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Exact diagonalisations of open spin-1 chains

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Abstract. We numerically compute the two lowest eigenvalues of finite length spin-1 chains with the Hamiltonian $H = \Sigma_i[\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} - \beta(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2]$ and open boundary conditions. For a range of β, including the value 0, we find that the difference of the two eigenvalues decays exponentially with the length of the chain. This exponential decay provides further evidence that these spin chains are in a massive phase as first predicted by Haldane. The correlation length ξ of the chain can be estimated using this exponential decay. We find estimates of ξ for the Heisenberg chain ($\beta = 0$) that range from 6.7 to 7.8 depending on how one extrapolates to infinite length.

1. Introduction

The antiferromagnetic spin-1 Heisenberg chain has been the subject of numerous numerical studies, motivated in large part by Haldane's prediction that this chain has radically different properties from the spin-$\frac{1}{2}$ chain [1]. He argued that the ground state of the spin-S Heisenberg antiferromagnetic chain is in a massive phase if S is an integer and in a massless phase if S is a half integer. The massive phase is characterised by a gap in the energy spectrum immediately above the ground state energy and an exponential decay of the truncated correlation functions. The massless phase is characterised by no gap and by a power law decay.

The ground state of these spin chains has been studied numerically by Monte Carlo simulation [2], exact diagonalisation [3, 4], and series expansions [5]. Exact diagonalisation studies usually impose periodic boundary conditions. With these boundary conditions the Hamiltonian is invariant under translations, and so one can search for the ground state in the subspace of translation invariant states. This reduces the dimension of the subspace by a factor roughly equal to the length of the chain. In this paper we use exact diagonalisation to study the lowest eigenvalues of the *open* spin-1 chain with Hamiltonian

$$H = \sum_{i=1}^{L-1} [\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} - \beta(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2] \tag{1}$$

for $-1 \leqslant \beta \leqslant 1$.

There are several values of β where the Hamiltonian (1) is solvable in some sense. The most important one for our purposes is $\beta = -\frac{1}{3}$. To see why $\beta = -\frac{1}{3}$ is special consider the terms in the Hamiltonian associated with a single bond, i.e., $\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} - \beta(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2$. This operator has three eigenvalues, a singlet with energy

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$-2-4\beta$, a triplet with energy $-1-\beta$, and a quintuplet with energy $1-\beta$. For $\beta > -\frac{1}{3}$ the singlet has the lowest energy while for $\beta < -\frac{1}{3}$ the triplet has the lowest energy. At $\beta = -\frac{1}{3}$, where the singlet and triplet are degenerate, Affleck *et al* [6] found the ground state exactly and rigorously proved that there is a unique infinite volume ground state, exponential decay of the truncated correlation functions in the ground state and a gap. Another special value of β is $\beta = 1$. This model is solvable by the Bethe *ansatz* and has no gap [7] with soft modes at $k = 0, \pi$. When $\beta = -1$ the operator $\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} - \beta(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2$ simply interchanges the spins at sites i and $i+1$. This model [8] has an SU(3) symmetry, no gap and soft modes at $k = 0, 2\pi/3, 4\pi/3$.

The initial motivation for the present work came from comparing the degeneracy of the ground state at $\beta = -\frac{1}{3}$ and $\beta = 0$. When $\beta = -\frac{1}{3}$, the chain with periodic boundary conditions (and more than two sites) has a unique ground state, but the chain with open boundary conditions has a fourfold degenerate ground state consisting of a singlet and a triplet. Loosely speaking, the open chain has a spin-$\frac{1}{2}$ degree of freedom at each end. These two spin-$\frac{1}{2}$'s combine to form the singlet and the triplet. Each of these four ground states yields the same infinite volume ground state. For $\beta = 0$ Lieb and Mattis [9] proved that the ground state of the open chain is a singlet if the number of sites is even and a triplet if the number is odd. The present numerical work was begun so as to understand what happens to the fourfold degeneracy of the ground state when one varies β from $-\frac{1}{3}$ to 0.

