gamma \leq \infty$ corresponds to $0 \leq \alpha \leq 1$. Due to the factor $1/\gamma$ in Eq. (2.20), the RG results for the order and the mass gap for this Hamiltonian differ only by a factor of 4, as shown in Fig. 2. The greatest error in the energy density is the 12% error at $\alpha = 0$, and the general shape of the curve is correct. According to Eq. (2.19b) the curve in Fig. 2 behaves as $\alpha^{1.6}$ for α near zero, whereas in fact both the gap[10] and the order[11] are known to vanish exponentially as $\alpha \to 0+$. This substitution of power law for exponential behavior is a common feature of simple block-spin calculations of this type and can be corrected by improving the calculation using variational techniques.[4] Except for this feature, the results of the simple RG calculation given here are completely consistent with the known properties of this model.

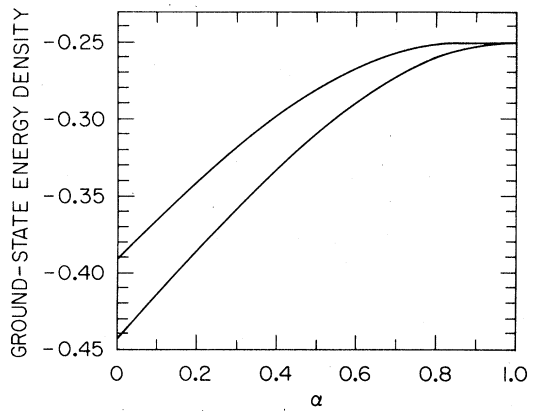

FIG. 1. Comparison of the exact ground-state energy density for H_{Orbach} (lower curve) with the result of the renormalization-group calculation (upper curve).

III. TWO-SITE CALCULATION FOR THE ISOTROPIC HEISENBERG MODEL

A rule of thumb for block-spin calculations states that theories involving half-integral spins or fermionic degrees of freedom should be treated using an odd

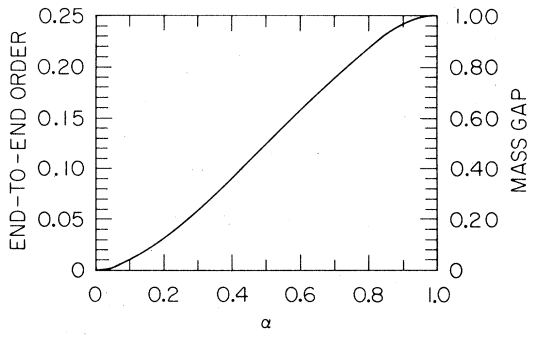

FIG. 2. Results of the renormalization-group calculation of the end-to-end order $|\langle \vec{S}(1)\cdot\vec{S}(N)\rangle|$ and the mass gap for H_{Orbach}.

number of sites per block to preserve these features. The consequences of ignoring this good advice will now be examined by applying a two-site blocking procedure to the isotropic Heisenberg model

$$H=\sum_{i=1}^{N-1}\vec{S}(i)\cdot\vec{S}(i+1)\ . \tag{3.1}$$

Decomposing the Hamiltonian into pieces which do and do not connect different two-site blocks yields:

$$\begin{aligned} H&=H_{\text{in}}+H_{\text{out}}\ ,\\ H_{\text{in}}&=\sum_k\vec{S}(k,1)\cdot\vec{S}(k,2)\ ,\\ H_{\text{out}}&=\sum_k\vec{S}(k,2)\cdot\vec{S}(k+1,1)\ . \end{aligned} \tag{3.2}$$

Anticipating that tensor operators will be useful in the description of the integer-spin block states, I write the operators appearing here in terms of raising and lowering operators:

$$\begin{aligned} \vec{S}(k,a)\cdot\vec{S}(k',a')=&S_0(k,a)S_0(k',a')\\ &-S_1(k,a)S_{-1}(k',a')\\ &-S_{-1}(k,a)S_1(k',a')\ , \end{aligned} \tag{3.3}$$

where $S_0\equiv S_z$ and $S_{\pm1}\equiv\mp(1/\sqrt{2})(S_x\pm iS_y)$.

