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Parity, precision and spin inversion within the density matrix renormalization group

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Abstract. A way of implementing the density matrix renormalization group (DMRG) method which simplifies the use of real-space parity as a conserved quantum number is discussed. The use of parity in the infinite-system DMRG calculations is often necessary in order to calculate more than the lowest excitation gap in a system. In addition, the use of parity reduces the computational overhead by a factor of two. Using parity as a symmetry we give numerical evidence that the infinite-system DMRG method in some cases displays a power-law convergence with the number of states retained. In particular we show that the often-used measure of the error in a DMRG calculation, $1 - P_m$, bears only a marginal resemblance to the true error. Spin inversion is shown to be a very useful symmetry when performing calculations in the $S^z_T = 0$ subspace, allowing for a distinction between even and odd multiplets even when using the finite-system method.

1. Introduction

The density matrix renormalization group [1] (DMRG) method allows one to perform calculations for one-dimensional systems with a precision that is unattainable with most other methods. The drawback is that one is forced to follow states by means of an iterative procedure as the system size is increased. It is hence often rather difficult to calculate more than the gap to the lowest-lying excitation, unless different excitations can be distinguished by differing quantum numbers. While it is straightforward to perform DMRG calculations within a subspace where the total particle number, N, or the total z-component of the spin, S^z_T, is conserved, more complicated quantum numbers are often rather difficult to implement [2, 3]. A particularly simple symmetry, that has been extensively used with the infinite-system DMRG method [4], is reflection with respect to the mid-point of the system with associated quantum numbers $+1$ and -1 for states that are parity even and parity odd respectively. In order to use this symmetry when performing a DMRG calculation it is useful to know how individual states transform under a reflection. While this is a trivial task if one is performing an exact diagonalization, it quickly becomes difficult to determine how a state transforms once an iteration with the infinite-system DMRG method has been performed. In the present paper we discuss a simple modification of the usual infinite-system DMRG scheme. This parity scheme allows for an explicit determination of how states will transform under a real-space reflection. Within the parity scheme the mapping between states and their parity-reflected partners is invariant under a DMRG iteration and can be calculated once and for all at the outset. The parity scheme can be applied equally

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well to open and periodic boundary conditions. In the following we consider mainly the infinite-system DMRG method which we shall refer to simply as the DMRG method.

The DMRG method involves truncating the Hilbert space representing half of the system by a factor which is necessarily $1/q$, where q is the number of degrees of freedom for the site that one is adding. Note that this site need not be a physical site in real space. After truncation, the half-Hilbert space contains a number of states usually denoted by m. Naturally, the precision of a calculation increases with the number of states retained, m. White [1] and Legeza and Fáth [5] as well as Kneer [6] have studied this error extensively and here we extend their results. It is important to understand exactly how the error depends on m and how convergence with m is obtained. This is a somewhat difficult task since one necessarily has to compare to exactly known models of which not many exist. In addition, the DMRG method is in most cases much more precise if open boundary conditions are used instead of periodic ones, thus necessitating the use of exact results for this case. While such results are available for many so-called matrix-product states, they are not of much use since the DMRG method is already *exact* for such states, as has been explicitly verified [7, 8] for the $S = 1$ Affleck–Kennedy–Lieb–Tasaki (AKLT) model [9] and the $S = 1/2$ Majumdar–Ghosh (MG) model [10]. We therefore focus on the familiar $S = 1/2$ Heisenberg model, with the Hamiltonian

$$H_{\mathrm{Heis}} = \sum_{j=1}^{L-1} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}. \tag{1}$$

It is well known that the one-dimensional Heisenberg model with periodic boundary conditions is solvable using the Bethe *ansatz* [11]. Perhaps less widely known is the fact that the same model is also solvable for many other boundary conditions and in particular for open boundary conditions [12]. Hence, this model is ideal for use in studying the relative and absolute errors for different values of m. Below, we present results for both this model, which is gapless, and for the gap in the MG model. In the latter model the first excited state is not known exactly, unlike the ground state. However, it is still possible to study the convergence of the DMRG method and we observe a power-law convergence in both cases.

