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Renormalization Group for the Linear-Chain Heisenberg Model*

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Several real-space renormalization group techniques are applied to the spin-1/2 linear-chain Heisenberg model. The particular schemes investigated renormalize blocks (or subchains) to new spin-1/2 sites, each coupled only to nearest neighbor (like-renormalized) sites. Iteration of the renormalization transformation eventually provides values for the per-site properties of an infinite chain. A first-order perturbational method, a related variationally optimized approach, and a cluster-expansion technique are applied using blocks of several different sizes. The first two of these schemes are found to give less accurate values and converge more slowly with block size than the cluster-expansion technique, though this last technique (unlike the first two) is not variationally bounded. A novel modification of the perturbation-variation scheme, where one renormalizes at each iteration only a single block at the end of the chain, is also noted as a possibility and is found to give variationally bounded results comparable to the cluster expansion.

INTRODUCTION

Renormalization »group« theory is a promising general technique, one application of which is to find ground-state characteristics of large molecular systems. The real-space version offers a conceptually appealing approach to the treatment of a large system in terms of (local) subsystems. Often, the focus has been on temperature-dependent renormalization and/or momentum-space renormalization,[1] but in principle it can also be used to treat ground states in coordinate space. However, earlier versions of real-space ground-state renormalization have met with only slight success, as noted by White and Noack.[2]

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Here, we investigate ways to improve the accuracy of a very simple renormalization mapping, as applied to a well-known but nontrivial many-body system: the linear-chain isotropic spin-1/2 Heisenberg (or valence-bond) model. This simple renormalization mapping carries the nearest-neighbor model into another similar rescaled nearest-neighbor model. That is, the mapping just shifts the zero of energy and rescales the interaction strength. In the real-space view, sets of sites are grouped together in *blocks*, each of which has first, a low-lying state of the same symmetry as a single original site; and second, all neighbor pairs of blocks related in symmetrically the same manner as pairs of original neighbor sites. The blocks give rise to renormalized sites, and the process is iterated. Our present cluster-expansion[3] and variational renormalization schemes both yield more accurate values than the earlier first-order perturbational scheme clearly reviewed by Casper.[4] Further, looking at blocks of varying size, we investigate extrapolations to the exact infinite block limit.

RENORMALIZATION

The Heisenberg model of present interest is

$$H = \sum_i A + \sum_{i-j} (B + 2J\vec{S}_i \cdot \vec{S}_j) \tag{2.1}$$

where the $\vec{S}_i$, are the usual spin operators (for site i) and the second sum is over nearest-neighbor pairs of sites, and the operators A and B are of the form of scalars A and B times unit operators. Often, the site and interaction shifts A and B are combined or deleted, though one can expect them to renormalize in different ways. The renormalized model is to be of the same form

$$H' = \sum_i A' + \sum_{i-j} (B' + 2J'\vec{S}_i \cdot \vec{S}_j) \tag{2.2}$$

but with the site indices and associated spin operators now referring to what previously were blocks, so that in fact the system now appears smaller. Since A and B merely shift the eigenspectrum, the new »exchange« coupling J' should depend solely on the previous strength J, and indeed the relation should be linear to preserve units. Similarly, B' associated with the new interaction should depend only on the previous one, through B and J, in a linear manner too. Finally, A' might depend on A, B and J since both several sites and bonds have been incorporated into the new site, and again we assume a linear relation. For the chain in which M sites (and M–1 bonds) are combined together into a block to give the new site, we then write

$$\begin{aligned} J' &= \gamma J \\ B' &= B + \beta J \\ A' &= MA + (M-1)B + \alpha J \end{aligned} \tag{2.3}$$

The different schemes considered here compute α, β and γ *via* different criteria, each of which may be applied to a range of block sizes M. In all cases, M is odd so that the chain of length M (comprising a block) has a spin doublet ground state, just as does

a single site. The most common scheme[4] determines α, β, γ *via* a first-order perturbational argument. But, as we see in the next two sections, there are other possibilities.

In any of these schemes, the equation (2.3) may be iterated. Denoting the parameter values at the n^{th} iteration with appropriate superscripts, we find (with $B^{(0)} = A^{(0)} = 0$)

$$\begin{aligned} J^{(n)} &= \gamma^n J^{(0)} \\ B^{(n)} &= \beta \frac{1-\gamma^n}{1-\gamma} J^{(0)} \\ A^{(n)} &= (M^n - \gamma^n)\frac{\alpha+\beta}{M-\gamma} J^{(0)} - \beta \frac{1-\gamma^n}{1-\gamma} J^{(0)} \end{aligned} \tag{2.4}$$

of course $A^{(n)}$ provides an energy estimate for a chain of M^n sites. Thus, our infinite chain energy per-site estimate (in units of $J^{(0)}$ is

$$\mathcal{E} = \lim_{n\to\infty} \frac{A^{(n)}}{M^n J^{(0)}} = \frac{\alpha+\beta}{M-\gamma} \tag{2.5}$$

and all that remains is the choice of α, β and γ.

