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Renormalization group and other calculations for the one-dimensional spin-1/2 dimerized Heisenberg antiferromagnet[a]

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A zero-temperature renormalization group (RG) approach is applied to the one-dimensional, spin-1/2 antiferromagnetic Heisenberg dimerized (alternating) chain. Specifically, the ground state energy and lowest-lying spectral excitations are examined. The calculation indicates the existence of a gap in the spectrum of the dimerized chain which vanishes only in the limit of a uniform spin chain, in contrast to a recent Green's function approach. The RG results are in reasonable agreement with numerical extrapolations on the exact eigenvalue spectrum of finite chains of up to 12 spins. Both methods are compared with several other approximate treatments of the Heisenberg system, and tested by comparison with exact results for the spin-1/2 XY dimerized chain.

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INTRODUCTION

Recent experimental studies of linear chain spin-Peierls systems such as TTF $CuS_4(CF_3)_4$ have been interpreted [1,2] in terms of a Hartree-Fock (HFA) treatment [3] of the dimerized spin-1/2 anti-ferromagnetic Heisenberg chain, whose Hamiltonian is

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

where we take $J_1 \geq J_2 > 0$. To the extent that this interpretation depends upon the existence of a gap in the dimerized Heisenberg system for all $J_2 < J_1$, it has been called into question by a recent calculation [4] based on a Green's function decoupling scheme, which produces a gapless excitation band.

In this paper we discuss and compare two very recent approximate calculations of the ground state energy and low-lying excitations of Hamiltonian (1). The first calculation, which we shall present in some detail, is a zero-temperature quantum renormalization group (RG) treatment based on a simple two-level truncation scheme [5]. However, since the dimer spectrum has a four-level (singlet-triplet) rather than a two-level character, a four-level quantum RG scheme which preserves the basic singlet-triplet character, has also been employed, to increase quantitative accuracy [7].

The second method consists of direct extrapolations on the exact eigenvalue spectrum of finite chains of up to 12 spins [6].

Finally the various results have been compared with several other approximate calculations.

THE RENORMALIZATION GROUP METHOD

In this section we describe calculations which are similar in approach to the lattice RG techniques frequently used to calculate critical behavior [8]. We shall establish recursion relations which define the Hamiltonian, and we shall find fixed-points of these recursion relations.

In this approach, the lattice is sub-divided into coupled blocks of N_s sites such that the eigenvalues and eigenvectors of each block may be calculated exactly. The basis of each block (2^{N_s} levels) is truncated to some number, N_L, of levels, and the coupling between adjacent blocks is written within the truncated basis. The blocks have thus become equivalent to single sites on a new lattice. Choosing the two lowest states of an odd-N_s block, for example, maps the block onto a single spin 1/2 in the new lattice, and allows us to write down explicitly a set of recursion relations which define an RG transformation for the ground state of the Hamiltonian, at least for small N_s.

In order to maintain the symmetries of the system throughout the iterative process, we cast the Hamiltonian into the form

$$\begin{aligned}H^{(n)} = J^{(n)}\sum_i\{&(S^+_{2i}S^-_{2i+1}+S^-_{2i}S^+_{2i+1})+2\mu^{(n)}S^z_{2i}S^z_{2i+1})\\&+\alpha^{(n)}(S^+_{2i+1}S^-_{2i+2}+S^-_{2i+1}S^+_{2i+2}+2\nu^{(n)}S^z_{2i+1}S^z_{2i+2})\\&+C^{(n)}(I_{2i}+I_{2i+1})\},\end{aligned} \qquad (2)$$

where I represents the 2 x 2 identity matrix. The initial conditions are

$$J^{(o)} = J_1,\quad \mu^{(o)} = \nu^{(o)} = 1,\quad \alpha^{(o)} = \alpha,\quad C^{(o)} = 0,$$
$$\text{where } \alpha = J_2/J_1. \qquad (3)$$

Associating the lattice sites into blocks of N_s spins, the Hamiltonian can be written as a sum of intrablock and interblock terms:

$$\begin{aligned}H^{(n)} = \sum_p\{&H^{(n)}_{2p}+H^{(n)}_{2p+1}+V^{(n)}_{2p,2p+1}+V^{(n)}_{2p+1,2p+2}\\&+C^{(n)}\sum_{i=1}^{N_s}(I_{2p,i}+I_{2p+1,i})\},\end{aligned} \qquad (4)$$