2. Parity

We begin by considering the implementation of parity. In order to do this we use the rather simple modification of the standard DMRG storage scheme, (a) in figure 1, schematically shown as (b) in figure 1. This is just a more convenient way of representing the Hamiltonian matrix if parity is to be implemented. Instead of using a reflection of the left-hand side as a representation of the right-hand Hamiltonian space we simply copy it identically, and connect the two subspaces in the somewhat more elaborate manner indicated in the figure. The matrix representing the bond interaction between sites $L/2$ and $L/2 + 1$ is however always trivial to calculate since it is never truncated with the DMRG method and is therefore always known exactly. Hence, there is no added complication. However, matrices representing the two half-spaces are now trivially identical which simplifies the DMRG calculation greatly. When performing DMRG calculations, matrices, H_L, H_R, representing the left-hand and right-hand half-spaces are needed. Before iterating with the DMRG method, these two matrices are identical for spin systems. After iterating with the DMRG method using the standard DMRG scheme shown as figure 1(a), the two matrices are no longer identical element by element, but one can be obtained from the other and therefore

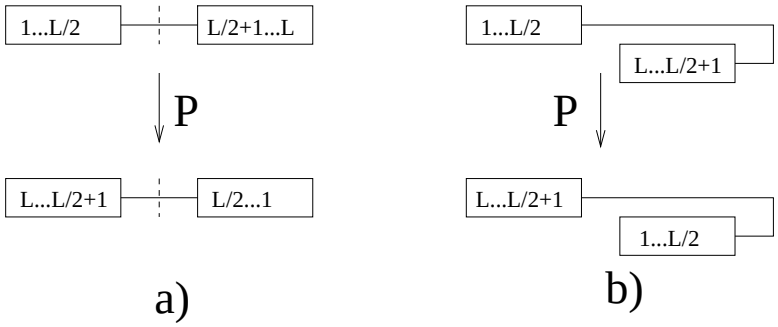

Figure 1. The effect of a real-space parity reflection in the two schemes. (a) The 'standard' scheme. (b) The 'parity' scheme.

one usually only stores one of them. Using the scheme shown as figure 1(b), the two matrices remain identical, which is an advantage.

When implementing parity as a symmetry one has to know how a given state transforms under a parity reflection. In particular one has to know how states transform in each of the two half-spaces describing the left-hand and right-hand sides of the system. If we work in a product basis and consider a half-space of three sites and symbolically denote a state by $|s_1s_2s_3\rangle$, then under parity it will transform into the state $|s_3s_2s_1\rangle$. If one knows how states transform in each of the half-spaces it is straightforward to determine how states for the complete system transform. What in figure 1 looks like a trivial modification of the DMRG scheme has an influence on how states transform under parity. As is shown in figure 1, a parity transformation of the complete system now just amounts to interchanging the two 'parts' of the state representing the right-hand and left-hand sides of the system. If we consider a system of six sites and work in a product basis, we see that before performing DMRG iterations a parity transformation of a given state would be given by

$$\begin{aligned} \mathcal{P}|s_1s_2s_3\rangle|s_4s_5s_6\rangle &\rightarrow |s_6s_5s_4\rangle|s_3s_2s_1\rangle \qquad \text{(a)} \\ \mathcal{P}|s_1s_2s_3\rangle|s_6s_5s_4\rangle &\rightarrow |s_6s_5s_4\rangle|s_1s_2s_3\rangle \qquad \text{(b)}. \end{aligned} \tag{2}$$

In other words, if states in the standard scheme (a) are represented as $|\Psi_a\rangle = |i\rangle|j\rangle$ and those in the parity scheme (b) are represented as $|\Psi_b\rangle = |\alpha\rangle|\beta\rangle$, then a parity transformation yields

$$\begin{aligned} \mathcal{P}|\Psi_a\rangle &= \mathcal{P}[|i\rangle|j\rangle] \rightarrow \mathcal{P}[|j\rangle]\mathcal{P}[|i\rangle] \qquad \text{(a)} \\ \mathcal{P}|\Psi_b\rangle &= \mathcal{P}[|\alpha\rangle|\beta\rangle] \rightarrow |\beta\rangle|\alpha\rangle \qquad \text{(b)} \end{aligned} \tag{3}$$

eliminating the need to know how states transform in the two half-spaces if the parity scheme (b) is used. Hence, in the parity scheme (b) it is trivial to write down the corresponding mapping between states no matter how many DMRG iterations have been performed and no matter how many states m are retained. One finds

$$\mathcal{P}|i + (j-1)qm\rangle \rightarrow |j + (i-1)qm\rangle. \tag{4}$$

Summarizing, the benefits of scheme (b) are as follows.