We find that the two lowest eigenvalues are a singlet and a triplet. For β near $-\frac{1}{3}$ the difference of these two eigenvalues is quite small and decays exponentially with the length of the chain. It is difficult to determine the exact range of β for which this holds, but the range appears to include $\beta = 0$. It is important to emphasise that our results do not in any way contradict Haldane's prediction of a gap. Based on our understanding of the ground states for $\beta = -\frac{1}{3}$, we expect that when $\beta \neq -\frac{1}{3}$ the four eigenstates associated with the two lowest eigenvalues are the same except for boundary effects at the two ends of the chain. Thus each of these four states will yield the same ground state in the infinite length limit [10]. The Haldane gap will be the difference between the second and third lowest eigenvalues.

2. Results

We have only studied the interval $-1 \leqslant \beta \leqslant 1$. First let us consider the interval $-\frac{1}{3} < \beta \leqslant 1$. Letting L denote the number of sites in the chain, we find that if L is even the ground state is a singlet and the next eigenvalue is a triplet. If L is odd the ground state is found to be a triplet, with the next eigenvalue a singlet. The difference between these two lowest eigenvalues is shown in table 1 for several values of $\beta > -\frac{1}{3}$. For β near $-\frac{1}{3}$, e.g. $\beta = -0.3, -0.2$, these differences are quite small and decrease rapidly with L. For $\beta = 0$ the difference still clearly decreases to 0 as $L \to \infty$, but for $\beta = 0.4$ the decrease of the difference with L is quite slow.

To see whether or not this eigenvalue difference is decaying exponentially to zero we plot $\frac{1}{2}\ln(s_{L-2}/s_L)$ as a function of $1/L$, where s_L is the difference in the two lowest eigenvalues (figure 1). If s_L decays as $\exp(-L/\xi)$, then this quantity should converge to $1/\xi$. If s_l decays as $1/L^p$ then this quantity will converge to 0. Thus exponential decay of this eigenvalue difference is equivalent to a non-zero intercept of the curves in figure 1 with the vertical axis. Not surprisingly, figure 1 shows that the points for even values of L lie on a different curve from the points for odd values of L. We expect that the

Table 1. The difference of the two lowest eigenvalues of the chain with open boundary conditions and L sites for several $\beta > -\frac{1}{3}$.

L	$\beta = -0.30$	$\beta = -0.20$	$\beta = -0.10$	$\beta = 0.00$	$\beta = 0.40$
4	0.039379	0.171777	0.329668	0.509170	1.331250
5	0.023224	0.147423	0.328731	0.546645	1.603914
6	0.011608	0.082462	0.184574	0.307786	0.927374
7	0.006364	0.066161	0.178889	0.330956	1.153717
8	0.003310	0.040809	0.110734	0.201879	0.696740
9	0.001774	0.031059	0.102979	0.212703	0.877509
10	0.000935	0.020254	0.068391	0.138331	0.548516
11	0.000497	0.014880	0.061122	0.141772	0.693475
12	0.000263	0.010015	0.042723	0.097142	0.445742
13	0.000140	0.007200	0.036921	0.096709	0.563294
14	—	0.004933	—	0.069165	—