The block Hamiltonian is introduced by

$$\begin{aligned} H_{\text{in}}&=\sum_k H_{\text{block}}(k)\ ,\\ H_{\text{block}}&=\vec{S}(1)\cdot\vec{S}(2)\ . \end{aligned} \tag{3.4}$$

The eigenstates of H_{block} form the familiar singlet and triplet which will be labeled as follows:

$$\left.\begin{aligned} |+\rangle&=|\uparrow\uparrow\rangle\ ,\\ |0\rangle&=\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle)\ ,\\ |-\rangle&=|\downarrow\downarrow\rangle\ , \end{aligned}\right\}\ E=+\tfrac{1}{4}\ ,$$

$$|\times\rangle=\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle)\ ,\quad E=-\tfrac{3}{4}\ . \tag{3.5}$$

The Hamiltonian must now be rewritten in terms of block-spin operators which act on the states (3.5). To keep rotational invariance explicit, it is useful to define spherical tensor operators of rank 1, Q_i, and T_i, $i=-1,0,+1$, by

$$Q_0=S_z,\quad Q_{\pm1}=\mp\frac{1}{\sqrt{2}}(S_x\pm iS_y)\ , \tag{3.6}$$

$$\begin{aligned} &\langle 0|T_0|\times\rangle=1\ ,\quad \langle\times|T_0|0\rangle=1\ ,\\ &\langle+|T_1|\times\rangle=1\ ,\quad \langle\times|T_1|-\rangle=-1\ ,\\ &\langle-|T_{-1}|\times\rangle=1\ ,\quad \langle\times|T_{-1}|+\rangle=-1\ , \end{aligned} \tag{3.7}$$

and all other matrix elements of $T_i=0$, where S_x, S_y, and S_z are the usual spin operators for a spin-1 particle whose states are $|+\rangle$, $|0\rangle$, and $|-\rangle$; these operators annihilate the spinless state $|\times\rangle$. Q_i thus acts only within the spin-1 subspace while T_i connects the spin-0 state to the spin-1 states. It is easy to check that the following relations between matrix elements of the spin-$\frac{1}{2}$ operators appearing in H_{block} and of the operators introduced in Eqs. (3.6) and (3.7) hold between any pair of the states $|+\rangle$, $|0\rangle$, $|-\rangle$, and $|\times\rangle$:

$$\langle S_i(1)\rangle=\tfrac{1}{2}\langle Q_i+T_i\rangle,\quad \langle S_i(2)\rangle=\tfrac{1}{2}\langle Q_i-T_i\rangle\ . \tag{3.8}$$

These relations may be inverted

$$\langle Q_i\rangle=\langle S_i(1)+S_i(2)\rangle,\quad \langle T_i\rangle=\langle S_i(1)-S_i(2)\rangle\ . \tag{3.9}$$

Thus, for example, $\vec{S}(k,2)\cdot\vec{S}(k+1,1)$ may be replaced by the scalar operator

$$\begin{aligned} &\tfrac{1}{4}\sum_i(-1)^i[Q_i(k)-T_i(k)][Q_{-i}(k+1)+T_{-i}(k+1)]\\ &\qquad\equiv\tfrac{1}{4}[Q(k)-T(k)][Q(k+1)+T(k+1)] \end{aligned}$$

It is also possible to record the diagonalization of H_{block} in the form

$$\langle\vec{S}(k,1)\cdot\vec{S}(k,2)\rangle=-\tfrac{3}{4}+\tfrac{1}{2}\langle Q^2(k)\rangle\ , \tag{3.10}$$

since $Q^2=2$ in the spin-1 subspace and $Q^2=0$ in the spin-0 subspace. Using Eqs. (3.8) and (3.10), the effective Hamiltonian after the first blocking may be written

$$\begin{aligned} H^{(0)}=&\sum_{k=1}^{N/2}[E_0+c_0\Delta_0Q^2(k)]\\ &+\sum_{k=1}^{(N/2)-1}c_0[Q(k)-g_0T(k)]\\ &\qquad\times[Q(k+1)+g_0T(k+1)]\ , \end{aligned} \tag{3.11}$$

where $E_0=-\frac{3}{4}$, $c_0=\frac{1}{4}$, $\Delta_0=2$, and $g_0=1$. It is important to realize that no approximation has been made yet because $|+\rangle$, $|0\rangle$, $|-\rangle$, and $|\times\rangle$ form a complete set of block states. A new basis in Hilbert space has simply been chosen, so that the Hamiltonian (3.11) now describes a lattice of length $\frac{1}{2}N$ with a spin-1 triplet state and a spin-0 singlet state at each site. The change of basis and its inverse are described by Eqs. (3.8)–(3.10).