(i) Matrices representing variables for the right-hand and left-hand sides of the system are completely identical as opposed to the case for scheme (a).

(ii) If the states are numbered $1, \ldots, q^2m^2$ with q the number of degrees of freedom per site, and the states for the right-hand and left-hand halves of the systems are numbered

$i, j, \ldots, qm$, then reflection around the mid-point of the system (parity), as shown in figure 1, will map states as detailed in equation (4).

(iii) By forming parity-invariant states

$$\Psi_P \propto \Psi \pm P\Psi \tag{5}$$

the DMRG calculation can easily be performed using parity as a quantum number in a manner completely analogous to what is done in an exact-diagonalization study—thus allowing states to be classified according to their parity and reducing the computational effort by a factor of roughly two. Here $\mathcal{P}$ denotes the parity operator. Note that in equation (5) one should, as usual, be careful with states that are invariant under parity.

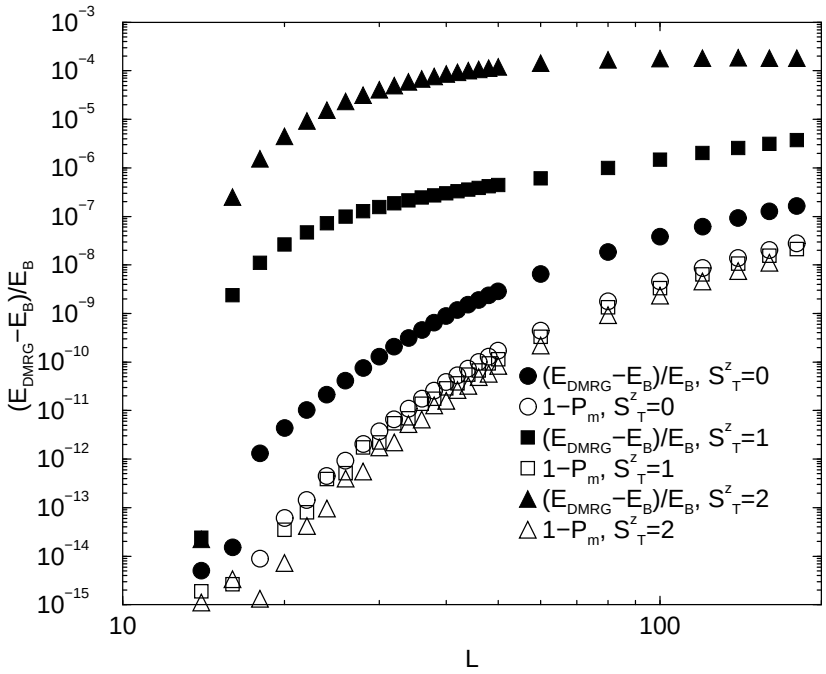

Figure 2. $\Delta E = (E_{\mathrm{DMRG}} - E_{\mathrm{Bethe}})/E_{\mathrm{Bethe}}$, the *relative* error, and $1 - P_m$ versus the system size, L. The results are for the Heisenberg model with $S^z_T = 0$, $P = (-1)^{L/2}$, $S^z_T = 1$, $P = (-1)^{L/2+1}$ and $S^z_T = 2$, $P = (-1)^{L/2}$; in all cases, $m = 64$ states were retained.

3. Precision

As explained in the introduction, the DMRG method involves a systematic truncation of the Hilbert space representing one half of the system down to a size m. The truncation is done in the space of eigen-vectors of the density matrix representing one half of the system, and one usually denotes the sum of the corresponding eigenvalues that are eliminated in a given DMRG iteration by $1 - P_m$. Sometimes $1 - P_m$ is used as an indication of the precision of a DMRG calculation. This would seem intuitively clear since a value of $1 - P_m$ of the order of 1 implies that a lot of information is lost in an iteration. Unfortunately, a very small value of $1 - P_m$ does not necessarily imply that the results obtained with the DMRG method are very precise. This is seen in figure 2 where a DMRG calculation for

