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# Gapless spectrum in a class of $S = 1$ exchange models with long-range interactions

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**Abstract.** We present evidence for the absence of a gap in a class of  $S = 1$  antiferromagnetic exchange models. The spin exchange is long ranged, of the type  $-(-1)^{i-j}/|i-j|^\alpha$  where  $1 < \alpha < 3$ . We have shown previously that without the alternating factor the model for  $\alpha = 2$  (the  $S = 1$  Haldane–Shastry model) has a gap, exponentially decaying correlation functions and exponentially small susceptibility at very low temperatures. In the case of the alternating interaction the stabilizing next-nearest-neighbour ferromagnetic interaction changes the behaviour of the system qualitatively. We have studied the ground state and first excited state using a modified Lanczos algorithm for system sizes up to 16 sites. Also, we performed exact diagonalization for systems up to 8 sites and obtained the thermodynamics. The correlation functions decay with distance like a power law. These models define a new class of integer spin chains that do not show a Haldane gap. The results may be relevant for describing impurity spins coupled by a RKKY interaction through a half-filled conduction electron band.

## 1. Introduction

It was proposed long ago that integer and half-odd-integer spin chains behave qualitatively differently [1]. The reason for this lies in a topological term in the action that prevails in the latter case. On general grounds, half-odd-integer spin chains are gapless and integer spin chains show a gap [2]. This leads to important differences in the correlation functions. In the first case these show power-law behaviour and in the second case exponential behaviour. There are however several models that do not follow this rule at special points in the space of interactions. In the case where  $S = 1$ , adding a quadratic term in the interaction and requiring the models to be integrable, a  $SU(2)$ -invariant model [3] and a  $SU(3)$ -invariant model (both solvable by the Bethe *ansatz*) [4] are gapless. Also, adding frustrating next-nearest-neighbour (nnn) interactions to the Heisenberg model, it has been found that for  $S = 1/2$  there is a critical value  $\alpha_{cr} \sim 0.2411$  (where  $\alpha = J_2/J_1$  is the ratio of the nnn interaction to the nearest-neighbour (nn) interaction) such that for  $\alpha < \alpha_{cr}$  the spectrum is gapless (as for  $\alpha = 0$ ) while for  $\alpha > \alpha_{cr}$  a gap appears [5]. This has been interpreted as a fluid–dimer transition. In particular, it has been shown that if the spin is half-odd-integer and the ground state is translationally invariant ( $k = 0$ ) the spectrum is gapless [6]. The dimer phase is consistent with the Lieb–Schultz–Mattis theorem [7] which states that if the spectrum is not gapless the ground state should be degenerate (for half-integer spin). Also, recently it has been argued that translationally invariant spin chains in an applied field can

be gapful without breaking translation symmetry, when the magnetization per spin,  $m$ , is such that  $S - m$  is an integer. It was then proposed that a Haldane gap phase can be found for half-integer spin [8]. It has also been shown recently that the  $S = 1/2$  dimer chain, the Majumdar–Ghosh chain and the  $S = 1$  Haldane chain are in the same phase [9].

Explicit tests of the validity of Haldane’s proposal have concentrated on models of short-range interactions. Recently, we have extended this analysis to the case of long-range interactions, considering the  $S = 1$  Haldane–Shastry model [10, 11]. Even though we might expect that the correlation functions should not decay faster than the interaction we found a finite gap and the corresponding exponential decay of the correlation functions. This may be the result of the frustrating nature of the interactions. The influence of frustration in the  $S = 1$  Heisenberg chain has also been studied recently [12].

The standard Haldane–Shastry model [13, 14] is a periodic version of  $1/r^2$  exchange. The  $S = 1/2$  case has attracted considerable attention [15, 16]. The ground-state energy and the correlation functions have been obtained [15, 13, 14] together with the thermodynamics [17]. The ground-state wavefunction is a spin singlet of the Jastrow–Gutzwiller form. The excitations are spin-1/2 spinons [17] that form a gas of a semionic nature [17, 18]. The asymptotic correlations decay algebraically with exponent  $\eta = 1$  without logarithmic corrections, in contrast to the Heisenberg case. This indicates the absence of spin exchange between the spinons rendering the models solvable in greater detail than in the short-range Heisenberg counterpart, solvable by the traditional Bethe *ansatz* method. The zero- $T$  susceptibility is finite [17] (and numerically the same as for the Heisenberg model) consistently with a singlet ground state and a gapless spectrum.

The  $S = 1$  case is not integrable (for either model). In reference [10] we studied the ground-state properties and the gap to the first excited state using a modified Lanczos method for small systems of size up to 16 spins. We obtained that the ground-state energy per spin is  $-1.267\,894$  and the value of the gap is  $0.554\,39$  (recall that for the Heisenberg model the gap has been estimated to be  $0.410\,50$ ). The general trend of the ground-state correlation functions is that they decay faster than those for the Heisenberg model (in the sense that the numerical values are smaller) both with distance for fixed  $N$  and as a function of the size of the system. The same happens for the  $S = 1/2$  case where the spectrum is gapless. A linear fit of  $\log C_{N/2}$  as a function of  $N$  yields a correlation length of the order of  $\xi = 3.1$ . This is an underestimate due to finite-size effects. Also, we performed complete diagonalization of systems up to eight sites to obtain the temperature dependence of the susceptibility and correlation functions [11]. The susceptibility is exponentially small at low  $T$  and the correlation functions also decay faster than those for the Heisenberg model as a function of temperature.

