# Spectral excitations in the one-dimensional spin-$\frac{1}{2}$ dimerized Heisenberg chain: A renormalization-group approach

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(Received 14 July 1978)

A zero-temperature lattice renormalization-group calculation is presented and applied to the antiferromagnetic one-dimensional dimerized spin-$\frac{1}{2}$ Heisenberg chain. The calculation indicates the existence of a gap in the spectrum of the dimer system, which vanishes only in the limit of a uniform spin chain. To improve the accuracy of the numerical estimates of the ground-state energy and gap, an iterative extension of finite-chain techniques is also applied. These approximate techniques are checked against the dimerized $XY$ chain, for which an exact solution is found.

## I. INTRODUCTION

The existence of a gap in the excitation spectrum of a dimerized antiferromagnetic spin-$\frac{1}{2}$ Heisenberg chain is not yet rigorously established. Recent magnetic measurements[1] on the spin-Peierls system (TTF)$(CuS_4C_4(CF_3)_4)$ (TTF = tetrathiafulvalene) provide motivation for consideration of this question. These measurements have been interpreted in terms of an earlier Hartree-Fock (HFA) treatment[2] of the dimer Heisenberg system, which does indicate the existence of a gap. More recent numerical calculations on finite chains[3,4] support the HFA calculation. However, a calculation[5] based on a Green's-function decoupling which conserves the spin isotropy of the dimer chain produces an acoustic band in addition to the band with gap of the HFA.

The Hamiltonian for the Heisenberg dimer chain with free ends is

$$H=\sum_{j=1}^{N}\left(J_1\vec{S}_{2j}\cdot\vec{S}_{2j+1}+J_2\vec{S}_{2j+1}\cdot\vec{S}_{2j+2}\right), \qquad (1)$$

where $\vec{S}_p$ is the spin-$\frac{1}{2}$ vector operator $(S_p^x,S_p^y,S_p^z)$ at site $p$, and

$$S^z=\frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \text{ etc.} \qquad (2)$$

We will also consider the $XY$ dimer chain, the Hamiltonian for which has the form (1), where $\vec{S}$ is a two-component vector $(S^x,S^y)$. In both cases, we consider the limit of a large number $2N$ of spins. We also take $J_1\geq J_2\geq 0$. There are two limiting cases about which exact statements can be made:

(i) For $J_2=0$, the chain breaks into $N$ noninteracting dimers. The Heisenberg ($XY$) ground-state energy per spin is $\phi_0\equiv E_0/2N=-\frac{3}{8}J_1$ $(-\frac{1}{4}J_1)$, and there is a gap $\Delta=J_1$ $(\frac{1}{2}J_1)$, corresponding to the energy required to excite a single dimer.

(ii) For $J_1=J_2$, both ground-state energy[6] and low-lying excitation spectrum[7] are known for the Heisenberg system. The ground-state energy per site is $\phi_0=-0.4431J$; and the spin-wave excitation spectrum is gapless, $\Delta=0$. For the $XY$ model,[8] these quantities are $\phi_0=-J_1/\pi$ and $\Delta=0$.

The $XY$ dimer system can be solved exactly for its ground-state energy and excitation spectrum, for all values of $\gamma\equiv J_2/J_1$. Details are presented in Appendix A.

This paper describes another approximation to the one-dimensional dimerized spin systems, utilizing a particular renormalization-group (RG) approach which has already proved useful on other quantum systems in particle theory[9] as well as statistical mechanics[10,11] and solid-state theory.[12,13] The present calculations do not require the full RG machinery; a critical-point analysis is not needed for the questions of interest here. As a test of this RG calculation, a second series of calculations, essentially an iterative extension of finite-chain techniques[4,14] (IFC), is presented. Unlike the RG calculation, which provides information on the scaling behavior of the system, the IFC approximation as applied here provides useful information only on the eigenvalues. The two treatments do share some common features, however. In both, the full lattice is viewed as a system of coupled finite blocks, each of which is to be solved exactly. The coupling between adjacent blocks is written in terms of a truncated basis which is a

 

subset of the full set of single-block eigenstates. Iteration of this scheme produces approximate eigenvectors and eigenvalues for arbitrarily large lattices.

Section II of this paper contains a more detailed exposition of the RG calculation and a discussion of results for both the $XY$ and the Heisenberg dimer chains. Section III describes the results of the IFC calculation for both models. The IFC and RG results are discussed and compared in Sec. IV.

## II. RENORMALIZATION-GROUP CALCULATION

### A. Description of the method

In this section we shall describe calculations which are similar in approach to the lattice renormalization-group techniques[15] frequently used to calculate critical behavior. We shall establish recursion relations on a set of parameters which define the Hamiltonian, and we shall find fixed points of these recursion relations. We shall not, however, carry out the usual analysis of trajectories about the unstable fixed point. In order to maintain the symmetries of the system throughout the iterative process, we shall cast the Hamiltonian into the form

$$H^{(n)}=(\tfrac{1}{2}J^{(n)})\sum_j [(S^+_{2j}S^-_{2j+1}+S^-_{2j}S^+_{2j+1}+2\mu^{(n)}S^z_{2j}S^z_{2j+1}) + \gamma^{(n)}(S^+_{2j+1}S^-_{2j+2}+S^-_{2j+1}S^+_{2j+2} +2\nu^{(n)}S^z_{2j+1}S^z_{2j+2}) + C^{(n)}(I_{2j}+I_{2j+1})] \ , \tag{3}$$

where $I$ represents the $2\times 2$ identity matrix. The initial conditions, compare Eq. (1), are

$$J^{(0)}=J_1 \ , \quad \mu^{(0)}=\nu^{(0)}=c \ , \quad \gamma^{(0)}=\gamma \ , \quad C^{(0)}=0 \ , \tag{4}$$

where $c=1$ for the Heisenberg system, $c=0$ for $XY$. We now proceed to demonstrate the recursion from $n$ to $n+1$.