CLUSTER EXPANSION

In the cluster expansion approach,[3,5] renormalized sites and interaction terms are determined so as to match exactly those of smaller clusters of blocks. The lowest order approximation (as for the simple renormalization mapping here) makes a fit just to clusters of one and two blocks. Of course, the blocks must be of an odd number M of sites if the doublet spin symmetry of the original sites is to be retained upon renormalization. The renormalization is entirely determined from cluster energies $E_{\text{D}}(M)J^{(0)}$, $E_{\text{S}}(2M)J^{(0)}$, and $E_{\text{T}}(2M)J^{(0)}$ for the lowest doublet, singlet and triplet states of M-site, $2M$-site and $2M$-site clusters, with $A^{(0)} = B^{(0)} = 0$. Then, from the solution of the 1- and 2-site renormalized Hamiltonians H' we have

$$\begin{aligned} A' &= E_{\text{D}}(M)J^{(0)} \\ 2A' + B' + J'/2 &= E_{\text{T}}(2M)J^{(0)} \\ 2A' + B' - 3J'/2 &= E_{\text{S}}(2M)J^{(0)} \end{aligned} \tag{3.1}$$

Thus, recalling Eq. (2.3), one may solve for α, β, and γ to obtain

$$\begin{aligned} \alpha &= E_{\text{D}}(M) \\ \beta &= \tfrac{1}{4}E_{\text{S}}(2M) + \tfrac{3}{4}E_{\text{T}}(2M) - 2E_{\text{D}}(M) \\ \gamma &= \tfrac{1}{2}E_{\text{T}}(2M) - \tfrac{1}{2}E_{\text{S}}(2M) \end{aligned} \tag{3.2}$$

and a consequent energy per site *via* equation (2.5).

VARIATIONAL ESTIMATE

In the variational approach, one utilizes block wavefunctions of the same symmetry as the site states and uses these wavefunctions to develop a renormalized interblock coupling. For the present case, these block wavefunctions are doublets Ψ_+ and Ψ_- having z components of spin $+1/2$ and $-1/2$, respectively. The renormalized Hamiltonian is to be that over the basis of products of the Ψ_+ and Ψ_- for each block. Each renormalization stage reduces to the same problem, expressible in terms of single-block matrix elements of H_{block}, s_i^μ and s_M^μ on the basis $\{\Psi_+, \Psi_-\}$ with $\mu = x, y, z$ or $\mu = z, +, -$. In fact, the various matrix elements for different μ are (symmetry) related by the Wigner-Eckart theorem, and if we also assume that Ψ_+ and Ψ_- are reflection-symmetric (as is the ground state), then we have just two relevant symmetry-independent matrix elements

$$E_\Psi(M) \equiv \langle \Psi_+ | H_{block} | \Psi_+ \rangle$$

$$\gamma_\Psi \equiv 2\langle \Psi_+ | s_M^z | \Psi_+ \rangle \tag{4.1}$$

Next, following the analysis reviewed by Caspers,[4] one finds (with $A^{(0)} = B^{(0)} = 0$)

$$A' = E_\Psi(M) J^{(0)}$$

$$B' = 0 \tag{4.2}$$

$$J' = \gamma_\Psi^2 J^{(0)}$$

and the infinite-chain energy per site becomes (in units of $J^{(0)} = J$)

$$\mathcal{E} = \frac{E_\Psi(M)}{M - \gamma_\Psi^2} \tag{4.3}$$

In the common first-order perturbative approach,[4] one utilizes exactly this formalism with Ψ_+, constrained to be the ground-state to the block Hamiltonian. However, (4.3) is an upper bound to the ground state regardless of this constraint.