## 2. The model

In this work we consider a class of models of long-range interactions of the type  $1/r^\alpha$  but with alternating signs [16]. A simple and convenient way to implement periodic boundary conditions is to use the chord distance (that is the distance between the points when the chain is wrapped into a closed circle). We consider then the Hamiltonian [19]

$$H = - \sum_{i < j} (-1)^{i-j} \frac{\mathbf{S}_i \cdot \mathbf{S}_j}{[d(i-j)]^\alpha} \quad (1)$$

where  $d(i-j)$  is the chord distance  $d(i-j) = |\sin(i-j)\phi|/\phi$  with  $\phi = \pi/N$ , where  $N$  is the number of lattice sites in the chain. The leading term (nn) is antiferromagnetic but the

next-nearest-neighbour term (nnn) is ferromagnetic which tends to stabilize the dominant term. We take  $1 < \alpha < 3$ .

This class of long-range spin exchange models may describe impurity spins in a metallic host interacting via a RKKY interaction  $\sim \cos[2k_F r]/r^\alpha$  if the conduction electron band is half-filled. The value of the exponent  $\alpha$  in the case of non-interacting electrons is  $\alpha = d$  (where  $d$  is the dimensionality of the lattice). The case of interacting electrons has also been considered. In the case of the magnetic screening cloud around a single Kondo impurity in a Luttinger liquid ( $d = 1$ ),  $\alpha = g_c < 1$  [20] and in the case of the coupling between two impurity spins ( $S = 1/2$ ) coupled to a 1d Hubbard chain,  $\alpha = 2$  [21], for example.

To study model (1) we use the modified Lanczos algorithm [22] to obtain the ground-state properties and the gap to the first excited state and we use complete diagonalization of the Hamiltonian matrix to obtain the thermodynamics. In the modified Lanczos algorithm the size of the vectors can be considerably reduced using the symmetries of the problem. The Hamiltonian commutes with the total spin operators  $(S_T)^2$  and  $S_T^z$ , with the translation operator  $T$ , the spin-flip operator  $R$  and the reflection operator  $L$  ( $i \rightarrow N + 1 - i, i = 1, \dots, N$ ). The ground state has total  $S_T^z = 0$  and one of the (degenerate) first excited states also has  $S_T^z = 0$ . One can then immediately reduce the states under consideration to this subspace only [10]. A similar procedure can be used for the finite-temperature behaviour. We calculate the susceptibility

$$\chi = \frac{\beta}{3N} \sum_{i,j} \langle S_i \cdot S_j \rangle \quad (2)$$

and the correlation functions

$$C_m = \frac{3}{N} \sum_{i=1}^N \frac{\langle S_i^z S_{i+m}^z \rangle}{S(S+1)}. \quad (3)$$

Both diagonalizations give the exact results for the various finite-size systems. The results for the infinite system can be estimated using standard extrapolation methods [23] like the VBS method [24] or the BST method [25]. In the first method we want to estimate the limit of a finite sequence  $P_n$  ( $n = 1, \dots, N$ ). Defining

$$P_n^{(m+1)} = P_n^{(m)} + \frac{1}{Q_n^{(m)} - Q_{n-1}^{(m)}} \quad (4)$$

$$Q_n^{(m)} = \alpha_m Q_n^{(m-1)} + \frac{1}{P_{n+1}^{(m)} - P_n^{(m)}} \quad (5)$$

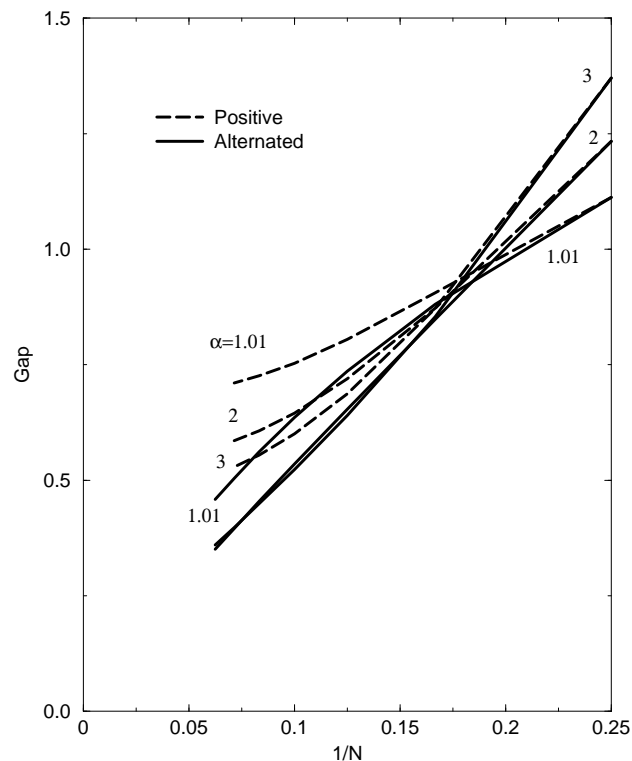
where  $Q_n^{(-1)} = 0$ ,  $P_n^{(0)} = P_n$ , we obtain an estimate of the sequence iterating. If  $\alpha_m = 0$  this is the Aitken–Shanks transformation which is adequate for exponential behaviour. To generate the Padé–Shanks transformation we select  $\alpha_m = 1$ . A power-law behaviour is well fitted choosing the Hamer and Barber transformation  $\alpha_m = -[1 - (-1)^m]/2$ . We get an estimate of the asymptotic value of the sequence  $P_n$  [23, 24] by selecting  $\alpha_m$  appropriately.