As mentioned above, the first step is to associate the lattice sites into blocks of $N_s$ sites. The Hamiltonian is written as a sum of intrablock and interblock terms

$$H^{(n)}=\sum_p \Big( H^{(n)}_{2p}+H^{(n)}_{2p+1}+V^{(n)}_{2p,2p+1}+V^{(n)}_{2p+1,2p+2} + C^{(n)}\sum_{i=1}^{N_s}(I_{2p,i}+I_{2p+1,i}) \Big) \ , \tag{5}$$

where $i=1,2,\ldots,\ N_s$ labels the position of the site within block $2p$ or $2p+1$. The intrablock terms have the form

$$H_{2p}=J(\vec{S}_{2p,1}\cdot\vec{S}_{2p,2}+\gamma\vec{S}_{2p,2}\cdot\vec{S}_{2p,3} +\cdots+\gamma\vec{S}_{2p,N_s-1}\cdot\vec{S}_{2p,N_s}) \ ,$$
$$H_{2p+1}=J(\gamma\vec{S}_{2p+1,1}\cdot\vec{S}_{2p+1,2}+\vec{S}_{2p+1,2}\cdot\vec{S}_{2p+1,3} +\cdots+\vec{S}_{2p+1,N_s-1}\cdot\vec{S}_{2p+1,N_s}) \ , \tag{6}$$

and the interblock couplings have the form

$$V_{2p,2p+1}=J\vec{S}_{2p,N_s}\cdot\vec{S}_{2p+1,1} \ ,$$
$$V_{2p+1,2p+2}=\gamma J\vec{S}_{2p+1,N_s}\cdot\vec{S}_{2p+2,1} \ . \tag{7}$$

In Eqs. (6) and (7) the labels $n$ are suppressed.

The diagonalization of the intrablock Hamiltonians and subsequent truncation of the bases are expedited[10] by the observation that $S^z_q$ commutes with $H^{(n)}_q$ (for $q=2p,\ 2p+1$), and thus that the eigenstates of $H^{(n)}_q$ may be chosen to be eigenstates of $S^z_q$, where $S^z_q$ is the total spin $z$ component in block $q$

$$S^z_q=\sum_{j=1}^{N_s}S^z_{q,j} \ . \tag{8}$$

We choose our new basis to contain the two states $\{|+\rangle_q,|-\rangle_q\}$, where $|+\rangle_q$ ($|-\rangle_q$) is the state of lowest energy $E_+$ ($E_-$) in the subspace $S^z_q=+\frac{1}{2}$ ($-\frac{1}{2}$). These states are the lowest-energy states of the old basis, and they may be expressed as

$$|+\rangle^{(n+1)}_{2p}=\sum_{\epsilon_1}\cdots\sum_{\epsilon_{N_s}}\lambda^{+(n)}_{\epsilon_1\cdots\epsilon_{N_s}}|\epsilon_1\cdots\epsilon_{N_s}\rangle^{(n)} \ ,$$
$$|+\rangle^{(n+1)}_{2p+1}=\sum_{\epsilon_1}\cdots\sum_{\epsilon_{N_s}}\Lambda^{+(n)}_{\epsilon_1\cdots\epsilon_{N_s}}|\epsilon_1\cdots\epsilon_{N_s}\rangle^{(n)} \ ,$$
$$|-\rangle^{(n+1)}_{2p}=\sum_{\epsilon_1}\cdots\sum_{\epsilon_{N_s}}\lambda^{-(n)}_{\epsilon_1\cdots\epsilon_{N_s}}|\epsilon_1\cdots\epsilon_{N_s}\rangle^{(n)} \ ,$$
$$|-\rangle^{(n+1)}_{2p+1}=\sum_{\epsilon_1}\cdots\sum_{\epsilon_{N_s}}\Lambda^{-(n)}_{\epsilon_1\cdots\epsilon_{N_s}}|\epsilon_1\cdots\epsilon_{N_s}\rangle^{(n)} \ , \tag{9}$$

where $\sum_{\epsilon_l}$ represents a summation over the two-spin states $|\pm\rangle^{(n)}_l$ at site $l$ of the block, and $|\epsilon_1\cdots\epsilon_{N_s}\rangle^{(n)}$ is the product state $|\epsilon_1\rangle^{(n)}\cdots|\epsilon_{N_s}\rangle^{(n)}$. From the symmetry of Eq. (6) it is easy to see that $E^{(n+1)}_+=E^{(n+1)}_-$ and that

$$\lambda^{\pm(n)}_{\epsilon_1\epsilon_2\cdots\epsilon_{N_s}}=\Lambda^{\pm(n)}_{\epsilon_{N_s}\cdots\epsilon_2\epsilon_1} \ . \tag{10}$$