the $S = 1/2$ Heisenberg model is compared to exact Bethe *ansatz* results [12] obtained using open boundary conditions. We show results for three different states with varying $S^z_T = 0, 1, 2$. The DMRG results are in all cases for $m = 64$, and hence can be improved upon rather easily. In order to make the most sensible comparison to $1 - P_m$, the solid points correspond to the *relative* error. From figure 2 it is clear that $1 - P_m$ is orders of magnitude smaller than the real error and in addition it shows hardly any dependence on S^z_T. The real error on the other hand depends strongly on S^z_T and increases rapidly with the system size. Another way of estimating the relative error of the energy for system size L is to use

$$1 - \prod_{l}^{L-4} P_m(l)$$

instead of simply $1 - P_m(L - 2)$ as we have done above. Here $P_m(l)$ is the sum of the eigenvalues that are retained when the system of size l is truncated. However, this expression gives only a small improvement in the estimate of the true error.

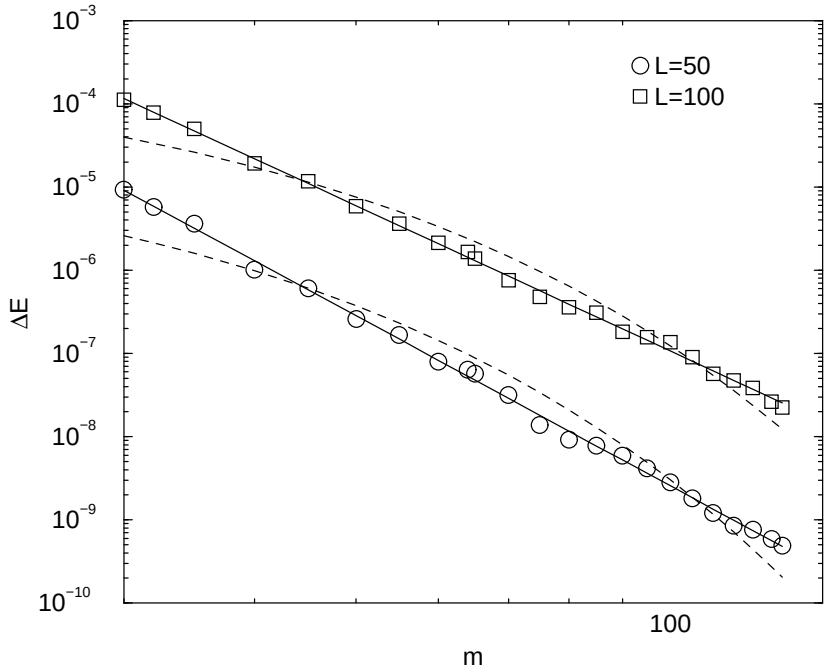

Figure 3. The absolute error $\Delta E = E_{\mathrm{DMRG}} - E_{\mathrm{Bethe}}$ versus the number of states retained, m, for the ground state, $S^z_T = 0$, $P = (-1)^{L/2}$, of the Heisenberg model. The error is shown for two different system sizes, $L = 50, 100$. The solid lines indicate power-law fits with exponents $-6.8(1)$ ($L = 50$) and $-5.8(1)$ ($L = 100$). The dashed lines indicate fits to an exponential form.

3.1. The infinite-system method—the Heisenberg model

In many cases one wishes to calculate gaps for a given model and to know the finite-size corrections to such gaps. The relevant quantities to study are therefore the total energies calculated and the *absolute* errors associated with such energies. In order to make a more

detailed study of this error we focus on the two system sizes, $L = 50, 100$, and study the absolute error as a function of m. In figure 3 we show results for the *absolute* error in the ground state for these two system sizes as m is increased from 30 to 128. For the results in figure 3 the calculations were always started at $L = 8$ and hence for some values of m the first few DMRG iterations were exact. As is clearly evident in figure 3, the exact result is approached as a *power law* in m. The exponents extracted for $L = 50, 100$, -6.8 and -5.8 depend slightly on L. It is also clear that the absolute error does not depend smoothly on m; some m-values work better than others. As stressed by White [1], this is probably due to the fact that the DMRG method will work better if complete multiplets of eigen-states of the density matrix and in particular of S^z_L are retained. Here S^z_L is the total z-component of the spin on the left-hand side. This is presumably the case for $m = s^n$ where s is the number of degrees of freedom per site in physical space. Note, that *absolute* errors are shown in figure 3. The precision obtained is therefore rather remarkable, especially in the light of the highly non-trivial nature of the Heisenberg model which has only algebraically decaying correlations.