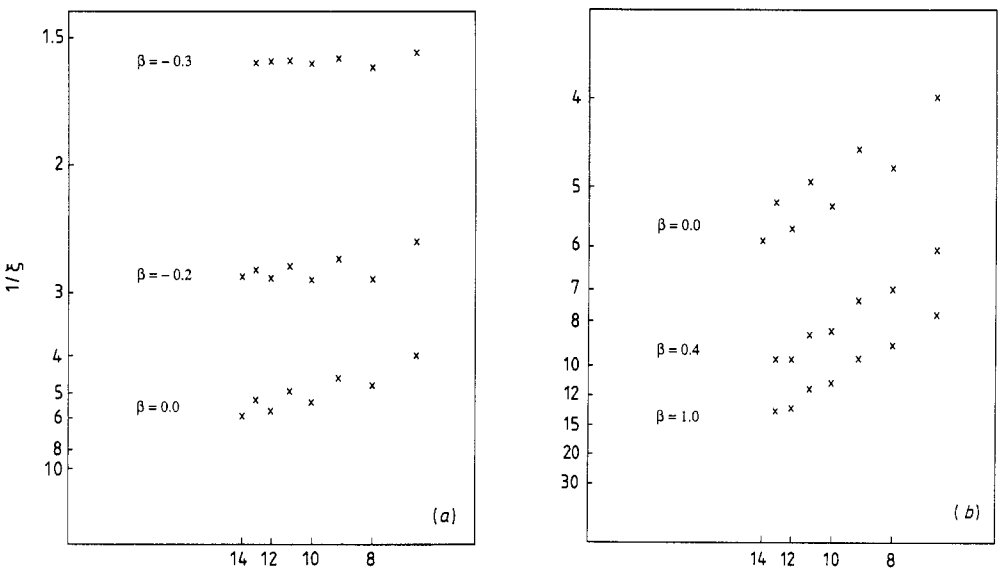

Figure 1. Plot of $\frac{1}{2}\ln(s_{L-2}/s_L)$ as a function of $1/L$, where s_L is the difference between the two lowest eigenvalues. The intersection of these curves with the vertical axis gives the inverse correlation length, so several correlation lengths are marked on the vertical axis. The horizontal axis is $1/L$, but the labels are values of L.

correlation length in the two cases should be the same, i.e. the two curves should have the same intercept with the vertical axis. This difference between even and odd length chains is the reason we consider the ratio s_{L-2}/s_L rather than s_{L-1}/s_L.

The value of β closest to $-\frac{1}{3}$ for which a curve is shown in figure 1(*a*) is $\beta = -0.3$. If we extrapolate this curve to $L = \infty$ the intercept with the vertical axis is clearly non-zero and the correlation length is fairly short, about 1.6. For $\beta = 0$ the intercept is much

Table 2. Various estimates of the inverse correlation length. The different estimates come from different methods of extrapolation to the infinite length limit and are explained in the text. The * indicates values for β for which the eigenvalues for $L = 14$ were computed.

β	Crude	Linear even	Linear odd	Linear LS	Quad LS
−0.33	0.880	0.966	0.954	0.961	0.891
−0.32	0.762	0.784	0.777	0.781	0.751
−0.31	0.685	0.700	0.691	0.696	0.685
−0.30	0.627	0.641	0.630	0.636	0.631
−0.20*	0.355	0.366	0.335	0.349	0.370
−0.10	0.243	0.207	0.204	0.205	0.245
0.00*	0.200	0.128	0.128	0.128	0.150
0.10	0.149	0.069	0.083	0.075	0.082
0.20	0.125	0.046	0.056	0.050	0.050
0.40	0.096	0.024	0.028	0.026	0.021
0.60	0.078	0.014	0.016	0.015	0.009
0.80	0.067	0.008	0.009	0.008	0.003
1.00	0.060	0.004	0.006	0.005	−0.001

smaller, but the curve would have to change drastically for larger values of L in order for the curve to have a zero intercept. (Note that the curves for $\beta = 0$ are slightly convex.) Although the intercept appears to be non-zero, the correlation length for $\beta = 0$ is rather long, between 6 and 8. In figure 1(*b*) we see that as $\beta \to 1$ the intercept continues to decrease (the correlation length increases). Whether the Haldane phase ends at some $\beta_c < 1$ or at the Bethe *ansatz* point, $\beta = 1$, has been the subject to some controversy. (See [4] and references therein for a discussion of this point.) Depending on how one extrapolates the curves in figure 1(*b*), one can conclude that β_c is anywhere from 0.4 to 1.0, so our results cannot shed any light on this question. Figure 1(*b*) does show that if the massive phase extends all the way to $\beta = 1$, then the correlation length in the interval $0.4 \leqslant \beta < 1$ is quite large.