Since the sum of two integer spins is again an integer, it will be possible to implement a two-site RG transformation under which Eq. (3.11) retains its form. In fact, restricting $H^{(0)}$ to a particular two-site

block produces a block Hamiltonian

$$H^{(0)}_{\text{block}} = 2E_0 + c_0\Delta_0[Q^2(1)+Q^2(2)] + c_0[Q(1)-g_0T(1)][Q(2)+g_0T(2)] \ . \tag{3.12}$$

According to the general rules for combining spins, H_{block} will have 16 eigenstates: two spin-0 singlets, three spin-1 triplets, and a spin-2 quintet. In order to preserve the form of Eq. (3.11) an effective Hamiltonian will be written for the subspace of states built from the lowest-lying singlet and triplet eigenstates of Eq. (3.12). These states are readily found to be

$$|0,0\rangle = (3+r_0^2)^{-1/2}(r_0|\times\times\rangle + |00\rangle - |+-\rangle - |-+\rangle), \quad E=E_1 \ , \tag{3.13a}$$

$$|1,1\rangle = (2+2s_0^2)^{-1/2}[s_0(|+\times\rangle + |\times+\rangle) + (|0+\rangle - |+0\rangle)] \ ,$$

$$|1,0\rangle = (2+2s_0^2)^{-1/2}[s_0(|0\times\rangle + |\times0\rangle) + (|-+\rangle - |+-\rangle)] \ ,$$

$$|1,-1\rangle = (2+2s_0^2)^{-1/2}[s_0(|-\times\rangle + |\times-\rangle) + (|-0\rangle - |0-\rangle)] \ ,$$

$$E=E_1' \ , \tag{3.13b}$$

where

$$r_0 = \{3+[(2\Delta_0-1)/g_0^2]^2\}^{1/2} + (2\Delta_0-1)/g_0^2 \ , \tag{3.13c}$$

$$s_0 = \{1+[(2\Delta_0-1+g_0^2)/4g_0]^2\}^{1/2} + (2\Delta_0-1+g_0^2)/4g_0 \ , \tag{3.13d}$$

$$E_1 = 2E_0 + c_0(4\Delta_0-2-r_0g_0^2) \ , \tag{3.13e}$$

$$E_1' = 2E_0 + c_0(4\Delta_0-1-2s_0g_0) \ . \tag{3.13f}$$

The next step is to define new tensor operators Q_i' and T_i' which act on the states (3.13a) and (3.13b) exactly as Q_i and T_i acted on the states (3.5): $\langle 0,0|T_0'|1,0\rangle = 1$, etc. The resulting relationships between matrix elements are

$$\langle Q_i(k,a)\rangle = u_a\langle Q_i'(k)\rangle + v_a\langle T_i'(k)\rangle \ ,$$

$$\langle T_i(k,a)\rangle = w_a\langle Q_i'(k)\rangle + z_a\langle T_i'(k)\rangle \ ,$$

$$u_1 = u_2 = \tfrac{1}{2} \ , \tag{3.14}$$

$$v_1 = -v_2 = 2(2+2s_0^2)^{-1/2}(3+r_0^2)^{-1/2} \ ,$$

$$w_1 = -w_2 = s_0/(1+s_0^2) \ ,$$

$$z_1 = z_2 = s_0(1+r_0)(2+2s_0^2)^{-1/2}(3+r_0^2)^{-1/2} \ .$$

The Hamiltonian (3.11) has the decomposition as $H_{\text{in}} + H_{\text{out}}$

$$H^{(0)} = \sum_{k=1}^{N/4} H^{(0)}_{\text{block}}(k) + \sum_{k=1}^{(N/4)-1} c_0[Q(k,2)-g_0T(k,2)] \times [Q(k+1,1)+g_0T(k+1,1)]$$

and use of Eqs. (3.13e), (3.13f), and (3.14) leads to a new, approximate, effective Hamiltonian of the same form as Eq. (3.11). In fact, the general RG equations are readily seen to be

$$H^{(m)} = \sum_k (E_m + c_m\{\Delta_m Q^2(k) + [Q(k)-g_mT(k)] \times [Q(k+1)+g_mT(k+1)]\}) \ , \tag{3.15a}$$