In the BST algorithm we look for the limit of a sequence of the type  $T(h) = T + a_1 h^\omega + a_2 h^{2\omega} + \dots$ , where  $h_N = 1/N$  is a sequence for the various system sizes,  $N$ . The value of the  $m$ th iteration for the sequence is obtained from

$$T_m^{(N)} = T_{m-1}^{(N+1)} + (T_{m-1}^{(N+1)} - T_{m-1}^{(N)}) / \left[ \left( \frac{h_N}{h_{N+m}} \right)^\omega \left( 1 - \frac{T_{m-1}^{(N+1)} - T_{m-1}^{(N)}}{T_{m-1}^{(N+1)} - T_{m-1}^{(N)}} \right) - 1 \right] \quad (6)$$

where  $\omega$  is a free parameter which is adjusted such that the estimate of the error

$$\epsilon = |T_{N_p-2}^{(1)} - T_{N_p-2}^{(0)}| \quad (7)$$



**Figure 1.** The gap as a function of  $1/N$  for the standard frustrating interaction (positive) and model (1) (alternating) for the values  $\alpha = 1.01, 2, 3$ .

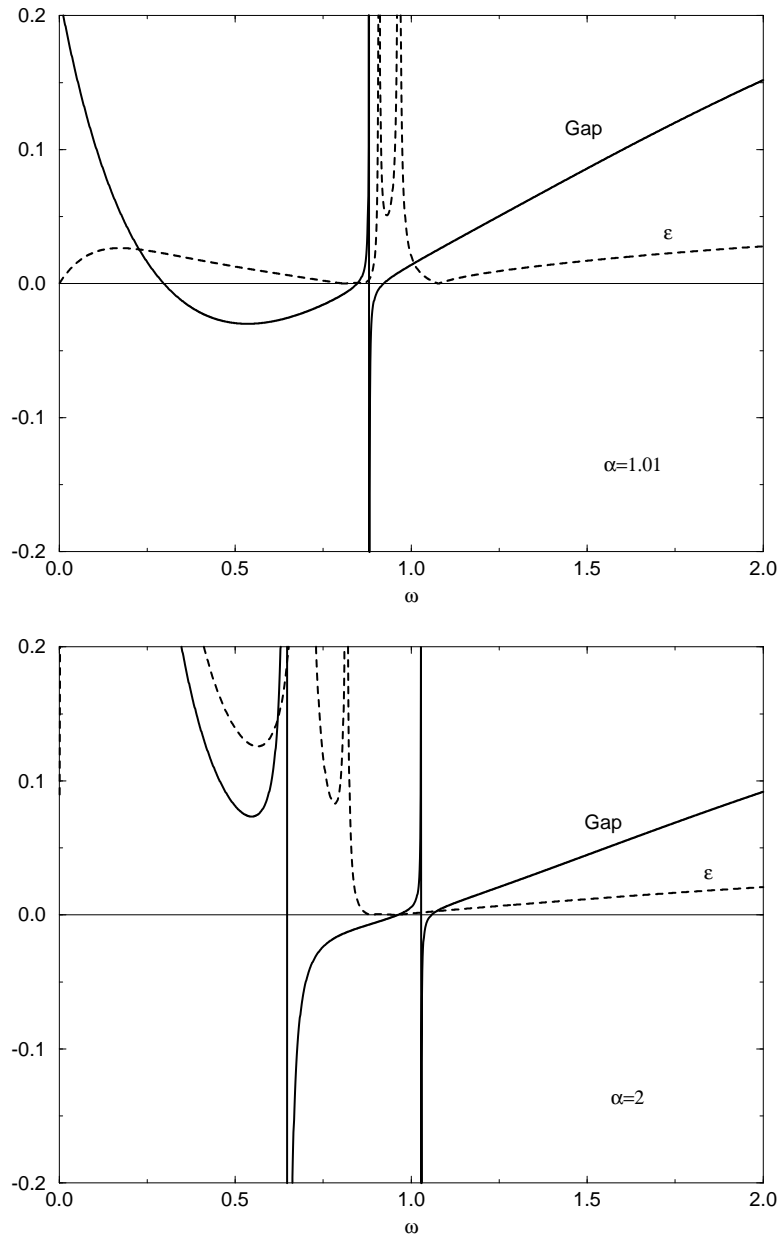
is a minimum (where  $N_p$  is the number of data points,  $T_{-1}^{(N)} = 0$  and  $T_0^{(N)} = T(h_N)$ ). It has been shown [25] that this algorithm has several advantages over the VBS algorithm, in particular for smaller sequences: it converges faster and it is less sensitive to rounding errors. In this paper we will use both methods to estimate the thermodynamic limit.