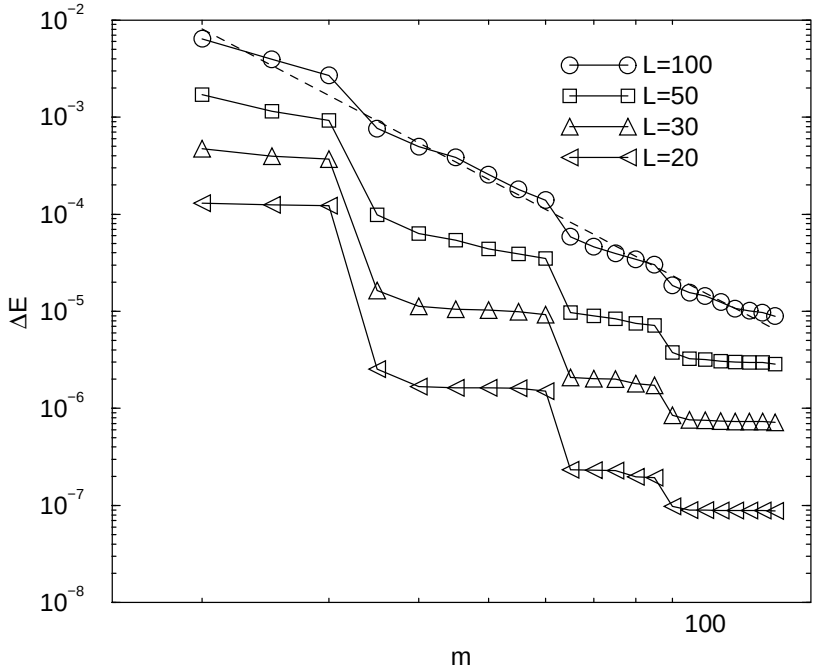

Figure 4. The absolute error $\Delta E = E_{\mathrm{DMRG}} - E_{\mathrm{Bethe}}$ versus the number of states retained, m, for the Heisenberg model. The calculation was performed in the $S^z_T = 1$, $P = (-1)^{L/2+1}$ subspace. The error is shown for different system sizes, $L = 20, 30, 50, 100$. For $L = 100$ the dashed line indicates a power-law fit with exponent $-3.9(1)$.

Higher-lying states do not display the same impressive precision as the ground state, as is already evident in figure 2. In figure 4 we show results for the first triplet. The calculation has been performed analogously to the one that produced the results shown in figure 3. We show results for four different system sizes, $L = 20, 30, 50, 100$. The initial numbers of sites for the results presented in figure 4 were in all cases $L = 8$. The absolute error now shows a pronounced dependence on the number of states retained. Some of the bigger features in the error seems to be associated with $m = s^n$ where s is the number

of degrees of freedom per site. This is perhaps not surprising and one may tentatively conclude that values of $m = 2^n$ in this case seem to be more useful. As the system size is increased, the features associated with particular values of m become less pronounced and a power-law dependence on m becomes apparent. However, the convergence is slower than for the ground state, with an exponent close to -4.

3.2. The finite-system method—the Heisenberg model

The results presented in the previous section can be improved upon by using what is usually referred to as the finite-system method. Here a sequence of asymmetric configurations $H_L(L-N-2)\bullet\bullet H_R(N)$ are used to describe a system of size L. Here $\bullet\bullet$ denotes the two sites added to the system. As N is varied, one obtains matrices $H_L(l)$, $H_R(l)$ progressively better and better adapted to describing l spins at one end of a finite system of L sites. We shall not discuss this method in detail here and refer the reader to reference [1].

