A density matrix renormalization group approach to interacting quantum systems on Cayley trees

1997 J. Phys.: Condens. Matter 9 9021

(http://iopscience.iop.org/0953-8984/9/42/016)

J. Phys.: Condens. Matter **9** (1997) 9021–9029. Printed in the UK PII: S0953-8984(97)83259-6

A density matrix renormalization group approach to interacting quantum systems on Cayley trees

Barry Friedman

Department of Physics, Sam Houston State University, Huntsville, TX 77341, USA† and Department of Physics and Texas Center for Superconductivity, University of Houston, Houston, TX 77204-5504, USA

Received 8 April 1997

Abstract. I have examined the nearest-neighbour quantum Heisenberg model on a Cayley tree using a simple density matrix renormalization group scheme. For spin 1/2 on a three-legged Bethe lattice I find indications of long-range antiferromagnetic order in agreement with the spin wave result. Preliminary calculations using a more complicated density matrix renormalization group scheme give promise that one can treat interacting quantum systems on Cayley trees very accurately.

1. Introduction

In this paper I will present a scheme to apply the density matrix renormalization group (DMRG) [1] to the Bethe lattice. In particular, we will study the quantum mechanical nearest-neighbour Heisenberg models on a sequence of growing Cayley trees using the DMRG. By applying this technique, I will address whether there is long-range antiferromagnetic order for the Bethe lattice with three legs.

During the last few years, the DMRG has enjoyed remarkable success in computing properties of the low-energy states of one-dimensional quantum mechanical many-body systems. Is it possible to generalize the DMRG in a straightforward way to higher-dimensional systems? Apparently, this is not possible for hypercubic lattices [2], however some success has been obtained in considering the properties of ladders [3, 4]. Another possible generalization away from one dimension is the Cayley trees (other fractal objects are possibilities as well, see [5]). This is natural since the one-dimensional lattice can be viewed as a Bethe lattice with two legs. Ultimately, I would like to consider the t–J and Hubbard models on Bethe lattices as examples of strongly correlated electron systems. The use of the Bethe lattice to study correlated electron systems dates back to the pioneering work of Brinkman and Rice [6]. Here, however, I restrict my considerations to the Heisenberg model, a simpler many-body system and the strong-coupling limit of the Hubbard model at half filling. At least on the surface it seems that if one cannot treat the Heisenberg model one cannot hope to deal with more complicated situations like doped Hubbard models.

Cayley trees are also interesting from another standpoint, that is, it has recently become possible to synthesize very large molecules [7, 8], referred to as dendrimers, that have the structure of Cayley trees. Although I am not aware of any studies of the electronic properties of dendrimers, it is not unreasonable that there should be some materials of this

† Present and permanent address.

0953-8984/97/429021+09$19.50

type that can be described by Hubbard type models. For, example, Hubbard models are successfully used to describe pi electron systems [9] and it is not necessary to consider extremely large systems to see interesting physics. As a cautionary note, observe that to due to 'congestion' at the boundary one cannot hope to 'grow' dendrimers to arbitrary size [10]. The limiting size is a function of the local chemistry of the cluster; in favourable cases dendrimers of generation 9 (using the notation of [8]) have been experimentally realized [8]. A dendrimer of generation 4 already has 94 'sites' and an interacting model on this relatively small dendrimer has a huge state space. It therefore seems dendrimers are a possible experimental realization of a strongly correlated system.

2. The model and a simple DMRG scheme

The model I consider is the spin $1/2$ nearest-neighbour Heisenberg model, that is

$$H = J \sum_{\langle i,j \rangle} S_i \cdot S_j$$

where S_i are spin $1/2$ operators, $\langle i, j \rangle$ refers to nearest-neighbours and $J > 0$ (I use units where $J = 1$). This Heisenberg model is defined on a Cayley tree. See figure 1 for a picture of a ten-site Cayley tree with three legs. Note there are two generations of points starting from the central point. Following [11] we call such finite objects Cayley trees and the large-system limit of Cayley trees will be referred to as the Bethe lattice. The points joined by only one bond are called boundary points. It is simple to see that as the number of generations goes to infinity the ratio boundary points/total points approaches a non-zero constant for any number of legs not equal to two. Consequently care must be used in deciding what is the proper observable to consider in the large-cluster limit.