**Table 1.** The ground-state energy per spin and gap as functions of  $N$  for  $\alpha = 1.01, 2, 3$ .

$N$	$\alpha = 1.01$	$\alpha = 1.01$	$\alpha = 2$	$\alpha = 2$	$\alpha = 3$	$\alpha = 3$
	$-E_N/N$	Gap	$-E_N/N$	Gap	$-E_N/N$	Gap
4	2.059 5832	1.111 8877	2.158 9760	1.233 7006	2.297 6817	1.370 2968
6	2.359 5499	0.889 9970	2.052 3213	0.848 0498	1.917 9450	0.854 1843
8	2.581 1593	0.736 3615	2.000 5515	0.654 0099	1.767 2689	0.640 2738
10	2.758 0452	0.635 9315	1.970 7343	0.535 3366	1.692 0636	0.523 2326
12	2.905 6771	0.561 6502	1.951 6741	0.454 5769	1.649 0979	0.449 1504
14	3.032 5603	0.504 2410	1.938 5998	0.395 7728	1.622 2435	0.397 9216
16	3.143 9108	0.458 4054	1.929 1615	0.350 9020	1.604 3433	0.360 3571

### 3. Results

In table 1 we show the values for the ground-state energy and gap as functions of  $N$  (for  $N = 4$  to 16 and  $N$  even) for the values  $\alpha = 1.01, 2, 3$  [26]. In figure 1 we show the gap as a function of  $1/N$  for the standard frustrating case compared to the behaviour of the gap in the alternating case. The results suggest that these two cases are in different classes since



**Figure 2.** The gap and estimate of the error as a function of  $\omega$  for model (1) for the values  $\alpha = 1.01, 2, 2.3, 2.5, 2.7, 3$ .

the slopes for the two cases are distinct. In particular, it suggests that the alternating cases may extrapolate to a zero value of the gap as  $N \rightarrow \infty$  while the standard frustrating cases suggest a finite value in agreement with the results previously obtained for  $\alpha = 2$  [10]. In table 2 we show the VBS estimated values for the gap using the various extrapolations. For small and intermediate values of  $\alpha$  the power-law fit (Hamer and Barber) consistently gives very small gaps suggesting that the spectrum is gapless. As  $\alpha$  grows further ( $\alpha \geq 2.7$ ) we

