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The density matrix renormalization group and critical phenomena

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Abstract. We adapt White's density matrix renormalization group (DMRG) to the direct study of critical phenomena. We use the DMRG to generate transformations in the space of coupling constants. We postulate that a study of density matrix eigenvalues leads to a natural identification of renormalized blocks, operators and Hamiltonians. We apply the scheme to the phase transition in the anisotropic spin-1/2 Heisenberg chain. In the simplest case where the two most probable states in odd-sized blocks are used to construct approximate renormalization group transformations, we find qualitative improvement upon the standard real-space renormalization group method for the thermal exponent ν.

1. Introduction

The advent of White's density matrix renormalization group (DMRG) method [1] has led to some very successful studies of low-lying excitations and static correlation functions in a number of one-dimensional quantum lattice systems [2]. The method represents a major improvement upon its precursor the (conventional, Wilson) real-space renormalization group (RSRG) method [3] which generally gives poor or slowly converging results for these quantities.

Both methods are truncated basis expansions in that a target state (such as the ground state) of a large lattice is built up from blocks of sites from which only a few *important* states are retained. The key difference between the two methods is the way in which the important states are determined—for the RSRG method states are retained on the basis of energy whereas in the DMRG method states are retained on the basis of how likely they are to be part of the target state being investigated.

It is well documented that the DMRG method works best when the system being studied is away from criticality—that is, when there is a substantial energy gap, or when the generic correlation functions decay exponentially, with a correlation length of only a few lattice spacings [1, 4, 5]. In fact, efforts to study zero-temperature phase transitions by using obvious approaches such as investigating the divergence of the correlation length [4] or the vanishing of an order parameter [5] have failed because it is very difficult to determine these quantities accurately near the critical point.

It is well known, however, that the RSRG method can be used to generate renormalization group transformations in the space of coupling constants [6]. Useful qualitative and even accurate quantitative results can be obtained for the positions of phase transitions and critical exponents [6, 7].

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A next step is to investigate whether the DMRG method can be used to generate such transformations and yield accurate phase diagrams and associated critical exponents, especially in cases where the RSRG method fails. That is, it would be useful to develop a DMRG scheme for coupling constant transformations which has the same accuracy, systematic improvability and portability as the DMRG scheme currently being used for the calculation of energies and correlation functions. Such a scheme might be very useful if applied to the investigation of critical phenomena in complex models such as coupled fermion chains.

Such an investigation has been carried out in a recent series of papers by Drzewiński and co-workers [8]. Results from the RSRG method were compared directly with those obtained from its DMRG analogue. In studies of anisotropic XY-models with transverse fields, it was generally concluded that the DMRG has no special advantage over the RSRG in calculating critical points and exponents. These studies cannot however be considered exhaustive. Firstly, the blocks and superblocks used were small—only a few sites. Secondly, the models did not afford the total z-spin as a good quantum number. This sometimes complicated the process of identifying important block states with renormalized block spin variables.

In this paper we consider a DMRG approach to coupling constant transformations which makes use of the fact that within DMRG algorithms we accurately calculate important states for very large blocks by retaining large numbers of states at each iteration. We apply this approach to a simple model, the anisotropic Heisenberg model, where critical properties are very well known [13]. The model has been studied using the RSRG [9] with less than encouraging results. We find that the DMRG approach yields qualitative improvement in the nature of the convergence of the thermal critical exponent ν as the block size is increased.

In the following sections we briefly outline the DMRG algorithm and describe how it can be used to generate coupling constant transformations. We then present our results for the anisotropic Heisenberg model and compare them with the RSRG results of [9]. We then conclude with some remarks on future directions.

2. The DMRG and coupling constant transformations

The DMRG algorithm has been described in great detail [1] so we will be brief in our description, concentrating on those points which are relevant to generating renormalization group transformations. We restrict ourselves to the infinite-lattice algorithm which we use in our calculations and we describe the algorithm in the context of the Heisenberg spin chain

$$\mathcal{H} = \sum_i \left[S_i^z S_{i+1}^z + \gamma \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right) \right] \tag{1}$$

where S_i is the spin operator of spin S for site i on the chain and γ is the anisotropy.