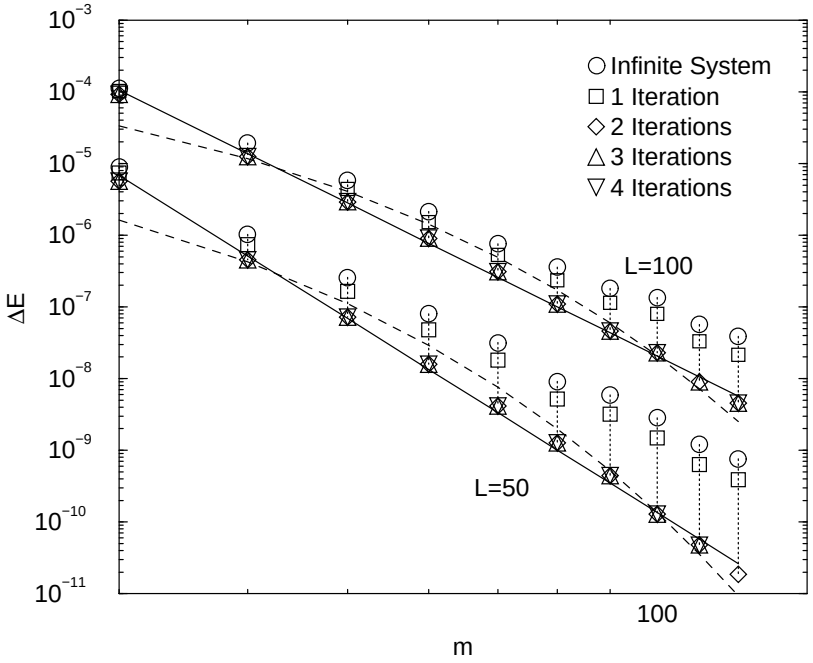

Figure 5. The absolute error $\Delta E = E_{\mathrm{DMRG}} - E_{\mathrm{Bethe}}$ versus the number of states retained, m, for the ground state of the Heisenberg model. The calculation was initially performed in the $S^z_T = 0$, $P = (-1)^{L/2}$ subspace and subsequently performed, using the finite-system method, in the $S^z_T = 0$ subspace without parity. Results are shown for the infinite-system method (○), after one iteration with the finite-system method (□), after two iterations (◇), after three iterations (△) and after four iterations (▽). The error is shown for two different system sizes, $L = 50, 100$. The solid lines indicate power-law fits to the results obtained after three iterations with the finite-system method, with exponents $-9.0(1)$ ($L = 50$) and $-7.1(1)$ ($L = 100$). The dashed lines indicate fits to an exponential form.

There are several ways in which one could imagine implementing the scheme for the finite system just described. Usually, the infinite-system method is applied until a system size of L is obtained, whereupon a number of complete sweeps with the finite-system method are performed to improve on the results obtained. Alternatively one can employ

the finite-system method at each iteration of the infinite-system method, performing several complete sweeps before adding additional sites to the system. The latter approach is rather time consuming and we have therefore used the former which is the one most often used in the literature.

Our results for the ground state of the Heisenberg model are presented in figure 5. For two different values of L, 50 and 100, four complete sweeps with the finite-system method were performed for $m = 20$–120. In all cases the initial system size was $L = 16$ as compared to $L = 8$ for the results presented in figure 3. The open circles (○) correspond to the initial results obtained before iterating with the finite-system method. They are essentially indistinguishable from the results in figure 3 even though the initial system size in this case was substantially larger. As is apparent from the results in figure 5, a few iterations with the finite-system method is sufficient to obtain convergence, and subsequent iterations lead to only marginal improvement. This is in agreement with previous work of White [1]. It should be noted that the results for the error shown in figure 5 are for the symmetric configuration with an equal number of spins in H_L, H_R. For larger values of m, significant improvement is obtained with the finite-system method, and for $L = 50$, a precision is obtained which is comparable to that of the numerical solution of the Bethe *ansatz* equations used to calculate the error. Hence, it is difficult to estimate the error for larger values of m. For both values of L the calculated error after the finite-system method has been used approximately follows a power law for the values of m considered, although a crossover to exponential behaviour for larger values of m cannot be excluded.