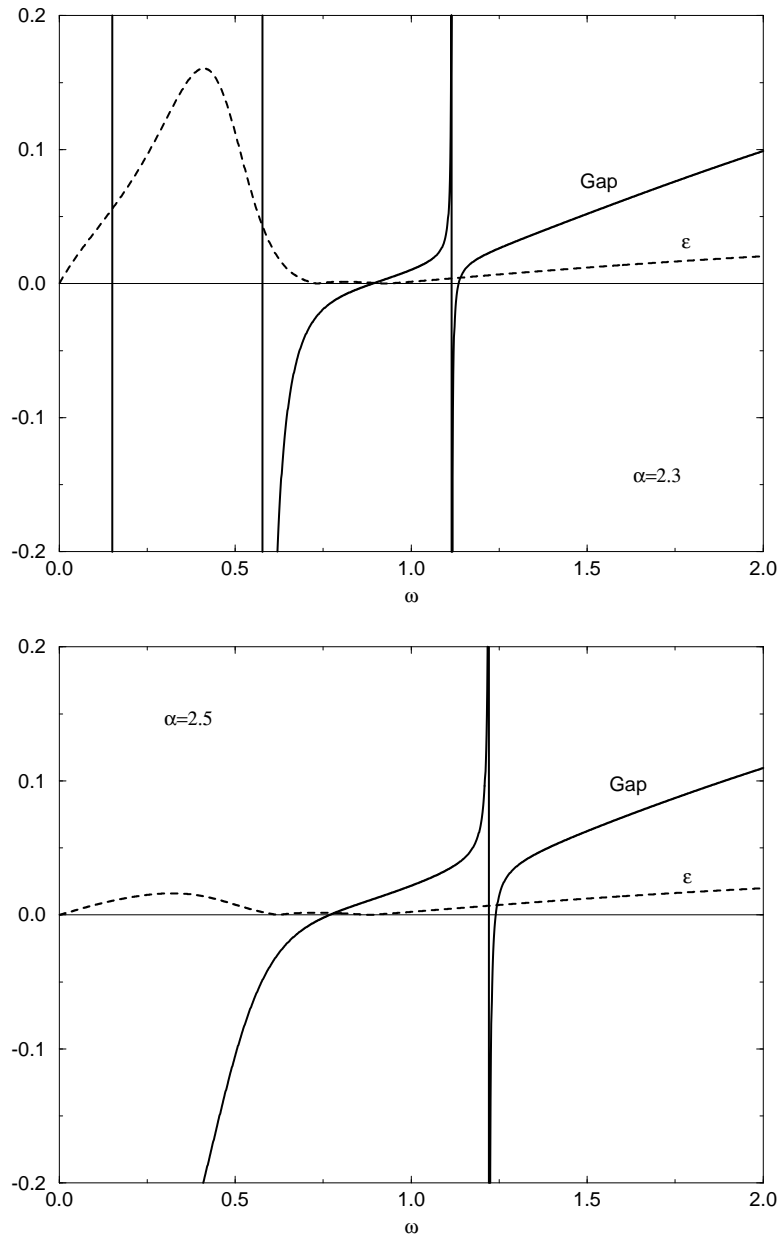
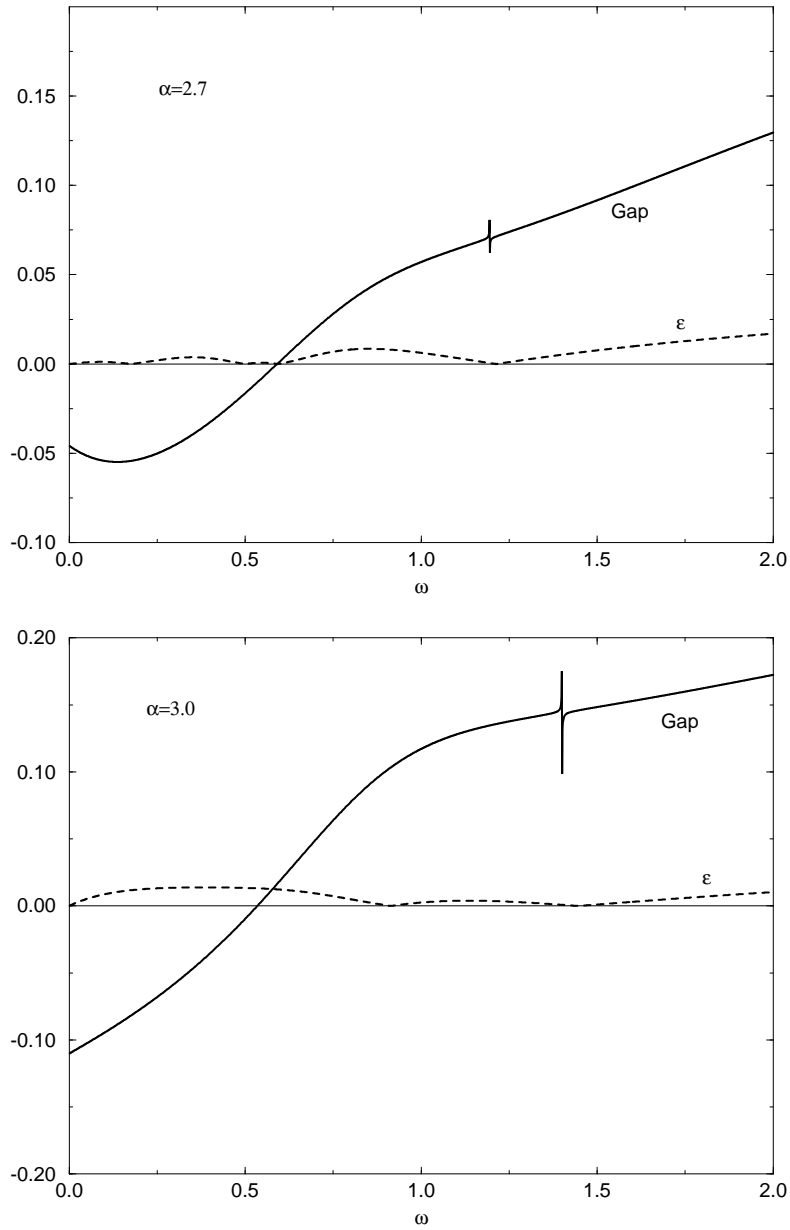


Figure 2. (Continued)

see that the gap increases and becomes apparently finite (we will return to this point later). The table shows consistently smaller gaps for the power-law fit as compared to the other two methods. If the spectrum is indeed gapless this is consistent since, for instance for the Aitken–Shanks transformation, one is trying to fit a power law with an exponential. In tables 3–5 we present the sequence of  $P_n^{(m)}$  obtained using the Hamer–Barber algorithm for  $\alpha = 2, 2.5, 3$ . The difference between the extrapolated value and the values for the previous iteration gives a measure for the error involved. Due to the small number of data points