The next step is to rewrite the interblock coupling terms. To this end, we calculate the matrix elements of $S_{q,l}^{+(n)}$ and $S_{q,l}^{z(n)}$ in the new basis

$$S_{2p,l}^{+(n)} = \xi_l^{(n)} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \xi_l^{(n)} S_{2p}^{+(n+1)} \tag{11a}$$

and similarly

$$S_{2p+1,l}^{+(n)} = \xi_{N_s-l+1}^{(n)} S_{2p+1}^{+(n+1)} , \tag{11b}$$

$$S_{2p,l}^{z(n)} = \eta_l^{(n)} S_{2p}^{z(n+1)} , \tag{11c}$$

$$S_{2p+1,l}^{z(n)} = \eta_{N_s-l+1}^{(n)} S_{2p+1}^{z(n+1)} , \tag{11d}$$

where

$$\xi_l^{(n)} = \sum_{\epsilon_1} \cdots \sum_{\epsilon_{l-1}} \sum_{\epsilon_{l+1}} \cdots \sum_{\epsilon_{N_s}} \lambda^{+(n)}_{\epsilon_1 \cdots \epsilon_{l-1},+,\epsilon_{l+1} \cdots \epsilon_{N_s}} \lambda^{-(n)}_{\epsilon_1 \cdots \epsilon_{l-1},-,\epsilon_{l+1} \cdots \epsilon_{N_s}} ,$$

$$\eta_l^{(n)} = \sum_{\epsilon_1} \cdots \sum_{\epsilon_l} \cdots \sum_{\epsilon_{N_s}} \epsilon_l \left| \lambda^{+(n)}_{\epsilon_1 \cdots \epsilon_l \cdots \epsilon_{N_s}} \right|^2 . \tag{12}$$

The coupling terms become

$$V_{2p,2p+1}^{(n)} \to \left(\tfrac{1}{2} J^{(n)}\right)\left[(\xi_{N_s}^{(n)})^2 (S_{2p}^{+} S_{2p+1}^{-} + \text{H.c.}) + 2\mu^{(n)} (\eta_{N_s}^{(n)})^2 S_{2p}^{z} S_{2p+1}^{z}\right] ,$$

$$V_{2p+1,2p+2}^{(n)} \to \left(\tfrac{1}{2} \gamma^{(n)} J^{(n)}\right)\left[(\xi_1^{(n)})^2 (S_{2p+1}^{+} S_{2p+2}^{-} + \text{H.c.}) + 2\nu^{(n)} (\eta_1^{(n)})^2 S_{2p+1}^{z} S_{2p+2}^{z}\right] . \tag{13}$$

The recursion may now be demonstrated. Putting Eq. (13) into Eq. (5), we obtain the original form, Eq. (3), where we have

$$J^{(n+1)} = (\xi_{N_s}^{(n)})^2 J^{(n)} , \qquad \gamma^{(N+1)} = \left(\frac{\xi_1^{(n)}}{\xi_{N_s}^{(n)}}\right)^2 \gamma^{(n)} ,$$

$$\mu^{(n+1)} = \left(\frac{\eta_{N_s}^{(n)}}{\xi_{N_s}^{(n)}}\right)^2 \mu^{(n)} , \qquad \nu^{(n+1)} = \left(\frac{\eta_1^{(n)}}{\xi_1^{(n)}}\right)^2 \nu^{(n)} ,$$

$$C^{(n+1)} = N_s C^{(n)} + E_{+}^{(n+1)} . \tag{14}$$

These recursion relations define a renormalization-group transformation for the ground state of the Hamiltonian. The parameters $J^{(n)}$ and $\gamma^{(n)}$ provide information on the splittings of the lowest states of the system, $\mu^{(n)}$ and $\nu^{(n)}$ determine the symmetries of the fixed point, and $C^{(n)}$ may be used to find the ground-state energy per site $\phi_0$ through the relation

$$\phi_0 = \lim_{n \to \infty} (C^{(n)}/N_s^n) . \tag{15}$$

In general the eigenvectors $|\pm\rangle^{(n+1)}$ and eigenvalues $E_{\pm}^{(n+1)}$, as well as the recursion coefficients of Eq. (14), are determined by machine. For the $XY$ system ($\mu^{(0)} = \nu^{(0)} = 0$) with $N_s = 3$, however, the algebra is simple and the results instructive; details may be found in Appendix B.

### B. Results

We have done the calculation for $N_s = 3, 5, 7$, and 9, finding always the fixed points corresponding to the limits discussed earlier.

(i) For $0 \leq \gamma^{(0)} < 1$, $\gamma^{(n)} \to 0$ and $J^{(n)} \to J^{\infty}$ as $n \to \infty$. The Hamiltonian at the fixed point describes a system of noninteracting dimers, with a nondegenerate ground state and gap $\Delta = J^{\infty}$ ($\frac{1}{2} J^{\infty}$) for the Heisenberg ($XY$) system $\mu^{(0)} = \nu^{(0)} = 1$ (0). (Strictly speaking, $E_{+}^{(\infty)} = E_{-}^{(\infty)}$ and the odd-$N_s$ approximation yields a doubly degenerate ground state. This degeneracy is due to the fact that the odd-$N_s$ block at $\gamma = 0$ contains a free spin.)

(ii) For $\gamma^{(0)} = 1$, $\gamma^{(n)} = 1$ for all $n$, and $J^{(n)} \to 0$. The system remains at the uniform limit, with a multiply degenerate ground state of finite energy.