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 (N_s odd)

$$\begin{aligned}H_{2p} &= 2J\{\vec{S}_{2p,1}\cdot\vec{S}_{2p,2}+\alpha\vec{S}_{2p,2}\cdot\vec{S}_{2p,3}+\ldots+\alpha\vec{S}_{2p,N_s-1}\cdot\vec{S}_{2p,N_s}\}\\H_{2p+1} &= 2J\{\alpha\vec{S}_{2p+1,1}\cdot\vec{S}_{2p+1,2}+\vec{S}_{2p+1,2}\cdot\vec{S}_{2p+1,3}+\ldots+\vec{S}_{2p+1,N_s-1}\cdot\vec{S}_{2p+1,N_s}\}\end{aligned} \qquad (5)$$

and the interblock couplings have the form

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

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$$V_{2p+1,2p+2} = 2\alpha J \vec{S}_{2p+1,N_S} \cdot \vec{S}_{2p+2,1}. \quad (6)$$

In equations (5) and (6) the labels n are suppressed.

The eigenstates of $H_q^{(n)}$, where q = 2p or 2p+1, may be chosen to be simultaneous eigenstates of the total z-component spin operator of the block q:

$$S_q^z = \sum_{i=1}^{N_S} S_{q,i}^z \quad (7)$$

The new basis is chosen to contain the two states $\{|+>_q, |->_q\}$, where $|+>_q$ ($|->_q$) is the state of lowest energy E_+ (E_-) in the subspace $S_q^z = +\frac{1}{2}$ ($-\frac{1}{2}$). These states are the lowest energy states of the old basis and may be expressed as

$$|\pm>_{2p}^{(n+1)} = \sum_{\varepsilon_1} \cdots \sum_{\varepsilon_{N_S}} \lambda^{\pm(n)}_{\varepsilon_1 \cdots \varepsilon_{N_S}} |\varepsilon_1 \cdots \varepsilon_{N_S}>^{(n)}$$
$$|\pm>_{2p+1}^{(n+1)} = \sum_{\varepsilon_1} \cdots \sum_{\varepsilon_{N_S}} \Lambda^{\pm(n)}_{\varepsilon_1 \cdots \varepsilon_{N_S}} |\varepsilon_1 \cdots \varepsilon_{N_S}>^{(n)}, \quad (8)$$

where $\sum_{\varepsilon_\ell}$ represents a summation over the two spin states $|\pm>_\ell^{(n)}$ at site ℓ of the block.

The next step is to rewrite the interblock coupling terms. We calculate the matrix elements of $S_{q,\ell}^{\pm(n)}$ and $S_{q,\ell}^{z(n)}$ in the new basis:

$$S_{2p,\ell}^{+(n)} = \xi_\ell^{(n)} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \xi_\ell^{(n)} S_{2p}^{+(n+1)} \quad (9a)$$

and, similarly,

$$S_{2p+1,\ell}^{+(n)} = \xi_{N_S-\ell+1}^{(n)} S_{2p+1}^{+(n+1)}, \quad (9b)$$

$$S_{2p,\ell}^{z(n)} = \eta_\ell^{(n)} S_{2p}^{z(n+1)} \quad (9c)$$

$$S_{2p+1,\ell}^{z(n)} = \eta_{N_S-\ell+1}^{(n)} S_{2p+1}^{z(n+1)} \quad (9d)$$

where

$$\xi_\ell^{(n)} = \sum_{\varepsilon_1} \cdots \sum_{\varepsilon_{\ell-1}} \sum_{\varepsilon_{\ell+1}} \cdots \sum_{\varepsilon_{N_S}} \lambda^{+(n)}_{\varepsilon_1 \cdots \varepsilon_{\ell-1},+,\varepsilon_{\ell+1} \cdots \varepsilon_{N_S}} \times \lambda^{-(n)}_{\varepsilon_1 \cdots \varepsilon_{\ell-1},-,\varepsilon_{\ell+1} \cdots \varepsilon_{N_S}},$$

and

$$\eta_\ell^{(n)} = \sum_{\varepsilon_1} \cdots \sum_{\varepsilon_\ell} \cdots \sum_{\varepsilon_{N_S}} \varepsilon_\ell (\lambda^{+(n)}_{\varepsilon_1 \cdots \varepsilon_\ell \cdots \varepsilon_{N_S}})^2. \quad (10)$$