The DMRG method is an iterative, truncated basis procedure whereby a large chain (or superblock) is built up from a small number of sites by adding a small number of sites at a time. At each stage the superblock consists of system and environment blocks (determined from previous iterations) in addition to a small number of extra sites. Also determined from previous iterations are the matrix elements of the block Hamiltonians and the *active* spin operators (those on the sites at the end(s) of the blocks) with respect to a truncated basis. Tensor products of the states of the system block, the environment block and the extra sites are then formed to provide a truncated basis for the superblock. The ground state $|\psi\rangle$ of the superblock is determined by a sparse-matrix diagonalization algorithm.

Next, a basis for an augmented block, consisting of the system block and a specified choice of the extra sites, is formed from tensor products of system block and site states. The augmented block becomes the system block in the next iteration. However, in order to keep the size of the superblock basis from growing, the basis for the augmented block is truncated. We form a density matrix by projecting $|\psi\rangle\langle\psi|$ onto the augmented block which we diagonalize with a dense-matrix routine. We retain the *most probable* eigenstates (those with the largest eigenvalues) of the density matrix in order to form a truncated basis for the augmented block that is around the same size as the system block basis. Matrix elements for the Hamiltonian and active site operators are then updated.

The environment block used for the next iteration is usually chosen to be a reflected version of the system block. The initial system and environment blocks are each chosen to consist of a small number of sites, usually one or two. The accuracy and computer requirements of the scheme are fixed by n_s, the number of states retained per block (of good quantum numbers) at each iteration. n_s determines the truncation error, which is the sum of the eigenvalues of the density matrix corresponding to states which are shed in the truncation process. The error in quantities such as the ground-state energy scale linearly with the truncation error [1].

Now, at each iteration we generate coupling constant transformations T as follows. After forming the system block of size L we construct a lattice $\mathcal{L}$ of size $2L$ consisting of two system blocks. A (small) subset B of the system block truncated basis states is identified with a complete basis for a renormalized block of spins of size L' where $L' = L/b$ and b is the renormalization factor. $B \otimes B$ is then clearly identifiable with a complete basis for a lattice $\mathcal{L}'$ of size $2L'$. Next, the matrix elements of $\mathcal{H}$, the Hamiltonian for $\mathcal{L}$, with respect to $B \otimes B$ (which are readily formed from the matrix elements of the block Hamiltonian and active site operator(s)) are identified with those of a renormalized Hamiltonian $\mathcal{H}'$ defined on $\mathcal{L}'$. T is then defined by

$$\gamma' = T(b|\gamma) \tag{2}$$

where γ and γ' are set(s) of coupling constant(s) which define the Hamiltonians $\mathcal{H}$ and $\mathcal{H}'$ respectively.

To complete the prescription we must have a suitable method for choosing the set B—its size and make-up—and hence the renormalization factor b, together with the type of renormalized block that it is identified as a basis for. We must then check that our identification is valid in that the Hamiltonian matrix element identification can in fact be made such that $\mathcal{H}'$ and $\mathcal{H}$, in a loose sense, have the same symmetries. Ideally, we would like $\mathcal{H}'$ and $\mathcal{H}$ to be of the same form. The resulting system of linear equations for the renormalized couplings γ' is typically overdetermined. This implies a consistency check of the identification.

As to the choice of B, just as the density matrix eigenvalues determine which states are to be retained in forming a new system block, so too can we use the spectrum of the density matrix in order to guide our choice as to the make-up of B. That is, we choose B from states that make up the bulk of the weight of the density matrix whose eigenvalues sum to unity.

Choice of the basis B. We commence with the simple example of an $S = 1/2$ model with $\gamma = 1$ (the isotropic case). We use a periodic superblock of the form ...–site–system–site–environment–... and augment the system block with both sites. The strongest density matrix eigenvalues are listed in table 1 for the case of $n_s = 20$. The initial system block is a single site so the blocks always have an odd number of sites. The strongest density matrix eigenvalues lie in the sector of the Hilbert space where the good quantum number

$S^z_{\mathrm{T}} \equiv \sum_i S^z_i$ has small magnitude. We see that there is a pair of strong eigenvalues in the $S^z_{\mathrm{T}} = \pm\frac{1}{2}$ sectors which make up the bulk of the weight of the density matrix.