In Table I we have listed, for the $XY$ system, the calculated values of $\phi_0$ and $\Delta$ for several values of $\gamma$ and for $N_s = 3, 5, 7$, and 9; also listed are the corresponding exact values, calculated from Eqs. (A9) and (A10). Figure 1 contains the exact results for $\Delta(\gamma)$ (solid line) and a more complete collection of $N_s = 7$ results (open circles). Observe that our approximate results for $\phi_0$ are in qualitative agreement with the exact results, and that agreement improves with increasing $N_s$; for $N_s = 9$ our results are within 5% of the exact values for all $\gamma$ (for fixed $N_s$, the error in $\phi_0$ increases as $\gamma$ increases to 1). On the other hand, results for $\Delta(\gamma)$ are relatively insensitive to $N_s$. The values of $\Delta(\gamma)$ at the limits $\gamma = 0, 1$ are correct, but the derivatives are not. The approximate curves approach $\gamma = 0$ as $(1+\gamma^2)^{-1}$ [compare Eq. (B7)] and approach $\gamma = 1$ as $(1-\gamma)^{\alpha}$ with $\alpha \simeq 0.72$ ($N_s = 7$), whereas the exact curve is described by the relation $\Delta = \frac{1}{2}(1-\gamma)$ [Eq. (A10)].

Table II contains RG values of $\Delta$ and $\phi_0$ for the Heisenberg system, as well as the HFA values.[2] The HFA (filled circles) and $N_s = 7$ (open circles) results for $\Delta(\gamma)$ are also presented in Fig. 2. Again, increasing $N_s$ decreases, and hence improves, the estimate

TABLE I. RG results (in units of $J_1$) for $XY$ ground-state energy per site and for the gap, for several values of $\gamma$, compared with exact values (Appendix A).

| $N_s$ | 3 | | 5 | | 7 | | 9 | | Exact | |
|---|---|---|---|---|---|---|---|---|---|---|
| $\gamma$ | $-\phi_0$ | $\Delta$ | $-\phi_0$ | $\Delta$ | $-\phi_0$ | $\Delta$ | $-\phi_0$ | $\Delta$ | $-\phi_0$ | $\Delta$ |
| 0.0 | 0.2500 | 0.500 | 0.2500 | 0.500 | 0.2500 | 0.500 | 0.2500 | 0.500 | 0.250 | 0.500 |
| 0.2 | 0.2501 | 0.481 | 0.2511 | 0.480 | 0.2514 | 0.480 | 0.2517 | 0.480 | 0.253 | 0.400 |
| 0.4 | 0.2513 | 0.429 | 0.2543 | 0.422 | 0.2559 | 0.420 | 0.2568 | 0.420 | 0.260 | 0.300 |
| 0.6 | 0.2557 | 0.351 | 0.2608 | 0.334 | 0.2638 | 0.325 | 0.2657 | 0.322 | 0.273 | 0.200 |
| 0.8 | 0.2649 | 0.237 | 0.2725 | 0.218 | 0.2769 | 0.207 | 0.2797 | 0.198 | 0.292 | 0.100 |
| 1.0 | 0.2828 | 0.0 | 0.2927 | 0.0 | 0.2983 | 0.0 | 0.3019 | 0.0 | 0.3183 | 0.0 |

of $\phi_0$. For $N_s=9$ the values for $\phi_0$ represent an improvement over the HFA; for $\gamma=1$ the approximate $\phi_0$ is within 5% of the exact value. As before, results for $\Delta(\gamma)$ are relatively insensitive to $N_s$ and correct at the limits $\gamma=0,1$. The results seem to approach $\gamma=1$ as $(1-\gamma)^\alpha$ with $\alpha\simeq 0.76$ ($N_s=7$).

Note that information concerning only the lowest states of each block at iteration $(n)$ is used to construct the blocks of iteration $(n+1)$, information concerning higher states being ignored. This would explain the poor convergence of the gap with increasing $N_s$.

## III. ITERATED FINITE-CHAIN APPROACH

In order to improve[11] our estimates of $\Delta$ and $\phi_0$, we have carried out another series of calculations, in which the truncated basis at each step is taken to be the $N_L>2$ states of lowest energy, regardless of symmetry considerations. Instead of identifying a new spin Hamiltonian $\{J^{(n)},\gamma^{(n)},\mu^{(n)},\nu^{(n)},C^{(n)}\}$ of given form at each iterative step, we consider a general matrix formulation of the problem. This scheme can be thought of simply as an extension of finite-chain techniques: one solves equivalent blocks (even $N_s$) on the original lattice, truncates the basis to $N_L$ states, couples adjacent blocks in pairs, and iterates the pairwise coupling. Details of the scheme may be found in Sec. III of Ref. 13(b).

We have carried out these calculations for $N_L=4$ and $N_L=8$, with original blocksize $N_s=4,6,8$. Results of these calculations for the $XY$-dimer chain are presented in Table III and in Fig. 1; for Heisenberg results, see Table IV and Fig. 2. In all cases we find one of three behaviors as $n\to\infty$: (i) For $\gamma<\gamma^*$, we have the gap $\Delta^{(n)}\to\Delta^\infty\neq 0$. The ground state is nondegenerate, and the lowest excited states highly degenerate, characteristic of the limit $\gamma=0$. (ii) For $\gamma=\gamma^*$, we have the gap $\Delta^{(n)}\to 0$, and the ground state has high degeneracy, characteristic of the uniform chain, with splittings $\sim 1/N$. The value of $\gamma^*$ is not exactly unity. (iii) For $\gamma>\gamma^*$, the ground state is four degenerate, with a finite gap to the highly degenerate excited states. This four degeneracy is characteristic of the limit $\gamma^*=\infty$, which creates two free spins, one at each end of the even-$N_s$ block.[16]