In figure 6 we show results for the state $S^z_T = 1$, $P = (-1)^{L/2+1}$. For the calculations performed with the finite-system method, the initial system size was $L = 18$. The results obtained before applying the finite-system method are indicated as open circles (○) in figure 6. For comparison, results from figure 4 are shown where the initial system size in all cases was $L = 8$. For the smaller values of m it is clear that it is advantageous to begin the calculation with the largest possible system for the infinite-system method also. With an exponent of -9.4, the use of the finite-system method leads to rather pronounced improvement in the precision for all values of m. As was the case for the ground state, results comparable to the Bethe *ansatz* results are obtained for the larger values of m. Tentatively, the data after two iterations with the finite-size method can be fitted with a power law as shown in figure 6. We have found that the maximal improvement in precision when using the finite-system method for these excited states is achieved when the initial system size was as large as possible.

3.3. The Majumdar–Ghosh model

The $S = 1/2$ Heisenberg model is somewhat particular since it is gapless. It is therefore reasonable to ask whether the power-law convergence with m is specific to such systems, and whether for a system with a gap an exponential convergence with m is possible. We have therefore investigated the MG model in detail, with the Hamiltonian

$$H_{\mathrm{MG}} = \sum_{j=1}^{L-1} \left[\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + \frac{1}{2} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2} \right]. \tag{6}$$

This model displays a gap and the ground state can be written as a matrix-product state. This simple structure is captured by the DMRG method which becomes *exact* for the ground state of these models. We have explicitly checked this, reproducing known results [7, 8]. While an analytic expression is available for the ground-state wave-function, no such expression is known for the lowest-lying gapped triplet excitation. The convergence is in this case

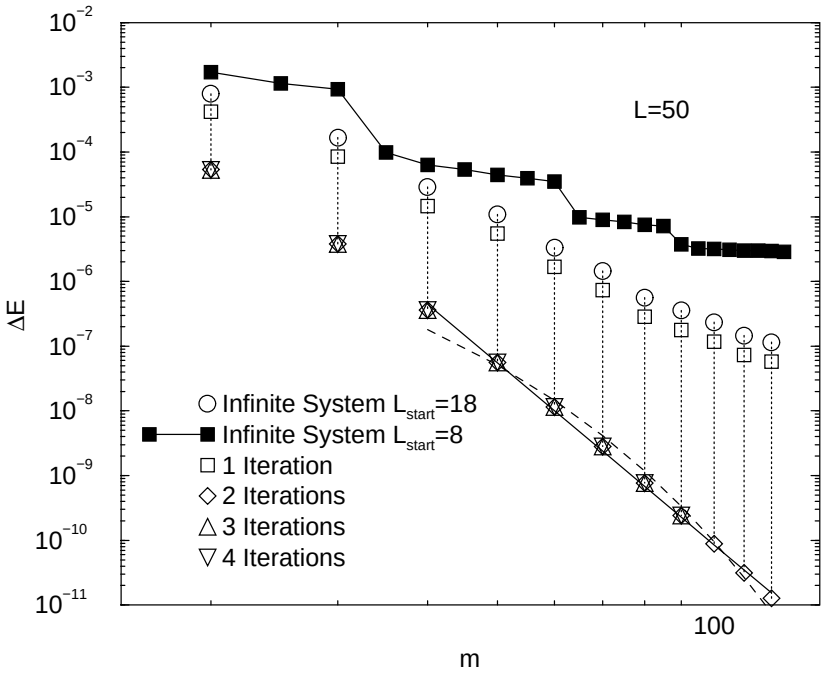

Figure 6. The absolute error $\Delta E = E_{\mathrm{DMRG}} - E_{\mathrm{Bethe}}$ versus the number of states retained, m, for the Heisenberg model. The calculation was initially performed in the $S^z_T = 1$, $P = (-1)^{L/2+1}$ subspace and subsequently performed, using the finite-system method, in the $S^z_T = 1$ subspace without using parity. Results are shown for the infinite-system method starting with $L_{\mathrm{start}} = 18$ sites (○), the infinite-system method starting with $L_{\mathrm{start}} = 8$ sites (■), after one iteration with the finite-system method (□), after two iterations (◇), after three iterations (△) and after four iterations (▽). The error is shown for the system size $L = 50$. The solid line indicates a power-law fit to the results after two iterations with the finite-system method, with exponent $-9.4(1)$ ($L = 50$). The dashed line indicates an exponential fit to the same data.