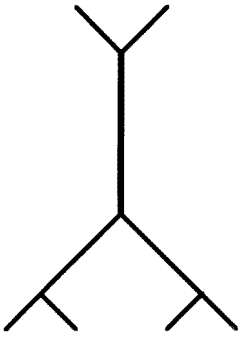

Figure 1. A ten-site Cayley tree. There are two generations and six boundary points.

I want to calculate the ground state of the Heisenberg model on the Cayley tree. The problem here is that the size of the state space grows exponentially with the size of the cluster as is the typical case in interacting quantum systems. To apply direct diagonalization to large clusters we therefore need some basis reduction scheme. I have used the density matrix renormalization group to implement this basis reduction. In particular, I have used a variant of Steve White's infinite-system algorithm [1]. To understand what I have done refer to figure 2. I start with the one generation 4 site cluster. The two circled sites are the system and the other sites are the environment. I calculate the density matrix for the block, diagonalize it and choose the eigenvectors corresponding to the largest eigenvalues.

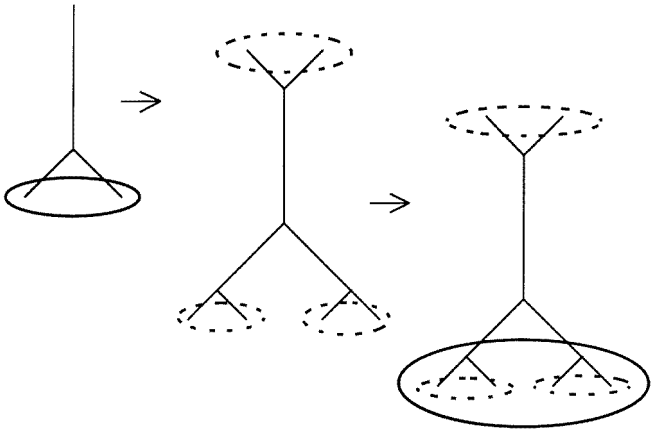

Figure 2. Simple DMRG scheme.

We now turn to the second generation 10 site cluster. The basis we use for the state space of this cluster is the direct product of the full state space of the sites not circled by dashed lines with the reduced state space (using the largest eigenvectors from the previous generation) of the circled sites. I next compute the density matrix for the ten-site cluster taking the six circled sites (solid 'circle') as the system and the four uncircled (by a solid circle, two sites are circled by a dashed circle) sites as the environment. I use the largest eigenvectors as a basis for the next cluster and then iterate the process as we move toward larger clusters.

Continuing in this way I never need diagonalize matrices of size larger than 16 n_b^3 where n_b is the dimension of the state space of the dashed circled block. These largest diagonalizations occur in computing the ground state of the cluster, which I assume has $S_z = 0$ (in an exact calculation this follows by spin rotation invariance) and thus the state space is in fact smaller than 16 n_b^3. The ground state is readily calculated using the Davidson algorithm [12]. As a practical matter I start the iterative process with the ten-site cluster which one can easily diagonalize. In computing the density matrix of the six-site block we target as many low-energy states as necessary to ensure non-zero eigenvalues of the density matrix. The problem here is that the environment in the ten-site case consists of four-sites, i.e. a state space of dimension 16. Since our largest calculations involve $\sim$30 states in a block and the number of non-zero eigenvalues is less than the dimension of the environment we need to target a few states in addition to the ground state. For the following iterations this is unnecessary since the state space of the environment is equal to 4 n_b.