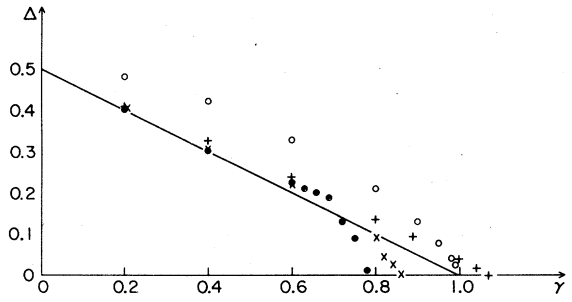


FIG. 1. Results for the $XY$ gap. The solid line represents the exact result. Open circles are the RG results, $N_s=7$. IFC results for various $(N_s,N_L)$ are also presented: filled circles for (4,4); crosses (+) for (4,8); crosses (×) for (8,4).

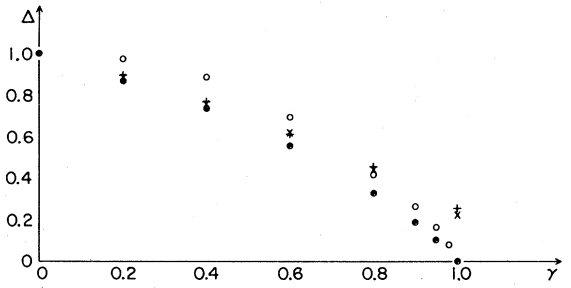


FIG. 2. Results for the Heisenberg gap. Filled circles represent the HFA results of Bulaevskii; open circles the RG results for $N_s=7$; crosses (+) the IFC results for $(N_s,N_L)=(4,8)$; crosses (×) the IFC results for $(N_s,N_L)=(6,8)$.

TABLE II. RG results (in units of $J_1$) for the Heisenberg ground-state energy per site and gap for several values of $\gamma$, compared with HFA results (Ref. 2).

| $N_s$ | 3 | | 5 | | 7 | | 9 | | HFA | |
|---|---|---|---|---|---|---|---|---|---|---|
| $\gamma$ | $-\phi_0$ | $\Delta$ | $-\phi_0$ | $\Delta$ | $-\phi_0$ | $\Delta$ | $-\phi_0$ | $\Delta$ | $-\phi_0$ | $\Delta$ |
| 0.0 | 0.3750 | 1.0 | 0.3750 | 1.0 | 0.3750 | 1.0 | 0.3750 | 1.0 | 0.3750[a] | 1.0[a] |
| 0.2 | 0.3748 | 0.976 | 0.3756 | 0.976 | 0.3760 | 0.976 | 0.3762 | 0.976 | 0.3764 | 0.885 |
| 0.4 | 0.3736 | 0.893 | 0.3771 | 0.884 | 0.3788 | 0.884 | 0.3798 | 0.884 | 0.3774 | 0.738 |
| 0.6 | 0.3729 | 0.747 | 0.3795 | 0.706 | 0.3836 | 0.697 | 0.3861 | 0.695 | 0.3825 | 0.557 |
| 0.8 | 0.3765 | 0.525 | 0.3867 | 0.460 | 0.3928 | 0.421 | 0.3969 | 0.402 | 0.3943 | 0.329 |
| 1.0 | 0.3913 | 0.0 | 0.4069 | 0.0 | 0.4157 | 0.0 | 0.4212 | 0.0 | 0.4196[b] | 0.0[a] |

[a]Exact result.

[b]Exact result (Ref. 6) is $-\phi_0 = 0.4431$.

TABLE III. IFC results for the $XY$ ground-state energy per site and for the gap, for several values of $\gamma$, compared with exact values. The last row contains our estimates for $\gamma^*$. Results are in units $J_1 = 1$.

| $N_s, N_L$ | 4,4 | | 4,8 | | 6,4 | | 6,8 | | 8,4 | | 8,8 | | Exact | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $\gamma$ | $-\phi_0$ | $\Delta$ | $-\phi_0$ | $\Delta$ | $-\phi_0$ | $\Delta$ | $-\phi_0$ | $\Delta$ | $-\phi_0$ | $\Delta$ | $-\phi_0$ | $\Delta$ | $-\phi_0$ | $\Delta$ |
| 0.0 | 0.2500 | 0.500 | 0.2500 | 0.500 | 0.2500 | 0.500 | 0.2500 | 0.500 | 0.2500 | 0.500 | 0.2500 | 0.500 | 0.250 | 0.500 |
| 0.2 | 0.2517 | 0.402 | 0.2522 | 0.408 | 0.2518 | 0.404 | 0.2522 | 0.408 | 0.2519 | 0.405 | 0.2522 | 0.407 | 0.253 | 0.400 |
| 0.4 | 0.2569 | 0.308 | 0.2588 | 0.327 | 0.2573 | 0.310 | 0.2589 | 0.327 | 0.2578 | 0.310 | 0.2589 | 0.324 | 0.260 | 0.300 |
| 0.6 | 0.2662 | 0.223 | 0.2698 | 0.239 | 0.2670 | 0.218 | 0.2700 | 0.245 | 0.2679 | 0.216 | 0.2701 | 0.237 | 0.273 | 0.200 |
| 0.8 | 0.2796 | 0.023[a] | 0.2842 | 0.135 | 0.2807 | 0.067 | 0.2855 | 0.153 | 0.2823 | 0.094 | 0.2850 | 0.136 | 0.292 | 0.100 |
| 1.0 | 0.3060 | 0.191[a] | 0.3048 | 0.039 | 0.3053 | 0.152[a] | 0.3060 | 0.027 | 0.3060 | 0.123[a] | 0.3065 | 0.041 | 0.3183 | 0.0 |
| $\gamma^*$ | 0.78 | | 1.07 | | 0.82 | | 1.05 | | 0.86 | | 1.08 | | 1.0 | |

[a]$\gamma > \gamma^*$, see text for discussion.