somewhat more complicated, since a subtraction of the exactly known ground-state energy leaves the gap in the thermodynamic limit. In general the numerically calculated energy with a given L, m can be written in the form $E(L, m) = E(L) + f(L; m)$, with f any function that tends to zero with m. Keeping L fixed, we can then study the functional form of f by calculating $\Delta E = E(L, m = m1) - E(L, m = m2) = g(L; m)$, for two different values of m. If f shows a power-law dependence on m for a given L, then so will g. We have performed such an analysis for the triplet state of the MG model, and find a behaviour equivalent to what is shown in figure 4. The error again approaches a power law as L is increased and one observes pronounced steps whenever $m = s^n$. The DMRG method is for this triplet gap extremely precise, and when plotting the gap as a function of L no discernible difference between the results from calculations performed with $m = 60$ and 128 is visible to the naked eye. Most of the error in calculating the gap therefore comes from the extrapolation to the thermodynamic limit. Assuming a dispersion relation of the form [4] $\omega(k) = \Delta + v^2(k - \pi)^2/2\Delta$ one finds that the energy of the gapped state should be

$$E(L) = \Delta + \frac{(v\pi)^2}{2\Delta(L+1)^2} + \mathcal{O}(L^{-3}).$$

Here v is the associated velocity. We have fitted our results using this form and the results are shown in table 1. The results for Δ are only weakly dependent on m and agree well with previous studies [7, 8]. The consistency of the values for the second coefficient allows for a determination of the velocity $v \simeq 1.43J \simeq \sqrt{2}J$; this is slightly different to that from the unfrustrated Heisenberg model, where $v = J\pi/2$. Here we have used $\Delta = 0.2340(1)$.

In order to study singlet excitations it is often quite useful to implement spin-inversion (particle–hole) symmetry [2], along with parity, in the S^z_T subspace. This symmetry is *extremely* useful since it allows for a clear distinction between low-lying singlets and triplets in the $S^z_T = 0$ subspace; hence the singlet gap can be calculated without difficulty. For the MG model we have calculated the singlet gap using this symmetry and we find $\Delta_{00} = 0.2340(1)$ with the same velocity as for the triplet excitation. Hence, the triplet and singlet excitations are degenerate. Spin inversion can be implemented along with parity, resulting in roughly a fourfold decrease in the computational effort. In addition this symmetry can be used with the finite-system method.

Table 1. The gap to the triplet excitation in the MG model, shown with associated fitting coefficients.

m	Δ	$(L+1)^{-2}$	$(L+1)^{-3}$
16	0.235 342	43.2	−434
32	0.233 995	43.3	−409
40	0.233 968	43.5	−419
50	0.233 983	43.2	−403
60	0.233 973	43.3	−409
64	0.233 965	43.4	−413
70	0.233 967	43.3	−411
80	0.233 968	43.3	−409
90	0.233 964	43.4	−412
100	0.233 953	43.5	−419
110	0.233 960	43.4	−414
120	0.233 961	43.4	−414
128	0.233 963	43.4	−412

4. Conclusions

In conclusion, we have presented a simple and hence very attractive way of implementing parity as a symmetry when performing DMRG calculations. We have shown that the DMRG method appears to converge as a power law in m, the number of states retained, for two non-trivial models. Kneer [6] has studied the absolute error in the 1D Hubbard model and interprets the results as having an exponential convergence in the number of states. However, an interpretation of his data in terms of a power-law convergence seems equally plausible. It is conceivable that more elaborate DMRG schemes will show faster convergence. In particular White and Affleck (reference [8]) seem to favour an exponential convergence for some quantities. It also remains a possibility that models where the gap is to a well-defined mode and not to a continuum, as is the case for the MG model, could display an exponential convergence with m. We also cannot exclude the possibility that for significantly larger values of m a crossover to exponential convergence occurs for the models considered here. However, an investigation of larger values of m would require an extensive analysis of round-off errors in the numerical calculation of the Bethe *ansatz*

results in order to allow a reliable comparison to the already very precise DMRG results.

Many variations of the finite-system method can be imagined and it would be desirable to have more complete results than the ones presented here, which are only meant to complement the results for the infinite-system method. It would also be interesting to repeat the above analysis of the precision of the DMRG method for disordered systems where a systematic convergence seems more doubtful. However, in this case exact results are rather more scarce. Recently, Andersson *et al* [13] have extensively analysed the error associated with calculating the correlation functions in the Heisenberg model.

Acknowledgments

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