Without checking anything, one might be quite suspicious since, in comparison with the one-dimensional case, in my DMRG scheme the number of sites in a block increases dramatically with each iteration. One could increase the number of sites in a block one at a time, the virtue of the present approach is that it is relatively simple to implement. Without further apology let us check the accuracy of this procedure. To do this, I have directly diagonalized the ground state of the 22-site (three-generation) cluster. This involves finding the ground state of a matrix of dimension $\sim$700 000 which is relatively simple to do with the Davidson algorithm. For the ground state energy per site I obtain $-0.380\,387\,19$. Note that the next-generation cluster of 46 sites has a state space of dimension $\sim 8 \times 10^{12}$. This is at present inaccessible to brute force diagonalization. In using the DMRG scheme in going from the ten-site to 22-site cluster I find for $n_b = 14$, 22, 29 an energy per site of

$-0.380\,272$, $-0.380\,280$, $-0.380\,385$, respectively (targeting the ground state with weight 0.9998 and the second and third (degenerate) excited states with weights 0.0001). We see we do not have exponential convergence with the number of states in the block. However, by choosing the dimension of the state space of the blocks large enough we get a decent approximation for the ground state energy per site. An optimistic view of the present DMRG scheme is that I can at least get qualitative information regarding the ground state.

3. Is there long-range antiferromagnetic order?

I now use the previously described DMRG to investigate whether there is long-range antiferromagnetic order in the ground state. Note that the Néel state is unfrustrated on a Cayley tree, so if long-range order does not exist, in some sense quantum fluctuations must suppress the order. I generate clusters up to the ninth generation (1534 sites) and calculate the correlation function $\langle S_0 \cdot S_m \rangle$ for each of these clusters. Here 0 denotes the middle of the cluster and m is a site m bonds away from the middle. It is very important here to consider the rotationally invariant quantity $\langle S_0 \cdot S_m \rangle$ rather than say $\langle S_0^z S_m^z \rangle$. This is due to the Lieb–Mattis theorem [13] which states that the total spin of an antiferromagnetic Heisenberg model on a cluster with N_a sites on the A sublattice and N_b sites on the B sublattice is $|N_a - N_b|/2$. As a consequence, the Cayley trees I consider have non-zero total spin, i.e. $S = 2$ for the ten-site cluster, $S = 4$ for the 22-site cluster, 2^{n-1} for the nth-generation cluster. Since the ground state is degenerate with respect to the z component of the total spin $\langle S_0 \cdot S_m \rangle \neq 3\langle S_0^z S_m^z \rangle$.

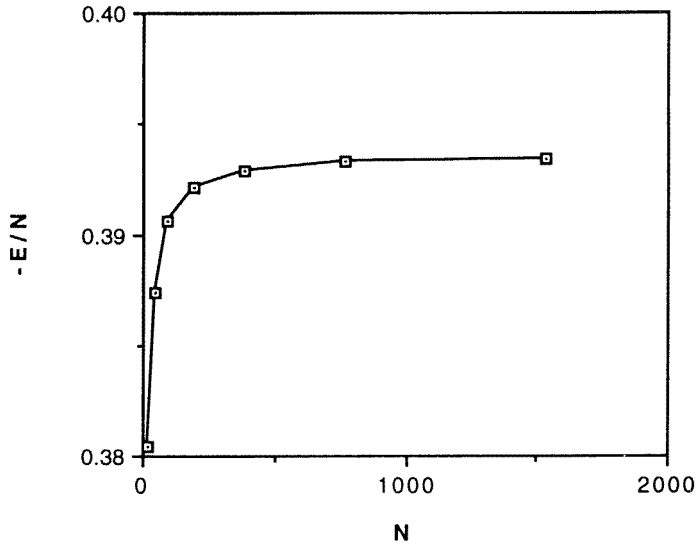

Figure 3. Energy per site against the number of sites.

In figure 3, I plot the ground state energy per site versus the number of sites for $n_b = 29$. The corresponding energies are given in table 1. These calculations involve finding the ground state of matrices of dimension $\sim$50 000. At least by the ninth generation we get a fair level of convergence with respect to system size. The energies in the table are upper bounds to the true energies due to the variational character of the DMRG. Let us now examine the spin–spin correlation function. Firstly, there is short-range antiferromagnetic

Table 1. Energy per site against number of sites in the cluster. The first row is the number of sites and the second row is the energy per site.