$$c_{m+1} = c_m\left[\frac{1+2g_ms_m+s_m^2}{2+2s_m^2}\right]^2 \ ,$$

$$g_{m+1} = \left[\frac{c_m}{c_{m+1}}\right]^{1/2}\frac{2+g_ms_m(1+r_m)}{(2+2s_m^2)^{1/2}(3+r_m^2)^{1/2}} \ ,$$

$$\Delta_{m+1} = \frac{c_m}{2c_{m+1}}(1-2g_ms_m+g_m^2r_m) \ , \tag{3.15b}$$

$$E_{m+1} = 2E_m + c_m(4\Delta_m - 2 - r_mg_m^2) \ ,$$

where

$$r_m = \{3+[(2\Delta_m-1)/g_m^2]^2\}^{1/2} + (2\Delta_m-1)/g_m^2 \ ,$$

$$s_m = \{1+[(2\Delta_m-1+g_m^2)/4g_m]^2\}^{1/2} + (2\Delta_m-1+g_m^2)/4g_m \ ,$$

$$E_0 = -\tfrac{3}{4}, \quad c_0 = \tfrac{1}{4}, \quad \Delta_0 = 2, \quad g_0 = 1 \ .$$

As usual, the energy per original lattice site is to be computed as $\lim_{m\to\infty} E_m/2^{m+1}$.

Numerical iteration of Eqs. (3.15) leads to a ground-state energy density of -0.4210, only 5% higher than the exact result of -0.4431. Because the isotropic Heisenberg model is massless, one would expect to find $c_m \to 0$. In fact, one finds that $g_m \to 1$, $\Delta_m \to 0$, but $c_m \to$ a nonzero constant! This limiting theory with $\Delta_\infty = 0$ can be solved exactly by using Eqs. (3.9) and (3.10) to rewrite it on an underlying spin-$\frac{1}{2}$ lattice (recall that this transformation is exact). The condition $\Delta_\infty = 0$ means that the two sites within any one block on the spin-$\frac{1}{2}$ lattice are uncoupled. The spin-$\frac{1}{2}$ couplings are therefore as shown in Fig. 3. This theory has a fourfold-

FIG. 3. Couplings for the spin-$\frac{1}{2}$ theory equivalent to the $m \to \infty$ integer-spin theory [Eqs. (3.15)].

degenerate ground state in which each coupled pair of sites has total spin 0 while the uncoupled sites at the ends of the lattice have total spin 0 or 1. There is a finite mass gap to the highly degenerate first excited state in which some pair of coupled spins have total spin 1, and additional mass gaps separate the higher excited states. Clearly this bears no resemblance to the physics of the isotropic Heisenberg model with its massless spin-wave excitations. What went wrong?

Recalling the calculation of Sec. II, suppose that here also the Heisenberg model $\Delta=2, g=1$ is an unstable fixed point of the more general model of Eqs. (3.15). The RG calculation should find this fixed point, but being an approximate calculation it need not locate it precisely at $\Delta=2, g=1$. In such a case the RG equations with Heisenberg-model initial conditions will iterate *away* from the unstable fixed point, toward a stable fixed point with totally different physics.

Figure 4 shows the qualitative behavior of the RG trajectories resulting from Eqs. (3.15) near the Heisenberg point $\Delta=2, g=1$ and supports the picture just sketched. The unstable fixed point is quite close, at $\Delta=1.7, g=0.84$, but the Heisenberg model iterates to the stable fixed point $\Delta=0$. There is also a stable fixed point at $\Delta=\infty$. At the unstable fixed point the Hamiltonian just rescales by a factor less than 1 at each iteration, leading to the correct massless behavior.

Recalling that the $\gamma=1$ unstable fixed point of the three-site calculation was located correctly as a consequence of rotational invariance, it is natural to ask whether the model (3.15a) possesses some symmetry at the Heisenberg point which is not preserved by the RG transformation. I now show that such a symmetry can be defined as invariance under a duality transformation.