Table 1. The strongest density matrix eigenvalues for the isotropic $S = 1/2$ model using $n_s = 20$ for various odd block sizes b using periodic boundary conditions and augmenting by two sites per iteration.

b	S^z_{T}	Strongest eigenvalues
3	$\pm 3/2$	0.0000, ...
3	$\pm 1/2$	0.5000, 0.0000, 0.0000, ...
5	$\pm 3/2$	0.0055, ...
5	$\pm 1/2$	0.4619, 0.0271, 0.0055, ...
9	$\pm 3/2$	0.0120, ...
9	$\pm 1/2$	0.4251, 0.0484, 0.0120, ...
21	$\pm 3/2$	0.0237, ...
21	$\pm 1/2$	0.3786, 0.0682, 0.0237, ...

An obvious choice for B then is the states corresponding to these eigenvalues. We identify them with the up and down z-spin states of a renormalized spin-1/2 operator. That is, the system block is renormalized to a single site—$b = L$. As we shall see, the advantage of such a choice of B is that $\mathcal{H}'$ is of the same form as $\mathcal{H}$.

Table 2. The strongest density matrix eigenvalues for the isotropic $S = 1$ model using $n_s = 20$ for various odd block sizes b using periodic boundary conditions and augmenting by two sites per iteration.

b	S^z_{T}	Strongest eigenvalues
4	± 1	0.027 52, 0.000 00, ...
4	0	0.917 46, 0.027 52, 0.000 00, ...
6	± 1	0.039 17, 0.000 03, ...
6	0	0.882 37, 0.039 17, 0.000 03, ...
10	± 1	0.052 04, 0.000 22, ...
10	0	0.843 10, 0.052 04, 0.000 22, ...
22	± 1	0.069 38, 0.001 04, ...
22	0	0.788 08, 0.069 38, 0.001 04, ...

Next, in table 2 we list the strongest density matrix eigenvalues for the case of an open-ended superblock of the form system–site–site–environment. We again augment the system with both sites. The initial system block is a pair of sites so the blocks are always even. We see that the simplest possible identification involves the four strongest eigenvalues—a pair in the $S^z_{\mathrm{T}} = \pm 1$ sectors and a pair in the $S^z_{\mathrm{T}} = 0$ sector. It is natural to form B from the four states corresponding to these eigenvalues and to identify B as a basis for a block of two spin-1/2 sites, i.e., $b = L/2$. Following [10] we identify the elements of B with singlet and triplet states. That is, we identify the $S^z_{\mathrm{T}} = \pm 1$ states with $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ and the strong- and weak-eigenvalue (low- and high-energy) $S^z_{\mathrm{T}} = 0$ states with $(1/\sqrt{2})(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ and $(1/\sqrt{2})(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ respectively. It is found that with this identification $\mathcal{H}'$ has the same form as $\mathcal{H}$.

Finally, in table 3 we list the strongest density matrix eigenvalues for a spin-1 model using odd-sized blocks, periodic boundary conditions, and augmenting by two sites at a time.

Table 3. The strongest density matrix eigenvalues for the isotropic $S = 1/2$ model using $n_S = 20$ for various even block sizes b using open boundary conditions and augmenting by two sites per iteration.

b	S^z_T	Strongest eigenvalues
3	± 2	0.000 00, ...
3	± 1	0.333 33, 0.000 00, ...
3	0	0.333 33, 0.000 00, 0.000 00, ...
5	± 2	0.005 20, ...
5	± 1	0.294 95, 0.005 20, ...
5	0	0.294 95, 0.071 81, 0.005 20, ...
9	± 2	0.005 79, ...
9	± 1	0.262 30, 0.005 79, ...
9	0	0.262 30, 0.154 10, 0.005 79, ...
21	± 2	0.003 88, ...
21	± 1	0.237 86, 0.003 89, ...
21	0	0.237 86, 0.226 96, 0.003 89, ...