The coupling terms become

$$V_{2p,2p+1}^{(n)} \to J^{(n)} \{[\xi_{N_S}^{(n)}]^2 (S_{2p}^+ S_{2p+1}^- + \text{h.c.}) + 2\mu^{(n)} [\eta_{N_S}^{(n)}]^2 S_{2p}^z \times S_{2p+1}^z\}$$

$$V_{2p+1,2p+2}^{(n)} \to \alpha^{(n)} J^{(n)} \{[\xi_1^{(n)}]^2 (S_{2p+1}^+ S_{2p+2}^- + \text{h.c.}) + 2\nu^{(n)} [\eta_1^{(n)}]^2 \times S_{2p+1}^z S_{2p+2}^z\}, \quad (11)$$

and hence

$$J^{(n+1)} = [\xi_{N_S}^{(n)}]^2 J^{(n)}; \quad \alpha^{(n+1)} = [\xi_1^{(n)}/\xi_{N_S}^{(n)}]^2 \alpha^{(n)};$$
$$\mu^{(n+1)} = [\eta_{N_S}^{(n)}/\xi_{N_S}^{(n)}]^2 \mu^{(n)}; \quad \nu^{(n+1)} = [\eta_1^{(n)}/\xi_1^{(n)}]^2 \nu^{(n)};$$
$$C^{(n+1)} = N_S C^{(n)} + E_+^{(n+1)}. \quad (12)$$

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

$$E_o = \lim_{n\to\infty} (C^{(n)}/N_S^{(n)}). \quad (13)$$

In general, the eigenvectors $|\pm>^{(n+1)}$ and eigenvalues $E_\pm^{(n+1)}$, as well as the recursion coefficients of equation (12), are determined by machine.

RESULTS

The RG calculation has been performed for N_S=3, 5, 7 and 9, for both the Heisenberg and the XY dimer systems. The uniform limit, $\alpha^* = 1$, is always found to be an unstable fixed point of the system. Initial values $\alpha^{(o)} < 1$ flow (with increasing n) into the stable fixed point $\alpha^* = 0$ (independent dimers). This result leads immediately to the conclusion that the alternating spectrum has a gap which vanishes only in the uniform limit $\alpha^{(o)} = 1$. This conclusion is supported by similar fixed point behavior in the case of the XY model, which is exactly solvable [9], and also shows a gap which vanishes only in the uniform limit. It is supported also by the direct finite chain extrapolations, which indicate a gap for both Heisenberg and XY dimerized systems [5, 6].

For both the ground state energy per spin (see Figs. 1 and 2) and the energy gap (see Fig. 3), the direct extrapolation method is believed to have the best quantitative accuracy for all degrees of dimerization. In Fig. 3, it is seen that the two-level RG method for N_S = 9 (the accuracy of this method improves as N_S increases) is qualitatively in agreement with extrapolation results near the uniform limit, but is rather seriously in error near the dimer limit. This is the result of preserving only two levels at each iteration step. In order to improve the RG estimates for the gap (and also for the ground state energy per spin) another type of RG calculation, in which the truncated basis at each step is taken to be four levels, preserving the singlet-triplet character, has been carried out, by way of a general matrix formulation of the problem which can be regarded as a variant on finite chain techniques [10, 11]. The result is a considerable quantitative improvement for both gap and ground state energy. However, this method yields an α^* which is approximately rather than exactly unity.

The "critical exponents" for the Heisenberg problem are (a) the deviation of E_o/J [where $J = \frac{1}{2}(J_1+J_2)$] from the uniform limit as a function of δ[where $\delta = (1-\alpha)/(1+\alpha)$], and (b) the vanishing of the gap Δ near the uniform limit, also as a function of δ. A very recent theory by Cross and Fisher based on the dimerized Luther-Peschel-Luttinger model [12] predicts that the deviation (from $E_o(\delta=0)/J$) $\mathcal{E}_o/J \sim \delta^{4/3}$, whereas an N_S = 3, two-level RG approach of de Braak et al [13] predicts $\mathcal{E}_o/J \sim \delta^{1.37744}$.