To extract a value for the correlation length from our data we have tried several methods of extrapolating to $L = \infty$ (Table 2). A very crude method of estimating ξ, which does not involve any extrapolation, is $1/\xi = \ln(s_L/s_4)/(L-4)$ where L is the length of the longest chain we compute. This estimate of ξ is shown in the column labelled 'crude' in table 2. The simplest extrapolation procedure is to take the straight line through the two points in figure 1 corresponding to the two largest even (or odd) values of L. For most values of β this means taking the lines through the points at $L = 11, 13$ and $L = 10, 12$. The two resulting values of ξ are shown in table 2 in the columns labelled 'linear even' and 'linear odd'. (For a few values of β we have computed the eigenvalues for $L = 14$. These values of β are marked with an * in table 2.)

Two other extrapolation methods are based on the assumption that the curves for even and odd values of L have the same intercept. Using the largest four values of L (10, 11, 12, and 13 in most cases) we find the two lines with the same intercept which best fit the four points. (There are three free parameters, the intercept and the two slopes, so we use a least squares fitting procedure to find the best two lines.) This estimate of ξ is referred to as 'linear LS' in table 2. Finally we use the six largest values of L to find the best fitting pair of parabolas with the same intercept with the vertical axis. The result is shown in the column labelled 'quadratic LS' in table 2.

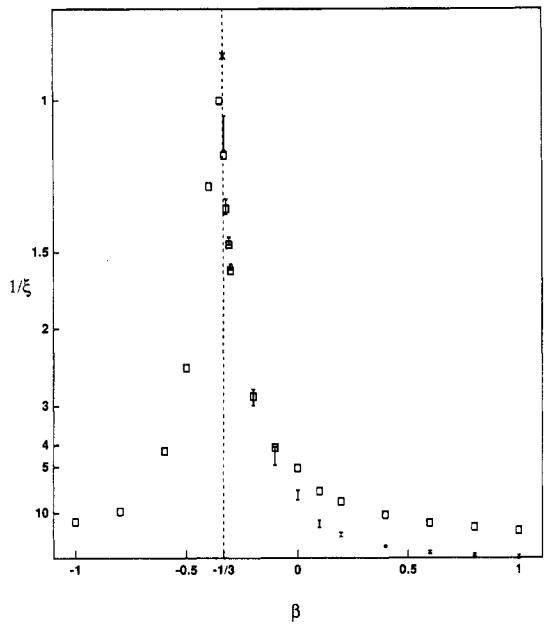

Figure 2. The inverse correlation length as a function of the parameter β in the Hamiltonian (1). (The labels on the vertical axis are correlation lengths rather than inverse correlation lengths.) The squares are the 'crude' estimates of the inverse correlation length described in the text. The vertical bars for $\beta > -\frac{1}{3}$ run from the smallest to the largest of the estimates of the inverse correlation length that we obtain from various methods of extrapolating to the infinite length limit. The $\times$ represents the exact value of $\ln 3$ at $\beta = -\frac{1}{3}$.

The usual definition of the correlation length would use the exponential decay of the two-point function. Although we expect that the correlation length we are computing is the same as this more standard definition, it is not inconceivable that they are different. The usual definition of the correlation length is difficult to compute numerically since one must worry about finite length effects. Moreo [3] computed the two-point function at a distance L in a periodic ring with $2L$ sites. She found a correlation length at $\beta = 0$ of approximately 5, but it should be emphasised that since the largest L was 16, this estimate is based on distances of no more than eight lattice spacings. Another approach to numerically computing the correlation length is to study the convergence of the ground state energy per bond to its infinite length limit. In a massive phase this convergence should be exponential. Again, we expect this correlation length to be the same as the other definitions, but it could be different. Affleck [11] used this approach and previously obtained exact diagonalisation and Monte Carlo calculations of the energy for up to 32 sites to estimate that the correlation length is 4.8. Zhang *et al* [12] used this approach and exact diagonalisation results up to 16 sites and estimated the correlation length to be 3.3.