We see that, for small L, the bulk of the density matrix is made up from the three strongest eigenvalues which lie in the $S^z_T = 0$ and $S^z_T = \pm 1$ sectors. When the corresponding states are (naturally) identified with the $|0\rangle$ and $|\pm 1\rangle$ states of a spin-1 operator, the resulting $\mathcal{H}'$ has the same form as $\mathcal{H}$. However, as L is increased, the second-largest eigenvalue in the $S^z_T = 0$ sector rapidly becomes comparable to those of the other retained states and the identification of the renormalized block with a spin-1 site becomes inconsistent. It becomes necessary to incorporate the corresponding state into B which, as in the previous example, is identified as a basis for a block of two spin-1/2 sites.

The renormalized $S = 1/2$ Hamiltonian $\mathcal{H}'$ is not however of the form (1), in that there are second- and third-neighbour interactions present with dimerization. This is consistent with White's analytic mappings between the spin-1 chain and coupled spin-1/2 chains [12]. That is, it becomes natural to identify the renormalized block with a single segment of coupled chains.

2.1. Discussion—systematic improvability of transformations

Now that we have described the procedure for generating coupling constant transformations, we discuss the question of its accuracy and systematic improvability. These issues are central to the success of the DMRG method in calculating energies and correlation functions. We consider how the algorithm should be scaled in order to obtain the most accurate results.

Now, suppose we choose B in the same way at each iteration, e.g., for a spin-1/2 system with odd blocks we always form B from two states—the most probable states in the $S^z_T = \pm\frac{1}{2}$ sectors. We have the guiding principle that, as long as we respect the basic symmetries of the Hamiltonian, then for a fixed basis size $|B|$, the accuracy of the transformations should increase with each iteration, with calculated quantities converging to their exact values as the block size is increased.

This principle stems from the fact that the ratio of intrablock to interblock components of the Hamiltonian decreases as the block size is increased and the exact ground state can asymptotically be written as a suitably symmetrized product of the B-states. The principle in fact appears to be borne out in the case of the spin-1/2 transverse Ising (ITF) model where slow but systematic convergence of critical exponents with block size is achieved

within a RSRG scheme whereby blocks of sizes 3, 5, 7, 9 and 11 are diagonalized and the basis B is formed from the states of lowest energy [11].

This principle as applied to estimates of critical exponents is however non-rigorous in general and within the DMRG scheme there is likely to be a limit to accuracy of infinite-lattice results imposed by the finiteness of n_s. That is, the finiteness of n_s imposes restrictions on how accurately we can determine important states of large blocks. In practice it may therefore be profitable to enlarge B and hence L'. This may have the undesirable side effect of leading to $\mathcal{H}'$ lying in an enlarged space with more interactions.

Finally, we describe how the approach considered here differs from that used in [8]. In [8], relatively small superblocks (of up to 12 sites) are diagonalized exactly, reduced density matrices are then constructed for small system blocks (of either 3 or 4 sites) and the basis B is formed from retaining the 2 (4) most probable states for 3- (4-) site system blocks. This is the direct DMRG analogue of the RSRG calculations [9]. In the approach considered here we again use only a handful of states to generate the RG transformation but many states are retained at each iteration for the purpose of constructing successive system blocks. That way we attempt to work with accurately determined *important* states of large blocks. Also, the density matrix eigenvalues are used in order to obtain a natural selection of the basis B.

3. Application to the spin-1/2 chain with anisotropy

We now apply our method to the $S = 1/2$ case of the Hamiltonian given in equation (1). This model is integrable and many properties have been calculated exactly [13]. We only consider $\gamma \geqslant 0$ here. In this regime the model has two trivial, stable fixed points. At $\gamma = 0$ (the Ising fixed point) the ground states are the classical Néel states and there is a finite energy gap and long-range antiferromagnetic order. At $\gamma = \infty$ (the XY fixed point) the model is equivalent to a spinless fermion gas [14], the spectrum is a gapless continuum and there is no long-range order. There is a phase transition at $\gamma = \gamma_c = 1$ (the isotropic, Heisenberg point). This critical point separates the gapless phase from the gapped, ordered doublet phase.