No of Sites	22	46	94	190	382	766	1534
E/N	−0.380 385 4	−0.387 39	−0.390 59	−0.392 12	−0.392 88	−0.393 25	−0.393 44

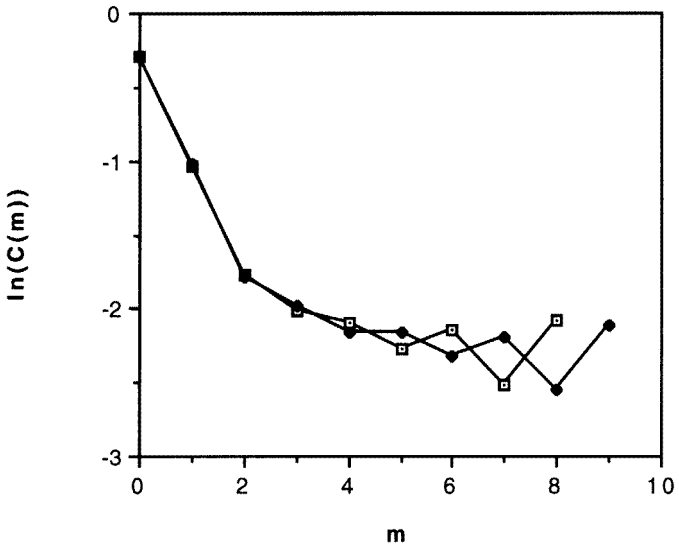

Figure 4. Spin–spin correlation function against the number of bonds between the sites. I have kept 29 states in each block and $C(m) = (-1)^m \langle S_0 \cdot S_m \rangle$. The points for the eighth-generation cluster are plotted as squares, while the points for the ninth-generation cluster are plotted as diamonds.

order in the sense that the signs of $\langle S_0 \cdot S_m \rangle$ change depending on what sublattice m is on in agreement with the Lieb–Mattis theorem. In figure 4 I have plotted the natural logarithm of $(-1)^m \langle S_0 \cdot S_m \rangle$ versus m for the eighth- and ninth-generation clusters. For an ordinary lattice, decay would, of course, mean no long-range order; unfortunately for a Bethe lattice one cannot conclude this due to the proliferation of boundary points. For example, for the valence bond solid (VBS) state on Bethe lattices the correlation function I have calculated decays exponentially but there is long-range order when there are more than four legs [14].

One way to define long-range order is to consider the expectation value of the central spin in the double limit of first system size going to infinity and then applied magnetic field going to zero (for more discussion see [15]). An alternative approach, which is natural for VBS states, is to fix the spins on the boundary and examine the expectation value of the central spin. Unfortunately, either of these definitions is difficult to implement in a numerical approach. I instead will investigate long-range order by studying the rate of exponential decay. If the correlation function decays sufficiently fast it is quite plausible that there is no long-range order. At first glance such an assertion seems absurd since for the VBS states of [14] $\langle S_0 \cdot S_m \rangle$ always decays as 3^{-m} whatever the number of legs. As pointed out in [14], the proper quantity to consider is not the spin correlation function itself, rather one should look at the product of the spin correlation function with the total number of spins on the boundary. If this quantity decreases with system size there is no long-range

order, while if it increases long-range order is present. In the VBS case the quantity to consider is then $3^{-m}(Z-1)^m$ which decays for $Z=3$ and increases with m for $Z \geqslant 5$. It also easy to check this criterion for the ferromagnetic Ising model: in this case $\langle S_0 \cdot S_m \rangle$ decays as $(\tanh K)^m$ where $K = J/kT$ [16] so the criterion is that $(\tanh K)^m(Z-1)^m$ either decays or grows with m. The boundary between order and disorder is $\tanh K(Z-1)=1$, the well known expression for the critical temperature of the Ising model on the Bethe lattice. The criterion therefore makes sense in an extreme quantum limit (VBS states) and for classical models, which suggests this criterion is of general applicability.

We then must read off the rate of decay from figure 4. To have long-range order the correlation function must decay slower than $e^{-\alpha m}$ where $\alpha < \ln 2 \approx 0.69$. The correlation function in figure 4 has a somewhat complicated behaviour, there is an initial rapid exponential decay, an 'intermediate' oscillatory exponential decay and an increase in the correlation function for the last point at the boundary. The quantity relevant to long-range order is the 'intermediate' exponential decay. This decay is significantly less than 0.69 and therefore the simple DMRG scheme indicates long-range order. One could question whether the decay is really exponential. However, the point is that if one assumes exponential decay, which is a reasonable assumption for the Bethe lattice, that decay is much slower than 0.69.