TABLE IV. IFC results for the Heisenberg ground-state energy per site and for the gap, for several values of $\gamma$, compared with HFA results (Ref. 2). The last row contains our estimates for $\gamma^*$. Results are in units $J_1 = 1$.

| $N_s, N_L$ | 4,4 | | 4,8 | | 6,4 | | 6,8 | | 8,4 | | 8,8 | | HFA | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $\gamma$ | $-\phi_0$ | $\Delta$ | $-\phi_0$ | $\Delta$ | $-\phi_0$ | $\Delta$ | $-\phi_0$ | $\Delta$ | $-\phi_0$ | $\Delta$ | $-\phi_0$ | $\Delta$ | $-\phi_0$ | $\Delta$ |
| 0.0 | 0.3750 | 1.0 | 0.3750 | 1.0 | 0.3750 | 1.0 | 0.3750 | 1.0 | 0.3750 | 1.0 | 0.3750 | 1.0 | 0.3750[a] | 1.0[a] |
| 0.2 | 0.3761 | 0.890 | 0.3766 | 0.893 | 0.3763 | 0.893 | 0.3766 | 0.892 | 0.3765 | 0.893 | 0.3765 | 0.895 | 0.3764 | 0.885 |
| 0.4 | 0.3799 | 0.757 | 0.3816 | 0.766 | 0.3807 | 0.762 | 0.3817 | 0.761 | 0.3813 | 0.762 | 0.3816 | 0.763 | 0.3774 | 0.738 |
| 0.6 | 0.3870 | 0.598 | 0.3907 | 0.618 | 0.3887 | 0.606 | 0.3909 | 0.621 | 0.3900 | 0.607 | 0.3908 | 0.613 | 0.3825 | 0.557 |
| 0.8 | 0.3983 | 0.403 | 0.4044 | 0.452 | 0.4012 | 0.413 | 0.4056 | 0.444 | 0.4034 | 0.427 | 0.4051 | 0.442 | 0.3943 | 0.329 |
| 1.0 | 0.4162 | 0.151 | 0.4248 | 0.260 | 0.4204 | 0.156 | 0.4270 | 0.226 | 0.4232 | 0.207 | 0.4254 | 0.253 | 0.4196[b] | 0.0[a] |
| $\gamma^* =$ | 1.07 | | 1.20 | | 1.07 | | 1.16 | | 1.15 | | 1.20 | | 1.00[a] | |

[a]Exact result.

[b]Exact result (Ref. 6) is $-\phi_0 = 0.4431$.

This behavior is equivalent to the situation (i) under interchange of $J_1$ and $J_2$ ($\gamma \rightarrow \gamma^{-1}$).

Unlike the RG approach, the IFC calculations reproduce the linear behavior of $\Delta(\gamma)$ for the $XY$ system; they also provide more accurate values of of $\phi_0$. These observations are in agreement with an earlier comparison of the two approximations, applied to the one-dimensional Ising chain in a transverse external field.[11] The improvement may be understood as the result of retaining a larger number of states per iteration in the IFC; the choice of states without regard to symmetry presumably accounts for the fact that $\gamma^*$ is only approximately unity. However, the general trend for $\gamma^*$ is improvement with either increasing $N_s$ or increasing $N_L$.

The $N_L = 4$ results for the $XY$ gap show unexpectedly strong behavior for all values of $N_s$ which we have considered. For $\gamma > 0.7$ the gap function is linear, extrapolating to zero at a value of $\gamma$ greater than one; however, at $\gamma \simeq 0.7$ a kink occurs, and we find $\gamma^* < 1$. The occurrence of the kink coincides with a level crossing which changes the degeneracies of the $N_s$-block eigenvalues, in ascending order, from (1,2,2,1,...) to (1,2,1,2,...), and thus affects the choice of states for $N_L = 4$. Neither the kink nor the difference in truncated basis appears for $N_L = 8$. In Table III we have listed, for the $N_L = 4$ calculations, the gap (with respect to the four-degenerate ground state) for $\gamma^* < \gamma \leq 1$.

For the Heisenberg system, the IFC approximation provides an improvement over the RG for both the estimate of $\phi_0(\gamma)$ and the agreement with the HFA on the gap for small $\gamma$. The IFC also provides greater accuracy (4% at $\gamma = 1$) in $\phi_0(\gamma)$ than the HFA. For these calculations, $\gamma^* > 1$ always. Also, it is difficult to discern trends in the results with increasing $N_L$ and $N_S$.

## IV. DISCUSSION

The major result of this work is a strong indication of the existence of a gap in the spectrum of the antiferromagnetic dimer Heisenberg chain. This is an immediate consequence of the fact that $\gamma = 1$ is an unstable fixed point of the system, while $\gamma = 0, \infty$ are stable fixed points. For $\gamma \neq 1$, the system is equivalent to a completely dimerized system $\gamma = 0$ (or $\infty$) insofar as its ground-state symmetries are concerned.