We propose to optimize our per-site energy estimate with regard to (symmetry preserving) variations in $\Psi = \Psi_\pm$. If variations are taken with respect to Ψ^* in (4.3), then

$$\delta\mathcal{E} = \langle \delta\Psi | \left\{ \frac{1}{M - \gamma_\Psi^2} H_{block} + \frac{2E_\Psi(M)}{(M - \gamma_\Psi^2)^2} \gamma_\Psi [s_1^z + s_M^z] \right\} | \Psi \rangle \tag{4.4}$$

Consequently, optimization is achieved if the eigensolution to

$$\left\{ H_{block} + \frac{2E_\Psi(M)}{M - \gamma_\Psi^2} \gamma_\Psi [s_1^z + s_M^z] \right\} | \Psi \rangle = \mathcal{E} | \Psi \rangle \tag{4.5}$$

is self-consistent in giving the expectations of (4.1) used in (4.5). Here, it is understood that to have Ψ retain the doublet spin symmetry of the ground state (and thereby enable the renormalization from (2.1) to (2.2), only parts of s_i^z and s_M^z not admixing other spin symmetries are to be used. This relevant symmetric part is given by[6]

$$[s_i^z] = 2\,\vec{s}_i \cdot \vec{S} \tag{4.6}$$

where $\vec{S}$ is the total spin operator (with a sum over M site spins). Now, an iterative procedure analogous to ordinary SCF theory is suggested: place an estimate of $E_\Psi(M)$ and γ_Ψ in (4.5), solve for Ψ, compute new estimates *via* (4.1), and iterate to convergence. The iteration could start, *e.g.*, with $\Psi_\pm$ from the first-order perturbative scheme.

Even further improvement might be obtained if the reflection symmetry of the ground state of a block were to be relaxed. Then, taking all blocks translationally equivalent, one obtains $\gamma = \gamma_\Psi \gamma_{\Psi'}$ with γ_Ψ and $\gamma_{\Psi'}$ being generally distinct spin-densities for the 1st and M-th spins in a block. Then, in place of (4.5) one obtains

$$\left[H_{\text{block}} + \frac{2E_\Psi(M)}{M - \gamma_\Psi \gamma_{\Psi'}} (\gamma_{\Psi'} [s_1^z] + \gamma_\Psi [s_M^z])\right] | \Psi\rangle = \mathcal{E} | \Psi\rangle \tag{4.7}$$

and the same self-consistent approach can be applied. If the asymmetry of the blocks were alternated, the alternating rescaling factors of γ_Ψ^2 and $(\gamma_{\Psi'})^2$ would arise and thereby give an apparently dimerized model.

NUMERICAL RESULTS

Using a range of block sizes, we have carried out computations for the three different renormalization schemes: the first-order perturbative scheme, the variational scheme, and the 2-site cluster-expansion scheme. Our numerical results for the energy per site (in units of J) are given in Table I, where also we report the corresponding value for a single block. In addition, we carried out the computations for the (M = 3 and 5) »nonsymmetric« variational scheme of Eq. (4.7), but optimization using this

TABLE I

Energies per site in units of J

M	$\mathcal{E}$			
block size	isolated block	1st order perturbation	variational	2-site cluster expansion
3	−0.6667	−0.7826	−0.7826	−0.8969
5	−0.7712	−0.8138	−0.8195	−0.8923
7	−0.8104	−0.8314	−0.8368	−0.8901
9	−0.8303	−0.8423	−0.8469	−0.8890
11	−0.8422	−0.8499		−0.8883
13	−0.8500	−0.8553		−0.8878
15	0.8556	−0.8593		
17	−0.8597	−0.8625		
19	−0.8629	−0.8650		

$\mathcal{E}_{\text{exact}} = -0.886294$

equation led back to the symmetric result, associated to Eq. (4.5). Even the first-order perturbation theoretic results obtained here extend significantly those earlier reported[7] up to $M = 9$. The numerical computations are made *via* an efficient »unitary group« technique.[8]

The data is sufficient that extrapolations as a function of block size M seem warranted. The block energies per site are naturally expected to deviate from the infinite block limit $\mathcal{E}_\infty$ by (end-correction) terms $\sim 1/M$. We anticipate a similar behavior for the first-order perturbative result, and then also for our variational result, which seems to approach closely the perturbative result as M increases. The behavior of the cluster-expansion renormalization result seems though a more delicate matter, which we have subjected to empirical test by plotting

$$\ln \{\mathcal{E}_{M+2}(\text{cluster}) - \mathcal{E}_M(\text{cluster})\} \text{ vs. } -\ln M \tag{5.1}$$

The resultant asymptotic slope of about 2.5 suggests that energies per site for this scheme seem to deviate from $\mathcal{E}_\infty$ by terms $\sim 1/M^{3/2}$. A similar plot for the first-order perturbative scheme gives an asymptotic slope of a little less than 2, and thence tends to verify earlier expectations for this case.