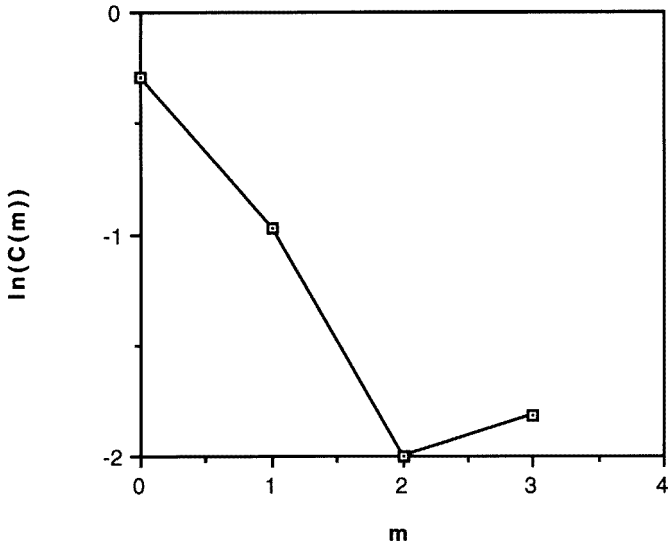

Figure 5. Spin–spin correlation function against the number of bonds between the sites for the 22-site cluster. The figure is the result of a exact diagonalization calculation and $C(m) = (-1)^m \langle S_0 \cdot S_m \rangle$.

I have checked my calculation by computing the spin–spin correlation function using exact diagonalization for the 22-site cluster. On the scale of figure 5, the results of the DMRG (for the 22-site cluster) are indistinguishable from the exact diagonalization results. There is an upturn at the boundary in the numerically exact calculation: it therefore seems the upturn in the DMRG calculation is not a total numerical artifact. It is also important to note that the 22-site cluster is too small to infer the long-distance decay: one only sees the initial decay of correlation.

Recently, Otsuka [17] has applied a similar DMRG approach to the Bethe lattice. In his scheme, one considers clusters of size 6, 14, 30, 62, 126, ... and these clusters have the nice feature that the ground state, by the Lieb–Mattis theorem, has spin 0. As a consequence, spin rotation invariance is respected by the calculation if all eigenstates of the density matrix with the same eigenvalue are kept. Otsuka points out that this means that the number of states that needs to be included grows exponentially with the size of the cluster. Consider the 14-site cluster where one calculates the density matrix for the seven-site block. By the Lieb–Mattis theorem one anticipates that the lowest eigenstates have spin $3/2$, i.e. the eigenstates are four-fold degenerate and this is borne out by explicit calculation. For the 126-site cluster the lowest eigenstates of the density matrix are 22-fold degenerate and calculations begin to become unwieldy. As a check on my calculation, I have computed the spin–spin correlation function for the 126-site cluster using Otsuka's method and all block eigenstates with weight $>10^{-4}$ are kept in the calculation. The results are plotted in figure 6 where I have plotted the 126-site cluster calculation results as open squares and the 94-site cluster results (using my scheme) as solid squares. We see a good agreement between the two calculations. This is fortunate, since for doped Hubbard or t–J models we do not have the Lieb–Mattis theorem to guide us in the choice of cluster shapes.