Support for this conclusion is provided by the IFC approximation, which we expect, from trial calculations on the $XY$ dimer system, to provide estimates of the gap which are quantitatively correct at small $\gamma$. In this region the IFC calculation supports the HFA results.[2] As $\gamma$ approaches unity the IFC values for the gap are larger than the HFA values; however, they are smaller than the values produced by the more standard finite-chain calculations, for equally sized blocks. For example, in the IFC for $N_L = N_s = 8$, the value of the gap is renormalized from 0.530 at the first iteration (corresponding to the standard calculation[14]) to 0.442 after several iterations. This is consistent with the renormalization of $J$ which occurs in the RG calculations, see Eqs. (14) and (B7).

Finally, we note that a similar RG study[17] of a more general system, the spin-$\frac{1}{2}$ dimer $XYZ$ chain, yields information which may be useful in understanding the special cases considered here.

*Note added in proof:* The program which produced the results listed in Table IV contained an error affecting later iterative steps. A correct treatment yields a slight further improvement in the ground-state energy and quantitative, though not qualitative, differences in the gap $\Delta(\gamma)$. Correct results for $N_L = N_S = 4$ are presented by Fields, *et al.*[18] Interestingly, for the Heisenberg dimer system, the $N_L = 4$ IFC calculation is equivalent to an $N_L = 4$ RG calculation. That $\gamma^* \neq 1$ is due to the lack of $J_1 \leftrightarrow J_2$ symmetry in the lattice block Hamiltonian for even $N_L$. The author thanks H. Blöte for suggesting the existence of an error.

## ACKNOWLEDGMENTS

The author wishes to thank M. Blume, J. C. Bonner, and V. J. Emery for useful discussions. In addition, he thanks R. Jullien for enlightening correspondence. This research was supported by the Division of Basic Energy Sciences, DOE, under Contract No. EY-76-C-02-0016.

## APPENDIX A: SOLUTION OF THE ANTIFERROMAGNETIC $XY$ DIMER CHAIN

We consider the Hamiltonian

$$H = (\tfrac{1}{2}J) \sum_{j=1}^{N} [S_{j,1}^{+} S_{j,2}^{-} + S_{j,1}^{-} S_{j,2}^{+} + \gamma (S_{j,2}^{+} S_{j+1,1}^{-} + S_{j,2}^{-} S_{j+1,1}^{+})] \ , \tag{A1}$$

where the index $i = 1, 2$ labels a particular site within the $j$th dimer unit cell. We impose periodic boundary conditions

$$\vec{S}_{j,i} = \vec{S}_{j+N,i} \ . \tag{A2}$$

Converting to fermionic operations $\psi_{j,1}$ and $\psi_{j,2}$ as in the treatment of the dimerized Heisenberg chain,[2] we rewrite Eq. (A1) in the form

$$H = (\tfrac{1}{2}J) \sum_{k} [a_k^{\dagger} b_k (1 + \gamma e^{ik}) + \text{H.c.}] \ , \tag{A3}$$

where we have

$$\psi_{j,1}=\left(\frac{1}{N}\right)^{1/2}\sum_k a_k e^{-ikj}\ ,$$
$$\psi_{j,2}=\left(\frac{1}{N}\right)^{1/2}\sum_k b_k e^{-ikj}\ , \tag{A4}$$

and

$$k=2n\pi/N,\quad n=1,2,\ldots,N\ . \tag{A5}$$

Note that we have taken the dimer length to be unity. The canonical transformation[2]

$$a_k=[1/(2)^{1/2}](\alpha_k+\beta_k)e^{-i\phi_k}\ ,$$
$$b_k=[1/(2)^{1/2}](\alpha_k-\beta_k)e^{i\phi_k}\ ,$$

and

$$\tan 2\phi_k=\frac{-\gamma\sin k}{1+\gamma\cos k}\ , \tag{A6}$$

takes the Hamiltonian (A3) into the form

$$H=\sum_k W_k(\alpha_k^\dagger\alpha_k-\beta_k^\dagger\beta_k)\ , \tag{A7}$$

$$W_k=(\tfrac{1}{2}J)[\cos 2\phi_k+\gamma\cos(k+2\phi_k)]\ . \tag{A8}$$

The ground state of the system consists of a filled $\beta$-particle band; its energy is

$$E_0=-\sum_k W_k=-\left(\frac{NJ}{\pi}\right)(1+\gamma)E\left(\frac{2\gamma^{1/2}}{1+\gamma}\right)\ , \tag{A9}$$

where $E$ is the complete elliptic integral of the second kind. The second equality in Eq. (A9) is obtained by converting the sum on $k$ into an integral, a correct approximation for large $N$.

The minimum excitation energy of the Hamiltonian (A7), which is the gap $\Delta$ in the original spin system described by Eq. (A1), is

$$\Delta=W_\pi=(\tfrac{1}{2}J)(1-\gamma)\ . \tag{A10}$$

In the limit $\gamma=0$, our results reduce to those expected for $N$ independent dimer pairs: $\phi_0/N=-\frac{1}{2}J$ and $\Delta=\frac{1}{2}J$. In the opposite limit of a uniform chain ($\gamma=1$), our results likewise agree with the results of Lieb, Schultz, and Mattis,[8] when account is taken of the increased periodicity of the lattice.