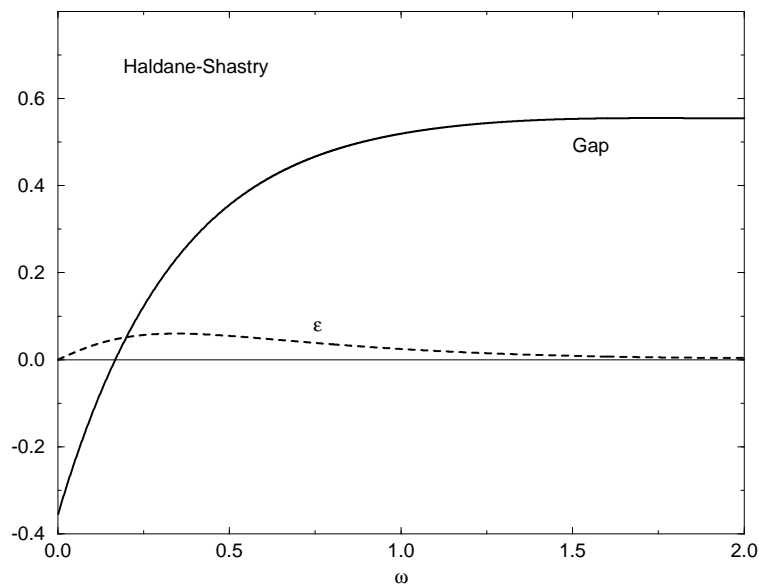


**Figure 2.** (Continued)

this difference is actually an order of magnitude larger than the extrapolated value itself (except for  $\alpha = 3$ ). Another possible criterion is to take the difference between the values for  $m = 2$ , but is also of the same order. The error in this procedure is therefore large.

To further clarify the nature of the spectrum and to have better control over the errors involved we consider now the BST algorithm, equation (6). In figure 2 we present the values of the gap as a function of the free parameter  $\omega$  for the various values of  $\alpha$  considered above. We also plot the error  $\epsilon$  defined in equation (7). In general, for each value of  $\alpha$  there are





**Figure 3.** The gap and estimate of the error as a function of  $\omega$  for the standard frustrating interaction (the Haldane–Shastry model).

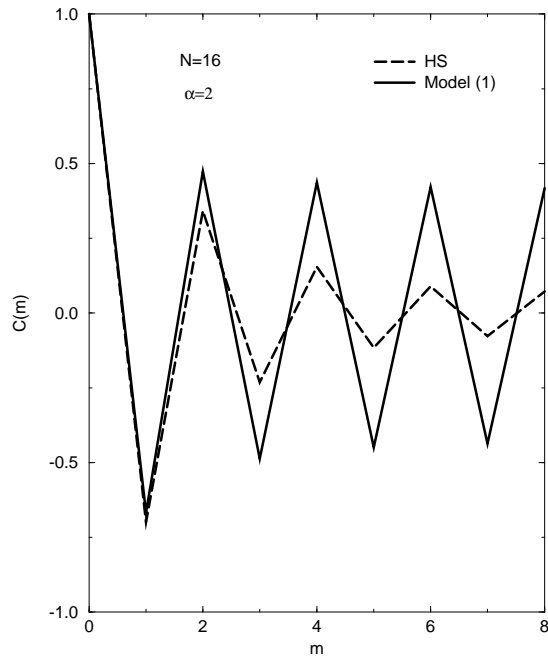
**Table 2.** Extrapolated values of the gap obtained using the VBS method.

	$\alpha_m = -[1 - (-1)^m]/2$	$\alpha_m = 1$	$\alpha_m = 0$
$\alpha = 1.01$	0.0658	0.2004	0.1254
$\alpha = 2.0$	-0.0142	0.1491	0.0742
$\alpha = 2.3$	0.0041	0.1571	0.0829
$\alpha = 2.5$	0.0065	0.1677	0.0925
$\alpha = 2.7$	0.0862	0.1850	0.1268
$\alpha = 3.0$	0.1701	0.2202	0.1845

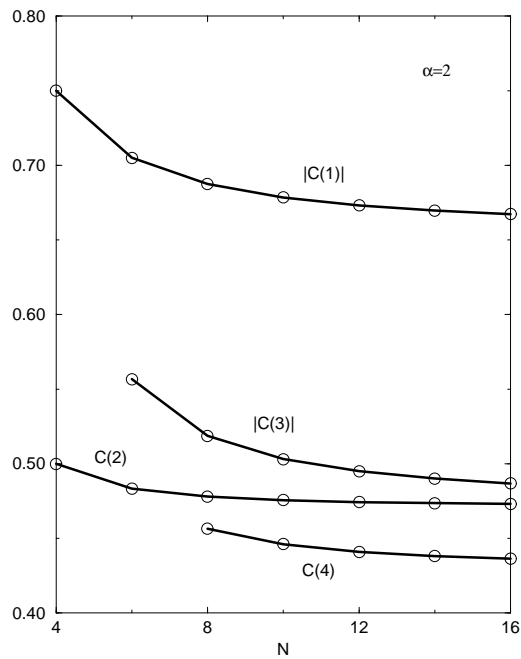
**Table 3.** Extrapolation iterations for the gap for  $\alpha = 2$  obtained using the Hamer–Barber algorithm.

$m$ :	0	1	2	3
	1.233 7006			
	0.848 0498	0.457 5103		
	0.654 0099	0.348 4716	0.181 7683	
	0.535 3366	0.282 5508	0.147 7233	-0.014 1768
	0.454 5769	0.238 2768	0.124 4493	
	0.395 7728	0.206 4011		
	0.350 9020			

several points in  $\omega$ -space where either the gap or the error go to zero or become very small. For each value of  $\alpha$  there is a point (actually a narrow region) where *both* are very small. First we take the value of  $\omega$  where the gap is very small and estimate its error, calculating  $\epsilon$  at that point. In table 6 we give the error  $\epsilon$  at the values of  $\omega$  chosen above for the values of



(a)



(b)

**Figure 4.** (a) The correlation functions  $C(m)$  as functions of  $m$  for  $N = 16$  and  $\alpha = 2$  for the Haldane–Shastry model (HS) and for model (1). (b) The correlation functions  $C(m)$  for  $m = 1, 2, 3, 4$  for  $\alpha = 2$  as functions of  $N$ .