It is important to note that power law corrections to exponential decays can make a large difference in the estimate of the correlation length. (Ignoring such power law corrections is like extrapolating figure 2 to $L = \infty$ by simply drawing a horizontal line through the last point.) If the eigenvalue difference s_L decays as $\exp(-L/\xi)/L^p$ then the plot of $\frac{1}{2}\ln(s_{L-2}/s_L)$ versus $1/L$ will be linear for large L with slope p. Using a power law correction of $L^{-1/2}$ and the same numerical data Affleck [13] found a correlation length of 7.2. It is worth noting that one advantage of our method of estimating the correlation length is that the quantity we are using decays to 0. If one uses the energy per bond, one must fit for the infinite length limit of this quantity as well as the correlation length.

Figure 2 shows the inverse correlation length as a function of β. With the exception of the 'crude' method, the various estimates of ξ are fairly close, so we do not attempt

Table 3. The difference of the two lowest eigenvalues for several β between $-\frac{1}{3}$ and -1.

L	$\beta = -0.40$	$\beta = -0.50$	$\beta = -0.60$	$\beta = -0.80$
4	0.075525	0.190628	0.309201	0.520651
5	0.010584	0.071468	0.239268	0.628191
6	0.007178	0.104629	0.251241	0.486708
7	0.007153	0.059699	0.150639	0.358247
8	0.003389	0.004440	0.087142	0.383921
9	0.000849	0.024437	0.123165	0.340393
10	0.000131	0.017035	0.074507	0.263762
11	0.000268	0.002529	0.032294	0.269265
12	0.000157	0.004593	0.060266	0.258896
13	0.000051	0.004438	0.037133	0.204449

to plot them individually. Instead we have plotted a box for the 'crude' estimate and plotted a vertical bar that runs from the largest to the smallest of the other estimates of ξ. The exact solution at $\beta = -\frac{1}{3}$ has an inverse correlation length of ln 3. This point is plotted with an $\times$. The inverse correlation length appears to converge to the exact value of ln 3 as $\beta \to -\frac{1}{3}$, but the most striking feature of this plot is the singular nature of this convergence. A small shift in β away from $-\frac{1}{3}$ can change the correlation length significantly.

The sharp peak in figure 2 suggests the following possible scenario. For $\beta \neq -\frac{1}{3}$ the true inverse correlation length might be significantly less than that shown in figure 2 and might not converge to ln 3 as $\beta \to -\frac{1}{3}$. Numerical studies of a finite chain with β near $-\frac{1}{3}$ would not see the true correlation length but would instead see behaviour similar to that at $\beta = -\frac{1}{3}$. If one could increase the length of the chain sufficiently one would then see a crossover to the true behaviour. As β moves away from $-\frac{1}{3}$ this crossover would occur at smaller L. However, we do not see any evidence of this crossover behaviour in any of the curves plotted in figure 1, so we do not believe this scenario is correct. In view of the sharpness of the peak in figure 2 this scenario should not be ruled out completely.

Next we consider the interval $-1 \leqslant \beta < -\frac{1}{3}$. Again the two lowest eigenvalues are a singlet and a triplet. Their difference is shown in table 3. For β near $-\frac{1}{3}$ this difference is small and decreases quickly as L increases. However, the dependence of the total spin of the ground state on the length L and the dependence of the difference of the two lowest eigenvalues on L is very different from that for $\beta > -\frac{1}{3}$. If we plot $\frac{1}{2}\ln(s_{L-2}/s_L)$ as a function of $1/L$ as we did in figure 1 for $\beta > -\frac{1}{3}$, the points do not form nice curves. We can still estimate the correlation length with the 'crude' method, $1/\xi = \ln(s_L/s_4)/L - 4)$. The results for $L = 11$, 12 and 13 are shown in table 4. The results for $L = 13$ are plotted in figure 2 with a rectangle. As one can see from table 4 this crude estimate of the inverse correlation length still shows a large dependence on L. One can try plotting this crude estimate as a function of $1/L$, but the points show a large scatter and no reasonable extrapolation to $L = \infty$ is possible.