## APPENDIX B: RG ON THE $XY$ DIMER, BLOCKS OF THREE SITES

We begin with the Hamiltonian of Eq. (5), with $N_s=3$,

$$H^{(n)}=\sum_p\left(H_{2p}^{(n)}+H_{2p+1}^{(n)}+V_{2p,2p+1}^{(n)}+V_{2p+1,2p+2}^{(n)}+C^{(n)}\sum_{l=1}^{N_s}(I_{2p,l}+I_{2p+1,l})\right)\ , \tag{B1}$$

where we have

$$H_{2p}=(\tfrac{1}{2}J)(S_{2p,1}^+S_{2p,2}^-+\gamma S_{2p,2}^+S_{2p,3}^-+\text{H.c.})\ ,$$
$$H_{2p+1}=(\tfrac{1}{2}J)\ (\gamma S_{2p+1,1}^+S_{2p+1,2}^-+S_{2p+1,2}^+S_{2p+1,3}^-+\text{H.c.})$$
$$V_{2p,2p+1}=(\tfrac{1}{2}J)(S_{2p,3}^+S_{2p+1,1}^-+\text{H.c.})\ , \tag{B2}$$
$$V_{2p+1,2p+2}=(\tfrac{1}{2}J)(S_{2p+1,3}^+S_{2p+2,1}^-+\text{H.c.})\ .$$

In Eqs. (B2), and henceforth, the superscript $n$ is suppressed.

The first step is to diagonalize the block Hamiltonians $H_{2p}$ and $H_{2p+1}$ within the invariant subspaces corresponding to $S^z=\pm\frac{1}{2}$, where $S^z$ denotes the total-spin $z$ component. The subspace for $S^z=+\frac{1}{2}$ is

$$\{|{+}{+}{-}\rangle,\ |{+}{-}{+}\rangle,\ |{-}{+}{+}\rangle\}\ ;$$

the subspace for $S^z=-\frac{1}{2}$ contains the complements of these states. The diagonalized is easily done. Denoting the states of least energy by $|\pm\rangle_q$ and the corresponding energies by $E_\pm$, we find

$$E_+=E_-=-(\tfrac{1}{2}J)(1+\gamma^2)^{1/2} \tag{B3}$$

and

$$|+\rangle_{2p}=(2)^{-1/2}\left(\frac{\gamma}{(1+\gamma^2)^{1/2}}|{+}{+}{-}\rangle-|{+}{-}{+}\rangle+\frac{1}{(1+\gamma^2)^{1/2}}|{-}{+}{+}\rangle\right)\ ,$$
$$|-\rangle_{2p}=(2)^{-1/2}\left(\frac{\gamma}{(1+\gamma^2)^{1/2}}|{-}{-}{+}\rangle-|{-}{+}{-}\rangle+\frac{1}{(1+\gamma^2)^{1/2}}|{+}{-}{-}\rangle\right)\ ,$$
$$|+\rangle_{2p+1}=(2)^{-1/2}\left(\frac{1}{(1+\gamma^2)^{1/2}}|{+}{+}{-}\rangle-|{+}{-}{+}\rangle+\frac{\gamma}{(1+\gamma^2)^{1/2}}|{-}{+}{+}\rangle\right)\ , \tag{B4}$$
$$|-\rangle_{2p+1}=(2)^{-1/2}\left(\frac{1}{(1+\gamma^2)^{1/2}}|{-}{-}{+}\rangle-|{-}{+}{-}\rangle+\frac{\gamma}{(1+\gamma^2)^{1/2}}|{+}{-}{-}\rangle\right)\ .$$

We now construct the new spin operators. Simple algebra leads to the result

$$\langle + | S^+_{2p,1} | - \rangle = \langle + | S^+_{2p+1,3} | - \rangle = \frac{-\gamma}{(1+\gamma^2)^{1/2}} ,$$
$$\langle + | S^+_{2p,3} | - \rangle = \langle + | S^+_{2p+1,1} | - \rangle = \frac{-1}{(1+\gamma^2)^{1/2}} , \quad \text{(B5)}$$

all other matrix elements being zero. Comparing Eq. (11), we have

$$\xi_1 = \frac{-\gamma}{(1+\gamma^2)^{1/2}} , \quad \xi_3 = \frac{-1}{(1+\gamma^2)^{1/2}} . \quad \text{(B6)}$$

Use of Eq. (14) gives the recursion relations

$$J^{(n+1)} = [1 + (\gamma^{(n)})^2]^{-1} J^{(n)} , \quad \text{(B7)}$$

$$\gamma^{(n+1)} = (\gamma^{(n)})^3 , \quad \text{(B8)}$$

$$\mu^{(n+1)} = \nu^{(n+1)} = 0 , \quad \text{(B9)}$$

$$C^{(n+1)} = 3C^{(n)} - \tfrac{1}{2} J^{(n)} [1 + (\gamma^{(n)})^2]^{1/2} . \quad \text{(B10)}$$

Equation (B8) is a recursion relation with two fixed points in the range $0 \leq \gamma_0 \leq 1$: an unstable fixed point $\gamma^* = 1$ and a stable fixed point $\gamma^* = 0$. [The stable fixed point $\gamma^* = 0$ is equivalent to $\gamma^* = \infty$, under change of scale from $J_1$ to $J_2$ in Eq. (1).] Machine calculations for larger $N_s$ indicate that Eq. (B8) has a simple generalization

$$\gamma^{(n+1)} = (\gamma^{(n)})^{N_s} . \quad \text{(B11)}$$

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