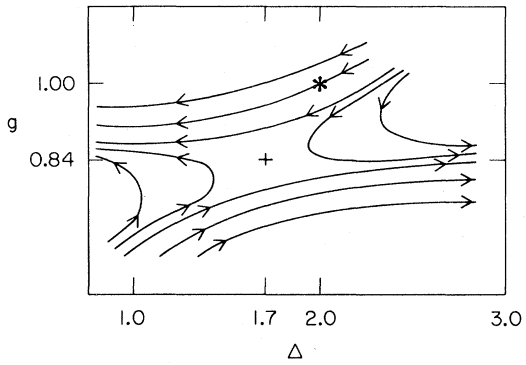

FIG. 4. Qualitative behavior of RG trajectories in the two-site calculation. The point * is the Heisenberg-model point and + is the unstable fixed point.

To define the duality transformation it is convenient to rewrite the Hamiltonian (3.15a) in the generic form:

$$H=\sum_k \{E+GQ^2(k)+AQ(k)Q(k+1) +BT(k)T(k+1) +D[Q(k)T(k+1)-T(k)Q(k+1)]\} , \tag{3.16}$$

where $G=c\Delta$, $A=c$, $B=-cg^2$, and $D=cg$. The change in notation is necessary because the duality transformation will not preserve the form of the nearest-neighbor couplings in the Hamiltonian (3.15a) except for special values of the parameters.

The first step is to use Eqs. (3.9) and (3.10) to write a spin-$\frac{1}{2}$ Hamiltonian equivalent to Eq. (3.16). This is the same trick used to solve exactly the fixed-point Hamiltonian. It yields a spin-$\frac{1}{2}$ Hamiltonian which, if blocked using two-site blocks, would reproduce (3.16). The spin-$\frac{1}{2}$ Hamiltonian is

$$H=\sum_k [E+\tfrac{3}{2}G+2G\vec{S}(k,1)\cdot\vec{S}(k,2)+(A+B)\vec{S}(k,1)\cdot\vec{S}(k+1,1)+(A+B)\vec{S}(k,2)\cdot\vec{S}(k+1,2) +(A-B-2D)\vec{S}(k,1)\cdot\vec{S}(k+1,2)+(A-B+2D)\vec{S}(k,2)\cdot\vec{S}(k+1,1)] . \tag{3.17}$$

The spin-$\frac{1}{2}$ lattice is now shifted one unit to the right by letting $(k,1)\to(k,2)$ and $(k,2)\to(k+1,1)$ (periodic boundary conditions are useful here). This shift interchanges interblock couplings with intrablock couplings. Finally, blocking the Hamiltonian back to the integer-spin form using Eqs. (3.8) and (3.10) produces the dual Hamiltonian

$$\tilde{H}=\sum_k \{\tilde{E}+\tilde{G}Q^2(k)+\tilde{A}Q(k)Q(k+1)+\tilde{B}T(k)T(k+1)+\tilde{D}[Q(k)T(k+1)-T(k)Q(k+1)] +\tilde{F}[Q(k)-T(k)][Q(k+2)+T(k+2)]\} , \tag{3.18}$$

where

$$\tilde{E} = E + \tfrac{3}{2}G - \tfrac{3}{4}(A - B + 2D) \ ,$$

$$\tilde{G} = \tfrac{1}{2}(A - B + 2D) \ ,$$

$$\tilde{A} = \tfrac{1}{2}(A + B + G) \ ,$$

$$\tilde{B} = \tfrac{1}{2}(A + B - G) \ ,$$

$$\tilde{D} = \tfrac{1}{2}G \ ,$$

$$\tilde{F} = \tfrac{1}{4}(A - B - 2D) \ .$$

Note that the dual gap parameter $\tilde{G}$ depends on the original couplings A, B, and D while the original gap parameter contributes to the dual couplings. Next-nearest-neighbor couplings have also appeared. H and $\tilde{H}$ clearly describe the same system in different ways and have the same spectrum and other properties. A system is self-dual in the sense that $H = \tilde{H}$ if its spin-$\frac{1}{2}$ form is translationally invariant. The self-duality condition reduces to $A - B = 2D = G$, which implies $\Delta = 2, g = 1$. Only multiples of the Heisenberg Hamiltonian are self-dual. Therefore, a calculation which respected translational invariance would lead to the correct physics for the Heisenberg model.