The total spin of the ground state is shown in table 5 for various values of L and β. Recall that in the interval $-\frac{1}{3} < \beta \leqslant 1$ the ground state has total spin 0 if L is even and 1 if L is odd. For $\beta = -0.34$ the ground state has total spin 0 if L is odd and total spin 1 if L is even as long as $L \leqslant 12$, but this pattern ends at $L = 13$. For $\beta = -0.35$ this pattern also holds for small L, but now ends at $L = 9$. For $\beta = -0.6$, -0.7, -0.8, -0.9 table 5

Table 4. Three 'crude' estimates of the inverse correlation length for $\beta < -\frac{1}{3}$ using maximum chain lengths of 11, 12 and 13.

β	Crude $L = 11$	Crude $L = 12$	Crude $L = 13$
−1.00	0.056	0.082	0.081
−0.80	0.094	0.087	0.104
−0.60	0.323	0.204	0.236
−0.50	0.618	0.466	0.418
−0.40	0.806	0.772	0.810
−0.35	1.025	1.001	1.002

Table 5. The total spin of the ground state. For β between $-\frac{1}{3}$ and 1 the total spin is 0 if the length of the chain is even and 1 if is odd.

	β								
L	−0.34	−0.35	−0.38	−0.40	−0.50	−0.60	−0.70	−0.80	−0.90
3	0	0	0	0	0	0	0	0	0
4	1	1	1	1	1	1	1	1	1
5	0	0	0	0	1	1	1	1	1
6	1	1	0	0	0	0	0	0	0
7	0	0	1	1	1	1	1	1	1
8	1	1	0	0	1	1	1	1	1
9	0	1	1	1	0	0	0	0	0
10	1	0	0	1	1	1	1	1	1
11	0	1	0	0	0	1	1	1	1
12	1	0	1	1	0	0	0	0	0
13	1	1	0	0	1	1	1	1	1

shows that the ground state is a singlet if L equals 0 mod 3 and a triplet otherwise. This period-3 behaviour is not surprising in light of the nature of the solution [8] at $\beta = -1$. Of course it is possible that this period-3 behaviour breaks down at some value of L beyond those we can compute. This period-3 behaviour suggests that we plot $\frac{1}{3}\ln(s_{L-3}/s_L)$ as a function of $1/L$. By analogy with figure 1 we hope to obtain three curves corresponding to $L = 0, 1, 2 \bmod 3$. The resulting plots for $\beta = -0.6$ and -0.8 are shown in figure 3. There are only two or three points on each of the three curves for a given value of β, so it is difficult to ascertain if the points really do lie on three curves and if the three curves have the same intercept with the vertical axis.

The computation of the two lowest eigenvalues is done as follows. Since the Hamiltonian is isotropic is spin space, each eigenvalue has an eigenvector with total S^z equal to zero, so we restrict our attention to that subspace. For the periodic chain one can use the translation invariance of the Hamiltonian to further restrict the dimension of the subspace, but this is not the case for the open chain. There are two symmetries of the Hamiltonian with open boundary conditions that we can exploit. One is the reflection of the chain about its midpoint. The three spin states at a single lattice site can be labelled as +, −, and 0 according to the eigenvalues of S_l^z. The other symmetry is the global spin