**Table 4.** Extrapolation iterations for the gap for  $\alpha = 2.5$  obtained using the Hamer–Barber algorithm.

$m$ :	0	1	2	3
	1.300 2061			
	0.847 8680	0.470 7043		
	0.642 1958	0.360 7076	0.198 8730	
	0.523 3554	0.295 2211	0.164 0630	0.006 4759
	0.445 2184	0.251 5429	0.140 6424	
	0.389 5432	0.220 2066		
	0.347 6438			

**Table 5.** Extrapolation iterations for the gap for  $\alpha = 3$  obtained using the Hamer–Barber algorithm.

$m$ :	0	1	2	3
	1.370 2968			
	0.854 1843	0.488 8593		
	0.640 2738	0.381 8190	0.243 082	
	0.523 2326	0.321 3966	0.216 709	0.170 0793
	0.449 1504	0.283 0859	0.202 198	
	0.397 9216	0.257 0883		
	0.360 3571			

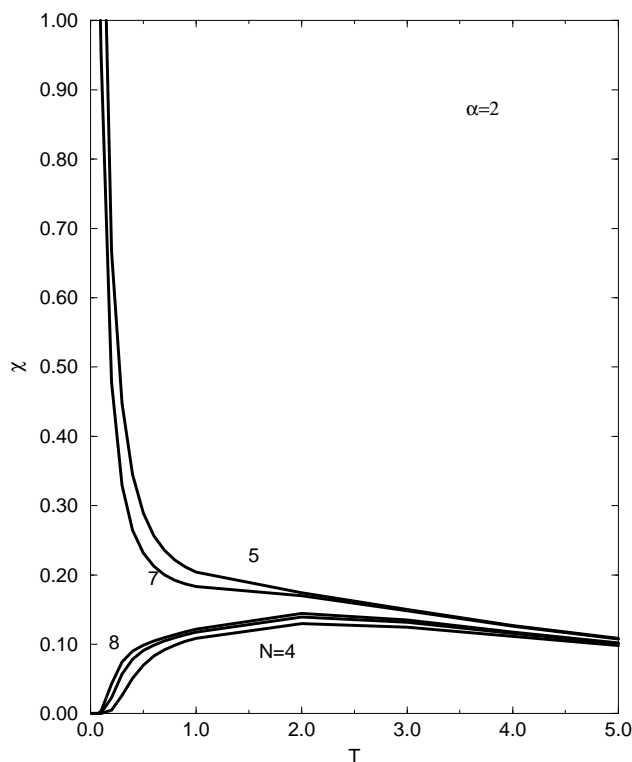
**Table 6.** Values of the error  $\epsilon$  defined in equation (7), for several values of  $\alpha$ , calculated at the values of  $\omega$  at which the gap goes through zero (smaller than  $1.0 \times 10^{-6}$ ) and where  $\epsilon$  is also small.

$\alpha$	$\omega$	Error ( $\epsilon$ )
1.01	0.846 448	0.000 68
2.0	0.962 115	0.000 17
2.3	0.890 129	0.000 66
2.5	0.768 180	0.001 58
2.7	0.590 684	0.000 05
3.0	0.534 526	0.013 18

$\alpha$ . We can also follow the standard method and select several local minima for  $\epsilon$  and take the gaps obtained at these points. The results are shown in table 7. They strongly suggest that the spectrum is gapless (at least for  $\alpha \leq 2.7$ ). The BST method is consistent with the VBS method for  $\alpha = 3$  in the sense that it suggests a finite gap (see however below).

Even though the results strongly suggest that the spectrum is gapless, it might appear that table 2 could be consistent with a finite gap (but a small one compared to that for the frustrated case [10]). However, if the gap were to be finite, the Hamer–Barber algorithm should yield a finite gap, as we obtained previously for the frustrated case [10], where all three algorithms correctly picked up the leading (finite) term of the sequence (see table 4 of reference [10]). As a further check we have used the BST algorithm to find the extrapolated gap for the standard Haldane–Shastry model ( $\alpha = 2$ , the frustrated case). The results are shown in figure 3. As a function of  $\omega$  the error decreases for  $\omega \sim 2$  and the gap is saturated to the value 0.554 05 (for  $\omega = 2$ ) very close to the (finite) result obtained previously [10].

When there is a true gap the extrapolation yields a finite value with a magnitude that is very close for the *four* algorithms (actually one might take the discrepancy of the extrapolations of table 2 as a sign that the gap is zero—i.e. there is no finite leading term in the sequence).