The phase transition is pathological in that the critical exponents are either zero or infinite. For example, the thermal exponent ν, describing the divergence of the correlation length ξ, is usually defined by

$$\xi \sim |\gamma - \gamma_c|^{-\nu} \qquad \text{as } \gamma \to \gamma_c. \tag{3}$$

However, for the $S = 1/2$ model we have the exact result [9]

$$\xi \sim e^{-A|\gamma - 1|^{-1/2}} \tag{4}$$

whence $\nu = \infty$.

As mentioned, the RSRG method has been applied to the $S = 1/2$ model [9]. Blocks of size $L = 3$, 5, and 7 were used and the basis B was comprised of the two low-energy states (in the $S^z_T = \pm 1/2$ sectors) and was identified with the up and down states of a spin-1/2 site. The estimates of ν so obtained were spurious in that $\nu \downarrow 2$ as $L \to \infty$.

Here we calculate ν from RG transformations derived within the DMRG scheme described above. We use the periodic superblock, augmenting by two sites per iteration with a single site as an initial system block (hence L is always odd). We choose $|B| = 2$ ($L' = 1$, $b = L$), identifying the most probable states in the $S^z_T = \pm 1/2$ sectors, which we denote by $|\uparrow\rangle$ and $|\downarrow\rangle$, with the up and down states of a single spin-1/2 site. The

renormalized Hamiltonian then has matrix elements

$$\langle\sigma'\rho'|\mathcal{H}'|\sigma\rho\rangle \equiv \langle\langle\rho'| \otimes \langle\langle\sigma'|\mathcal{H}|\sigma\rangle\rangle \otimes |\rho\rangle\rangle. \tag{5}$$

$\mathcal{H}'$ has sixteen matrix elements; i.e., $B \otimes B$ has four elements. However, the DMRG algorithm preserves certain symmetries of the Hamiltonian at every iteration. From conservation of total z-spin we have

$$\langle\sigma'\rho'|\mathcal{H}'|\sigma\rho\rangle = 0 \qquad \text{if } \sigma' + \rho' \neq \sigma + \rho. \tag{6}$$

From spin-flip symmetries we also have the following obvious relations:

$$\langle\uparrow\uparrow|\mathcal{H}'|\uparrow\uparrow\rangle = \langle\downarrow\downarrow|\mathcal{H}'|\downarrow\downarrow\rangle \tag{7}$$

$$\langle\uparrow\downarrow|\mathcal{H}'|\uparrow\downarrow\rangle = \langle\downarrow\uparrow|\mathcal{H}'|\downarrow\uparrow\rangle \tag{8}$$

$$\langle\uparrow\downarrow|\mathcal{H}'|\downarrow\uparrow\rangle = \langle\downarrow\uparrow|\mathcal{H}'|\uparrow\downarrow\rangle. \tag{9}$$

These symmetries reduce the number of independent matrix elements to three, namely: $\langle\uparrow\uparrow|\mathcal{H}'|\uparrow\uparrow\rangle$, $\langle\downarrow\uparrow|\mathcal{H}'|\downarrow\uparrow\rangle$ and $\langle\uparrow\downarrow|\mathcal{H}'|\downarrow\uparrow\rangle$.

The identification of $\mathcal{H}'$ is simple. We can write $\mathcal{H}'$ in the same form as $\mathcal{H}$ (up to a scale factor J' an additive constant C'):

$$\mathcal{H}' = J'\left[S_1^z S_2^z + \gamma'\left(S_1^x S_2^x + S_1^y S_2^y\right)\right] + C'I \tag{10}$$

where I denotes the identity operator and J', C' and γ' are uniquely determined from the three independent matrix elements. As mentioned, in general the identification is overdetermined.