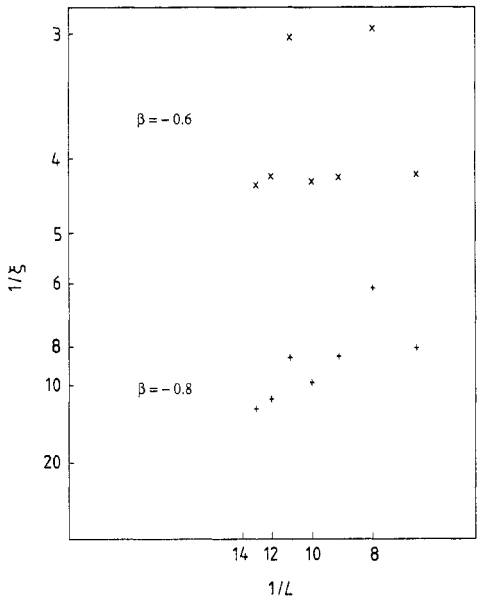

Figure 3. Plot of $\frac{1}{3}\ln(s_{L-3}/s_L)$ as a function of $1/L$, where s_L is the difference between the two lowest eigenvalues. The top curve is $\beta = -0.6$ and the bottom curve is $\beta = -0.8$. As in figure 1 the intersection of the curves with the vertical axis gives the inverse correlation length, so several correlation lengths are marked on the vertical axis.

flip that interchanges + and − and leaves 0 alone. Together these two symmetries reduce the dimension of the subspace we must consider by a factor of 4. More importantly the two lowest eigenvectors belong to different symmetry classes. One of them is even under both of these symmetries and the other is odd under both of these symmetries. Which is which depends on β and the length of the chain. One can extract this information from table 5 by the following rule. If the total spin is 0 and the length of the chain is even, or the total spin is 1 and the length of the chain is odd, then the eigenstate is even under both symmetries. Otherwise it is odd under both of them. Since the two eigenstates we seek belong to different symmetry classes we need only to compute the lowest eigenvalue in each of the two subspaces. This is done by the power method.

The calculations were done on a SUN 3/50. As is always the case with exact diagonalisations the time and memory required increase at least geometrically with the number of sites. The dimension of the subspace is about 50 000 for $L = 13$ and about 150000 for $L = 14$. The number of non-zero entries in the matrix in about 800000 for $L = 13$ and about 2 500 000 for $L = 14$. Several hundred iterations of the power method are required. The exact number depends on L and β. Most of the time is spent on the power method as opposed to setting up the basis and matrix. For $L = 13$ it takes 13 min to set up the basis and matrix and about 6 h to compute a single eigenvalue. For $L = 14$ the basis and matrix take 54 min while the power method takes about 60 h.

3. Conclusions

For a range of β including $\beta = -\frac{1}{3}$ the ground state of the open spin-1 Hamiltonian (1) is essentially fourfold degenerate. The two lowest eigenvalues are a singlet and a triplet and their difference decreases to zero exponentially fast as the length of the chain goes to infinity. Thus the Haldane gap for the open chain is the difference between the second and third lowest eigenvalues, not between the first and second lowest. It is difficult to

determine exactly where this range of β begins and ends, but it appears to include $\beta = 0$ (the usual Heisenberg Hamiltonian) and may extend all the way between the two special values $\beta = -1$ and $\beta = 1$. The exponential decay of the difference of the two lowest eigenvalues provides further evidence that these spin chains are in a massive phase. This exponential decay was used to estimate the correlation length of the chain as a function of β. While the correlation length is quite short ($1/\ln 3$) at the solvable point, $\beta = -\frac{1}{3}$, it grows rapidly as one moves away from this special point. At $\beta = 0$ our estimates of the correlation length range from 6.7 to 7.8 depending on how we extrapolate to the infinite length limit.

Acknowledgments

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Note added in proof. Two recent Monte Carlo simulations [14, 15] of the spin-1 chain with $\beta = 0$ both found correlation lengths of 6.2 lattice spacings by studying the decay of the correlation functions.

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