The RG transformation will *not* preserve self-duality (translational invariance). Indeed, RG calculations of this type treat intrablock and interblock couplings quite differently. The former are diagonalized and contribute to the gap parameter at the next iteration, while the latter contribute to the new couplings. In the present calculation the initial Hamiltonian was self-dual while the $\Delta = 0$ fixed point which was finally reached was not. This fixed point corresponds to $A - B = 2D \neq 0$, and $G = 0$. It is dual to the point $A = B = 2D = 0$, and $G \neq 0$ which is the $\Delta = \infty$ fixed point of Fig. 4. The $\Delta = \infty$ fixed point corresponds to Fig. 3 with the coupling pattern shifted one unit to the right.

Several remarks should be made regarding the problem with this calculation and its resolution as discussed above.

(i) Although the RG equations, naively applied, lead to the wrong fixed point, a glance at the trajectories of Fig. 4 is sufficient to reveal the problem and indicate the correct physics. Unfortunately, models with long-range interactions such as Eq. (1.1) involve an infinite number of different couplings, so that RG trajectories cannot be mapped out. Without the trajectories there is no way to locate unstable fixed points. Thus, the two-site calculation of this section cannot be reliably used to study the phases of the model (1.1) even though it may well yield a good ground-state energy density.

(ii) The problem encountered in the two-site calculation is clearly very general: it may occur in any theory when the first RG blocking embeds the theory at or near an unstable fixed point of a more general model. However, the following considerations suggest a rule for determining which of several possible calculations may be most seriously affected by the failure of the RG technique to preserve self-duality. In the two-site calculation, the ground state in a block was a singlet. In order to get the correct massless physics it would have been necessary for *both* the gap parameter G and the couplings A, B, and D to iterate to zero. This did not happen because the RG calculation treats gaps and couplings asymmetrically. In the three-site calculation the ground state in a block was a doublet, and the subspace of lattice states formed from these doublet block states was isomorphic to the space of states of the original Heisenberg model. This would remain true even in a three-site calculation using all eight block states. As long as all *couplings* iterate to zero in such a calculation, this subspace contains massless excitations yielding the correct spectrum *even if* nonzero gaps separate the lowest doublet from the other states in one block. This suggests the following rule of thumb: given a choice, one should prefer that calculation for which the ground state in a block has the highest multiplicity. This maximizes the number of lattice states that can be constructed from the block ground states alone. Physics which depends on this sector of lattice states only will be independent of gaps between block states, and therefore independent of asymmetrical treatment of gaps and couplings.

(iii) The duality transformation introduced here has applications beyond this particular model. Such a transformation can be defined in any calculation in which all the block states are kept at the first blocking, so that the blocking is "reversible". In a two-site calculation the square of the duality transformation is unity; in a calculation using m-site blocks the duality transformation generates a Z_m symmetry group.

(iv) In addition to its utility in classifying fixed points, the duality transformation may be used to increase the accuracy of the RG calculation itself. Consider the following scheme. Beginning with the Hamiltonian $H^{(0)}$ of Eq. (3.11), one blocks as usual to obtain $H^{(1)}$. $H^{(2)}$ is obtained by blocking the *dual* Hamiltonian $\tilde{H}^{(1)}$ (note that this blocking removes the next-nearest-neighbor couplings introduced by the duality transformation) and one continues by alternately applying the duality transformation and the blocking procedure. Since the underlying spin-$\frac{1}{2}$ lattice is shifted to the right at each iteration of this scheme, one might hope that more translationally invariant states than usual are being constructed and that edge effects due to the walls of the blocks are being "smeared out." This scheme does in fact improve the energy density found in the two-site calculation very slightly.

IV. IMPROVING THE THREE-SITE CALCULATION

One might try to improve the three-site calculation for the isotropic Heisenberg model ($\gamma = 1$ in the notation of Sec. II) in a variety of ways. One method is to keep more than two of the block states (2.4). One might keep both spin-$\frac{1}{2}$ doublets, or even all eight states in which case a duality transformation could be employed. Alternatively one might try to select a better pair of states to keep, which need not be eigenstates of H_{block}. In this problem, symmetry considerations make this impossible: rotational symmetry forbids mixing spin-$\frac{3}{2}$ with spin-$\frac{1}{2}$ states, and parity rules out a linear combination of the two spin-$\frac{1}{2}$ multiplets. A third course is to use larger blocks. In this section, I describe a way to improve the three-site calculation by using it to approximate a nine-site calculation.