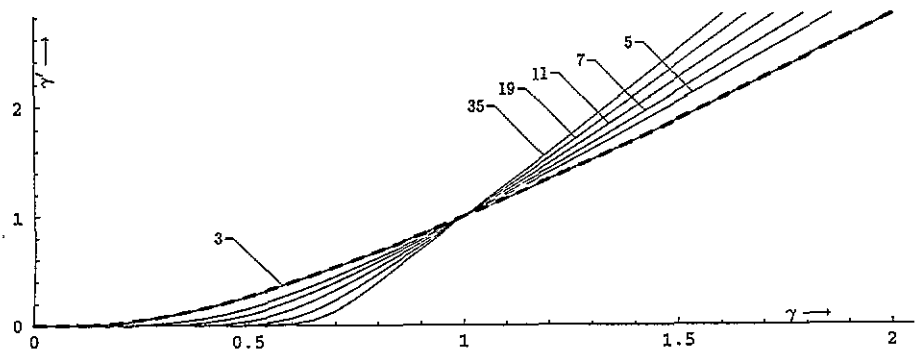

Figure 1. The renormalization group transformation $\gamma' = T(b|\gamma)$ for the anisotropic spin-1/2 chain from the DMRG method with $n_s = 50$ for various block sizes b. The thick dashed curve is the RSRG result for $b = 3$.

It is found that the renormalization group transformation $\gamma' = T(b|\gamma)$ converges quite rapidly and uniformly with n_s. We plot the transformation for various block sizes b (or L) in figure 1 in the case where $n_s = 50$. We also include a plot of the RSRG result [9] for $b = 3$, namely

$$T(3|\gamma) = \frac{16\gamma^3}{1 + \sqrt{1 + 8\gamma^2}}. \tag{11}$$

We see that the RSRG and DMRG results are almost identical for $b = 3$. We shall see, however, that a marked difference emerges for larger b.

We see that the transformation has trivial fixed points at $\gamma = 0$ and $\gamma = \infty$ and the critical point $\gamma = \gamma_c = 1$ is recovered as an unstable fixed point. This is to be expected, again from symmetry considerations—that is, $\mathcal{H}$ only has full rotational symmetry at $\gamma = \gamma_c$.

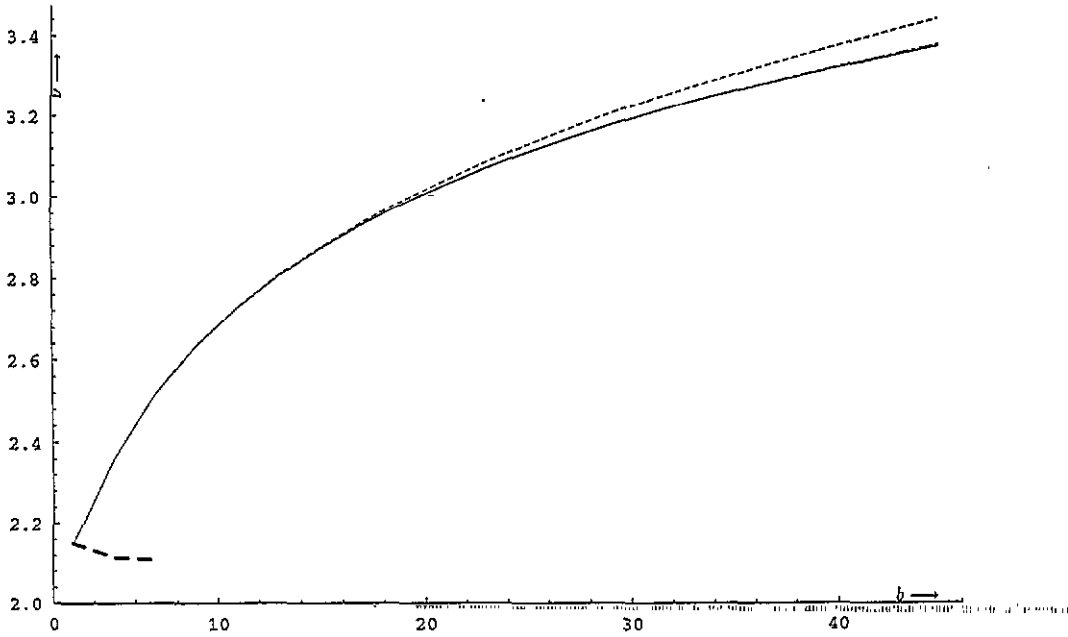

Figure 2. DMRG estimates of the critical exponent ν as a function of block size b for $n_S = 20$ (dashed line), $n_S = 35$ (dot-dashed line) and $n_S = 50$ (solid line). The thick dashed curve is the RSRG result.