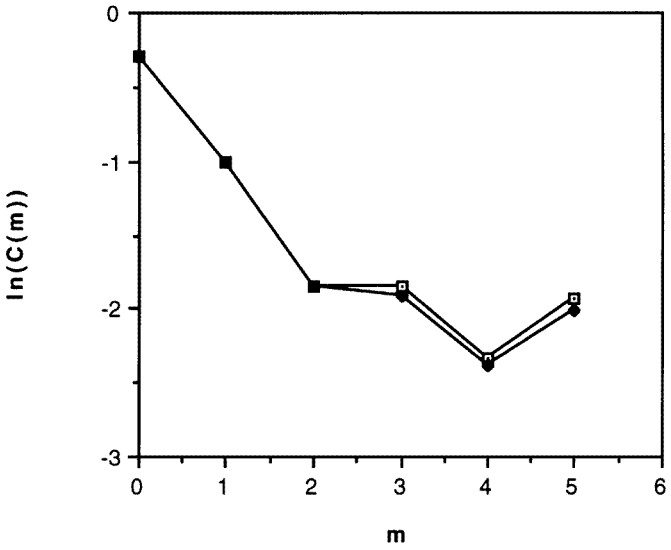

Figure 6. Spin–spin correlation function against the number of bonds between the sites. The solid (open) squares are for the 94- (126-) site cluster.

There are a number of rigorous results in regard to the Heisenberg model on hypercubic lattices (see for example [18] and [19]). The rigorous results do not, to my knowledge, cover the spin $1/2Z = 3$ Bethe lattice. I have therefore done a simple spin wave calculation to check for long-range order. I closely follow the formulation and notation of [20]. Firstly, replace the spin operator S_r by boson creation and annihilation operators, a_r, a_r^+, b_r, b_r^+ where a are operators on the A sublattice and b are operators on the B sublattice (for the definition of a_r and b_r in terms of S_r see [20]). Linearizing one gets the following Hamiltonian

$$H = -S^2 J 3N/2 + 3JS \sum_r n_r + JS \sum_{\langle r,r' \rangle} a_r b_{r'} + a_r^+ b_{r'}^+.$$

Here S is the magnitude of the spin, J is the coupling constant and N is the number of sites. For hypercubic lattices the next step would be to introduce the Fourier transform to decouple the sites in the third term of H. This does not work for the Bethe lattice; observe however, that plane waves are eigenstates of a nearest-neighbour tight-binding model on a hypercubic lattice. A way to handle the Bethe lattice is to introduce a new basis consisting of eigenstates of a nearest-neighbour tight-binding model on the Bethe lattice. Doing this, one sees that H is equivalent to

$$H = C_1 \sum_n (a_n b_n + a_n^+ b_n^+)\varepsilon_n + C_2 \sum_n n_n$$

where $C_1 = JS$ and $C_2 = 3JS$ and ε_n is an eigenvalue of the tight-binding Hamiltonian. One can now proceed exactly as in the hypercubic case (introduce a Bogoliubov transformation [20]). I find that the staggered magnetization per site is given by $1/2 - \varepsilon$ where

$$\varepsilon = \frac{1}{N} \sum_n \frac{1}{\sqrt{1 - (\varepsilon_n / Z)^2}} - 1$$

Z is the number of nearest-neighbours and the sum is over positive eigenvalues of a tight-binding model on the Bethe lattice (this formula works for the hypercubic case as well when the ε_n are taken to be tight-binding eigenvalues of the hypercubic lattice). Using the density of states for the $Z = 3$ Bethe lattice [21] one finds $\varepsilon = 0.18$. This value is slightly lower than the value obtained ($\varepsilon = 0.20$) for a 2D square lattice [20] (recall in one dimension ε diverges, reflecting the lack of long-range order). Therefore the spin wave calculation predicts long-range order in agreement with the DMRG calculation.

4. A more complicated DMRG scheme

In this section I will investigate whether it is possible to devise a DMRG scheme that is more accurate than the calculations in section 2. We can see why my first scheme has trouble by looking again at figure 2. The problem is that the environment the system sees when computing the density matrix is quite different from the environment the block encounters for the next larger cluster. Concretely, the six-site system sees a four-site environment. This environment looks quite a bit different from the environment the six-site block encounters when it is imbedded in the 22-site cluster. One way around this difficulty is to use the full state space for one six-site block (64 states) in the 22-site cluster and use a small number of states to describe the two other six-site blocks. The states I use to describe the two other blocks are taken as the eigenfunctions with largest eigenvalues of the density matrix of the six-site block imbedded in the ten-site cluster. One can then treat the 64-state block in the 22-site cluster as the system and recompute the density matrix, finding new eigenfunctions to use as a basis for the environment blocks. One can repeat this process until it converges. At this point one takes the largest eigenfunctions for all the blocks and diagonalizes the Hamiltonian a final time.