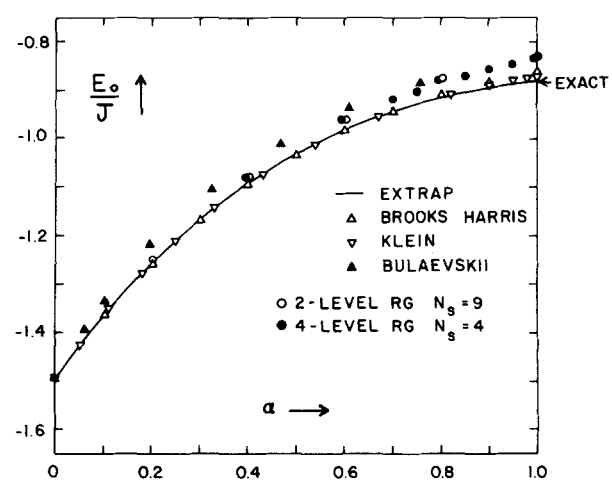

Fig. 1. Comparison of ground state energy per spin for various models

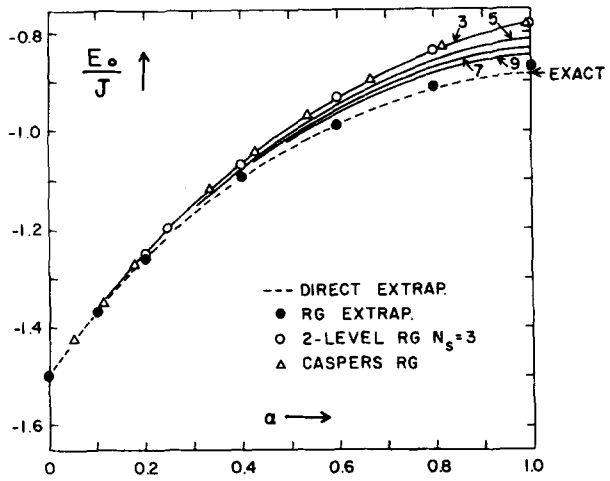

Fig. 2
Extrapolations of 2-level RG groups for N_s = 3, 5, 7, and 9 in comparison with direct extrapolations.

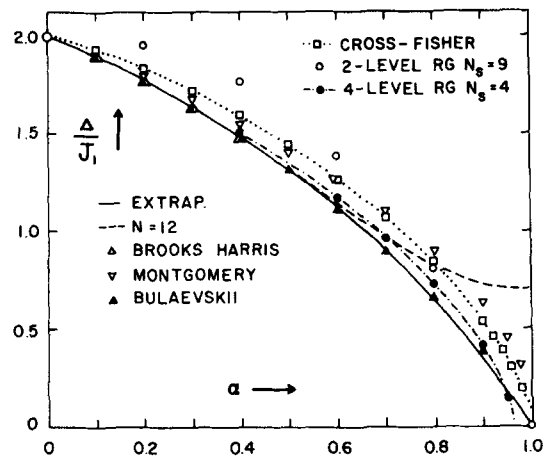

Fig. 3
Comparison of various approximate theories for the alternating antiferromagnetic excitation energy gap. The direct extrapolations are shown as a solid curve. As an aid to the eye, a dotted line has been drawn through the Cross-Fisher points and a dot-dashed line through the N_s = 4, N_L = 4 RG points.

The finite chain extrapolations are consistent with either prediction, yielding an exponent $1.36^{+.01}_{-.02}$. The N_s = 7, two-level RG approach, featured here gives a larger value of 1.5 (approx.). These four approaches are not consistent with the Bulaevskii HFA [3] which predicts $\mathcal{E}_o/J \sim \delta^2 \ell n^2 \delta$.

For the case of the excitation energy gap the Cross-Fisher theory [12] predicts $\Delta/J \sim \delta^{2/3}$, whereas our N_s = 7 RG approach gives $\Delta/J \sim \delta^{0.76}$ (approx). These two approaches are in reasonable agreement. However, from Fig. 3, it appears that the finite chain extrapolations are predicting a somewhat larger exponent, but apparently < 1. Extrapolation uncertainties do not permit a quantitative estimate, however.

Finally, we discuss a variety of other approximate calculations, In Fig. 1, the ground state energy per spin, E_o/J, is compared to the Bulaevskii HFA [3], and an appreciable quantitative discrepancy is observed for all α. (The exact result [14], for the uniform limit only, is indicated by the arrow.) Much better agreement is achieved by a third-order perturbation calculation of Brooks Harris [15] and a Kekulé state calculation of García-Bach and Klein [16]. It is interesting that the Harris calculation is a perturbation about the dimer limit (α=0) and yet does quite well near α=1. The 2-level RG result for N_s = 9 and the 4-level RG results for N_s = 4 are intermediate in accuracy. However, in Fig. 2, the 2-level RG sequence for N_s = 3, 5, 7, and 9 is extrapolated and the result gives much better agreement with the direct extrapolations. (The N_s = 3 RG calculation is equivalent to the RG calculation of ref. 13).

In the case of the energy gap (Fig. 3), the Bulaevskii HFA [3] shows the best agreement with the direct extrapolations. The Cross-Fisher calculation [12] is inherently incapable of predicting amplitudes, and is therefore presented with arbitrary normalization. As mentioned above, the 2-level, N_s odd, RG calculations are poor near the dimer limit. The 4-level, N_s = 4, RG calculation with singlet-triplet symmetry is accurate for $\alpha \lesssim 0.4$, but vanishes at $\alpha^* = 0.962$ instead of $\alpha^*=1$. An older, quasi-boson calculation of Montgomery [17] gives a gap which vanishes as $(1-\alpha)^{\frac{1}{2}}$ or equivalently, $\Delta \sim \delta^{0.5}$.

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