Extrapolated estimates for the infinite-block energy per site are now made in Figure 1 by plotting

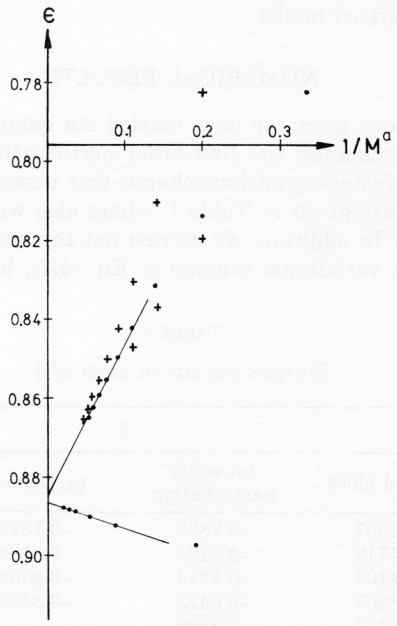

Figure 1. Energies per site as computed using different size M blocks plotted versus $1/M^a$. The positive slope line is estimated from the first-order perturbational points, just above and below wich there respectively occur the monomer block and variational points. The negative slope line is estimated from the cluster-expansion renormalization points.

$$\mathcal{E} \text{ vs. } 1/M^a \tag{5.2}$$

where $a = 1$ is taken for the first three columns of energies of Table I, and $a = 3/2$ is taken for the last column. The monomer energies, first-order perturbative energies and cluster-expansion energies seem, respectively, to extrapolate to near –0.889, –0.885 and –0.8863. Especially, the last extrapolation is near the exact result ≈–0.886294 of Hulthén.[9]

DISCUSSION

It seems that the earlier studied[4,7] first-order perturbative renormalization scheme can be improved upon. In addition to taking this older scheme to larger block sizes (*via* the efficacious computational technique of ref. 8), the variational scheme described here (in section 4) gives some improvement while maintaining a variational bound. Even more accurate energies, though now not variationally bounded ones, are obtained with our simple cluster-expansion technique of section 3.

There is much promise for further applications of our renormalization schemes. Of course, linear-chain systems with next-nearest-neighbor interactions and/or bond alternation are treatable by our improved renormalization schemes – and indeed such systems are of much interest, more so since the exact solution of Hulthén no longer applies. Also, computations for the ground states of Heisenberg models for 2-dimensional lattices are quite feasible (and are of interest, because of their possible relation to high-temperature superconductivity).

Further, there are also possibilities that our methods can be extended to deal with more complicated (and presumably more accurate) renormalization mappings. Higher-order perturbative and higher-order cluster-expansion approaches would yield new Hamiltonians (not just shifted and rescaled) with nonnearest neighbor interactions of varying strengths. Similar techniques, we believe, should be applicable to other models, such as Hubbard or PPP models.

Even within the constraint of renormalization mappings limited to no more than nearest neighbor couplings, there are conceivable improvements. One such already mentioned is that of lowering the translational symmetry leading to alternating bond strengths. Another type of previously unconsidered scheme iteratively renormalizes just the M sites at the end of a chain to a new site. This leads to models with the single bond at the (renormalizing) end of the chain being of a different strength than all the others, and for $M = 3$ yields the per-site energy of –0.8737. Indeed, this value is quite good for a variational bound, *e.g.* in comparison to the variational renormalization bounds of Table I, or a number of other bounds as listed in Ref. 4.

In conclusion, it seems that the renormalization schemes described here are of promise for application to other systems and, in addition, it seems that there are methodological extensions and alternatives of much promise too. Further investigation of such ground-state renormalization-group schemes seems warranted.

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SAŽETAK

Renormalizacijska grupa za Heisenbergov model linearnog lanca

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Nekoliko tehnika renormalizacijske grupe u stvarnom prostoru primijenene su na Heisenbergov model linearnog lanca sa spinom 1/2. Ispitanim shemama renormaliziraju se blokovi (ili pod-lanci) u nova mjesta sa spinom 1/2, tako da svako bude povezano samo s najbližim susjednim (na isti način renormaliziranim) mjestima. Iteriranje renormalizacijske transformacije pouzdano daje vrijednosti svojstava beskonačnog lanca, normirane na broj mjesta u lancu. Ispitana je perturbacija prvog reda, kao i sličan varijacijski optimiran pristup te razvoj u grozdove, upotrebljavajući blokove nekoliko različitih veličina. Ustanovljeno je da prve dvije tehnike daju manje točne vrijednosti i sporije konvergiraju s veličinom bloka nego razvoj u grozdove, premda ova zadnja tehnika (za razliku od prethodnih) nije varijacijski ograničena. Uočena je nova modifikacija perturbacijsko-varijacijske tehnike kojom se u svakoj iteraciji renormalizira samo blok na kraju lanca. Ovom tehnikom dobivaju se varijacijski određene granice usporedive s onima iz razvoja u grozdove.