I have used this procedure in going from the ten-site to 22-site cluster with 64 states for the system block and 12 states for the environment blocks. In the final stage I use 21 states in all the blocks since after these first 21 states the eigenvalues of the density matrix drop rapidly: the 21st eigenvalue is of order 10^{-7} while the 22nd is of order 10^{-12}. It turns out by comparison to the exact result ('exact' up to round-off errors, i.e. 10^{-13}–10^{-14}), the procedure is remarkably accurate. The exact result and the DMRG result for the energy per site of the 22-site cluster agree to 10^{-13}. In implementing the DMRG procedure we at most had to find the ground state of a matrix of order 2×10^4 where a brute force calculation

requires handling matrices of order 7×10^5. This scheme can be extended to larger clusters although it becomes somewhat awkward to handle a block of size $4\ n_b^2$ where n_b is of order 20.

5. Conclusions

I have studied the nearest-neighbour quantum spin $1/2$ Heisenberg model on a Cayley tree using the density matrix renormalization group. The scheme I use seems to be at least qualitatively accurate and is simple enough to generalize to more complicated models, i.e. the Hubbard or t–J model. For spin $1/2$ on a three-legged lattice I find long-range antiferromagnetic order in agreement with spin wave calculations. I have also done preliminary calculations using a more complicated DMRG scheme based on the idea that we can treat the environment in a fairly sloppy way if we treat the system very accurately. This more complicated scheme gives hope that one can use DMRG to do quantitatively accurate calculations of quantum interacting systems on Cayley trees.

Acknowledgments

I thank Dr Guozhong Wen for many helpful conversations. This work was partially supported by the Texas Center for Superconductivity at the University of Houston under Prime Grant No MDA 972-88-G-002 from the Defense Advanced Project Agency and the state of Texas and the Sam Houston State University research enhancement fund.

References

[1] White S R 1993 *Phys. Rev.* B **48** 10 345
[2] Liang S and Pang H 1994 *Phys. Rev.* B **49** 9214
[3] White S R, Noack R M and Scalapino D J 1994 *Phys. Rev. Lett.* **73** 886
[4] Dagotto E and Rice T M 1996 *Science* **271** 618
[5] Tomczak P 1996 *Phys. Rev.* B **53** R500
[6] Brinkman W F and Rice T M 1970 *Phys. Rev.* B **2** 1324
[7] Tomalia D A 1995 *Sci. Am.* May 62
[8] Tomalia D A, Naylor A M and Goddard W A III 1990 *Angew. Chem. Int. Edn Engl.* **29** 138
[9] Heeger A J, Kivelson S, Schrieffer J R and Su W P 1988 *Rev. Mod. Phys.* **60** 781
[10] DeGennes P G and Hervet H J 1983 *Phys. Lett. (Paris)* **44** 351
[11] Baxter R J 1982 *Exactly Solved Models in Statistical Mechanics* (London: Academic)
[12] Davidson E R 1993 *Comput. Phys.* **7** 519
[13] Lieb E H and Mattis D 1962 *J. Math. Phys.* **3** 749
[14] Affleck I, Kennedy T, Lieb E H and Tasaki H 1988 *Commun. Math. Phys.* **115** 477
[15] Thompson C J 1982 *J. Stat. Phys.* **27** 441
[16] Simon B 1993 *The Statistical Mechanics of Lattice Gases* (Princeton, NJ: Princeton University Press)
[17] Otsuka H 1996 *Phys. Rev.* B **53** 14 004
[18] Dyson F, Lieb E H and Simon B 1978 *J. Stat. Phys.* **18** 335
[19] Kennedy T, Lieb E H and Shastry B S 1988 *J. Stat. Phys.* **53** 1019
[20] Manousakis E 1991 *Rev. Mod. Phys.* **63** 1
[21] Economou E N 1983 *Green's Functions in Quantum Physics* 2nd edn (Heidelberg: Springer)