Note that the same argument applies in the spin-1 case. As mentioned, however, it was found that the self-mapping for the $S = 1$ case rapidly became inconsistent as b was increased. This is consistent with exact diagonalization results [15] where it is found that the $S = 1$ model is not critical at $\gamma = 1$ but rather at $\gamma = 1.167(7)$.

Results for the thermal exponent ν. Following [9] we use the following standard relation in order to obtain the thermal exponent:

$$\nu = \frac{\log b}{\log T'(b|\gamma_c)}. \tag{12}$$

We plot the estimates of the exponent as a function of block size b in figure 2 for various values of n_s. We also include the RSRG results from [9]. We see that the DMRG results are qualitatively more consistent with the exact result $\nu = \infty$ in that the DMRG result increases with b whereas the RSRG result monotonically decreases with b. Further, the DMRG result may increase without bound as $b \to \infty$. We plot e^{ν} versus b for the $n_s = 50$ case in figure 3. This function appears to be linear for large b, consistent with ν diverging logarithmically with b.

4. Discussion

In this paper we have presented a scheme for using the DMRG algorithm to generate RG transformations in the space of coupling constants. The scheme allows us to study critical phenomena directly using the DMRG method. The scheme makes use of the fact that the *important* states of large blocks are accurately calculated within the DMRG algorithm. Also, a natural solution to the perennial problem of the choice of renormalized block and

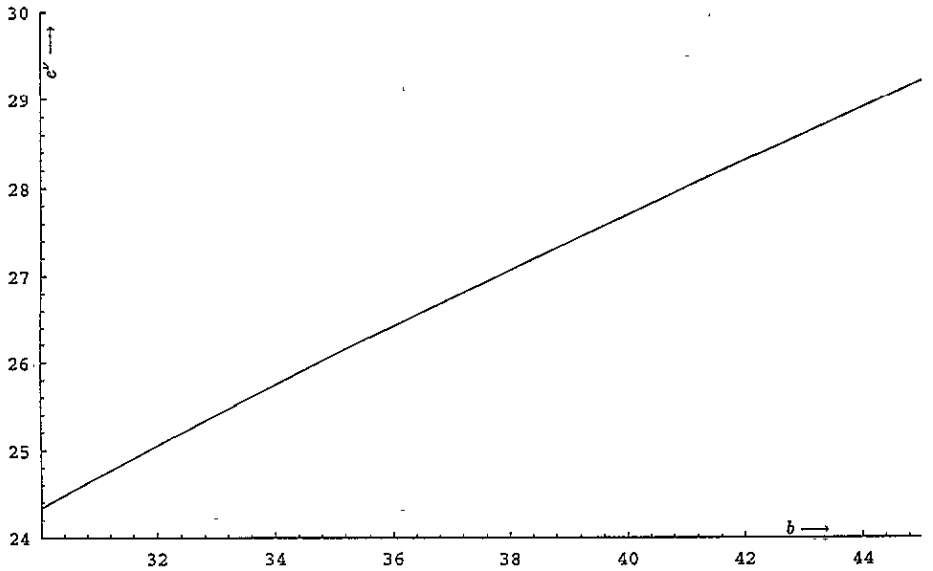

Figure 3. e^{ν} versus b for the $n_S = 50$ case.

the identification of the renormalized Hamiltonian is proposed in terms of the density matrix spectrum. This allows us to distinguish the different universality classes of the isotropic point in the anisotropic spin-S Heisenberg model. For $S = 1/2$, the RG transformation is a self-map with the isotropic point as a critical point. For $S = 1$ the model maps onto an $S = 1/2$ model with dimerization and longer-ranged interactions that can be identified with a coupled $S = 1/2$ chain.

We have applied the method to the pathological phase transition in the $S = 1/2$ model. Results for the thermal exponent ν are qualitatively better than the comparable RSRG results. That is, the exact result is $\nu = \infty$. The RSRG method yields $\nu \downarrow 2$ as $b \rightarrow \infty$ (where b is the block size) whereas the DMRG method has ν increasing with b, seemingly without bound.

We believe that the scheme described here may be useful in studying critical phenomena in quasi-one-dimensional systems with many states per unit cell, such as coupled spin or fermion chains, extended Hubbard-type models with a charge transfer gap and spin or fermion models with dimerization and frustration.

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