Consider performing a nine-site calculation by keeping only the lowest-lying spin-$\frac{1}{2}$ doublet of eigenstates on a block at each iteration. Such a calculation can only be done with the aid of a computer. However, two iterations of the three-site calculation have the effect of constructing a pair of spin-$\frac{1}{2}$ states on a nine-site block. The $S_z = \frac{1}{2}$ member of this pair is [cf. Eq. (2.4)]

$$\begin{aligned}|\psi\rangle = \frac{1}{\sqrt{6}}\big(&2|\tfrac{1}{2},\tfrac{1}{2}\rangle_1|\tfrac{1}{2},-\tfrac{1}{2}\rangle_1|\tfrac{1}{2},\tfrac{1}{2}\rangle_1 \\ &-|\tfrac{1}{2},\tfrac{1}{2}\rangle_1|\tfrac{1}{2},\tfrac{1}{2}\rangle_1|\tfrac{1}{2},-\tfrac{1}{2}\rangle_1 \\ &-|\tfrac{1}{2},-\tfrac{1}{2}\rangle_1|\tfrac{1}{2},\tfrac{1}{2}\rangle_1|\tfrac{1}{2},\tfrac{1}{2}\rangle_1\big)\ ,\end{aligned} \tag{4.1}$$

where

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

and

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

If the Hamiltonian on a nine-site block is written in the form

$$\begin{aligned}H_{\text{block}} &= H_0 + V\ , \\ H_0 &= \vec{S}(1)\cdot\vec{S}(2) + \vec{S}(2)\cdot\vec{S}(3) \\ &\quad + \vec{S}(4)\cdot\vec{S}(5) + \vec{S}(5)\cdot\vec{S}(6) \\ &\quad + \vec{S}(7)\cdot\vec{S}(8) + \vec{S}(8)\cdot\vec{S}(9)\ , \\ V &= \vec{S}(3)\cdot\vec{S}(4) + \vec{S}(6)\cdot\vec{S}(7)\ ,\end{aligned} \tag{4.2}$$

then $|\psi\rangle$ is an eigenstate of H_0 with eigenvalue -3. To the extent that V can be regarded as "small", $|\psi\rangle$ approximates an exact nine-site eigenstate. In actuality V will mix $|\psi\rangle$ with the additional states $V|\psi\rangle$, $V^2|\psi\rangle$, etc., of which the most important will be $V|\psi\rangle$ if V is "small." It is then reasonable to do a nine-site blocking calculation using as the $S_z = \frac{1}{2}$ state the lower-lying state obtained by diagonalizing the matrix of H_{block} in the subspace spanned by $|\psi\rangle$ and $V|\psi\rangle$ only. This is a 2×2 matrix, and the calculation is not difficult. It yields a ground-state energy density in error by 5.4% as compared to 11.7% for the three-site and 5.0% for the two-site calculation. Like the three-site calculation, it also yields the correct massless spectrum. Although perturbative in spirit, this method is not a consistent expansion to some particular order in V as is the method of Ref. 12. However, it can easily be improved further by diagonalizing the matrix of H_{block} in a larger subspace spanned by more of the states $|\psi\rangle$, $V|\psi\rangle$, $V^2|\psi\rangle$, ..., and choosing the lowest-lying state. Eventually these states will span the entire spin-$\frac{1}{2}$, $S_z = \frac{1}{2}$, even parity subspace on nine sites, and one is back to the exact nine-site calculation. This technique should also be suitable for studying the model (1.1) with long-range interactions.

V. CONCLUDING REMARKS

In this paper block-spin calculations for the isotropic Heisenberg model employing both two-site and three-site blocks have been discussed in great detail. The three-site calculation and its nine-site generalization gave good results and should be suitable for studying the model (1.1) with long-range interactions. The two-site calculation is not reliable for this purpose. Results of the three- and nine-site calculations for the long-range model will be presented in a subsequent paper. The duality transformation introduced in Sec. III can be defined for models other than the one studied here, and it is hoped that it will be useful in other calculations of this type.

After this work was completed, I learned from Marvin Weinstein that improving the two-site calculation by variational techniques suffices to obtain the correct massless spectrum. In such an improved calculation, the block states are allowed to depend on one or more variational parameters. These parameters are adjusted to minimize the ground-state energy computed after many RG iterations, rather than to diagonalize the block Hamiltonian. This "feedback" mechanism allows the physics at scales much larger than the block size to influence the selection of block states.

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