**Figure 5.** The susceptibility as a function of temperature for  $\alpha = 2$  for  $N = 4, 5, 6, 7, 8$ .

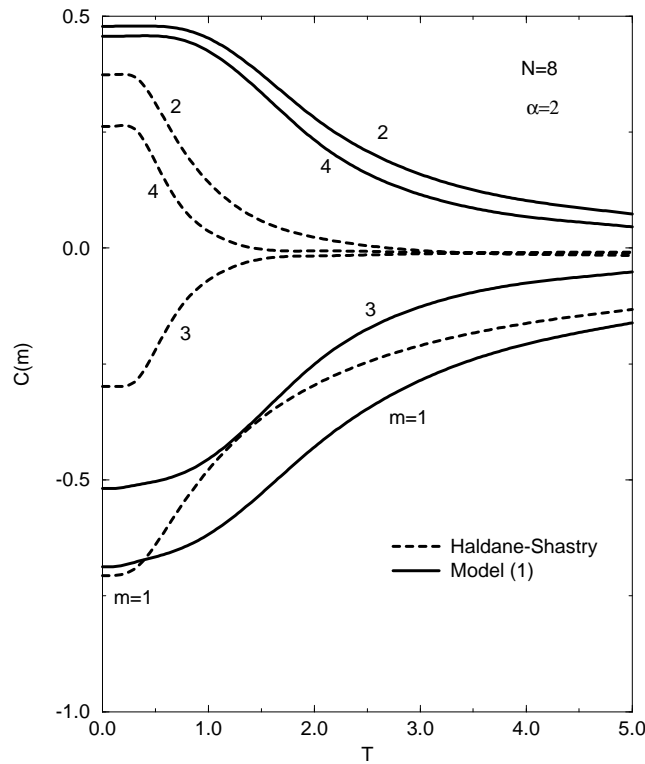
**Table 7.** Minima of the error  $\epsilon$ , equation (7), for several values of  $\alpha$  and the corresponding values of the gap. The minima of  $\epsilon$  (smaller than  $1.0 \times 10^{-5}$ ) that are close to the set of values of  $\omega$  shown in table 6 are highlighted in bold type. The absolute values of these results for the gap are the error estimates within the method.

	$\omega_1$	Gap	$\omega_2$	Gap	$\omega_3$	Gap
$\alpha = 1.01$	0.810	-0.007 4257	<b>0.864</b>	<b>0.007 9885</b>	1.077	0.025 4297
$\alpha = 2$	0.886	-0.006 7272	<b>0.955</b>	<b>-0.000 7323</b>		
$\alpha = 2.3$	0.733	-0.023 9250	<b>0.928</b>	<b>0.003 4268</b>		
$\alpha = 2.5$	0.622	-0.029 1923	<b>0.883</b>	<b>0.010 9872</b>		
$\alpha = 2.7$	0.500	-0.016 3724	<b>0.592</b>	<b>0.000 2422</b>	1.213	0.071 3413
$\alpha = 3$	<b>0.914</b>	<b>0.103 3700</b>	1.445	0.145 8258		

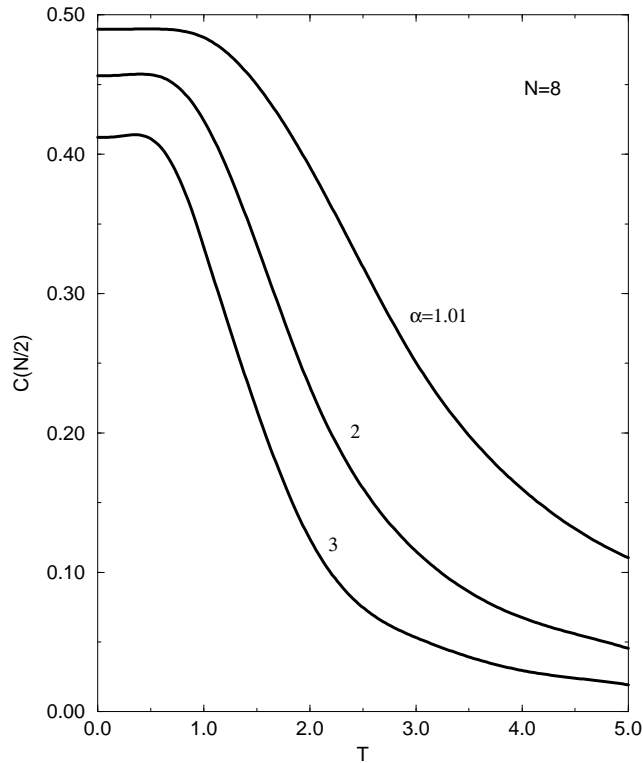
In table 8 we present the ground-state correlation functions for  $\alpha = 2$ . In figure 4(a) we show the ground-state correlation functions for  $\alpha = 2$  and  $N = 16$  for both cases showing that the decay is considerably slower in the alternating case. In figure 4(b) we show the correlation functions  $C(m)$  for  $m = 1-4$  as functions of  $N$  for  $\alpha = 2$ . The behaviour of  $|C(1)|$  is similar for the positive and alternating interactions (it is slightly smaller in

**Table 8.** The correlation functions  $C(m)$  for  $\alpha = 2$  for the set of values  $N = 4$  to 16 with  $N$  even.

$m$	$N$ :	4	6	8	10	12	14	16
1		-0.750 00	-0.705 02	-0.687 49	-0.678 51	-0.673 18	-0.669 70	-0.667 28
2		0.500 00	0.483 40	0.477 98	0.475 60	0.477 36	0.473 63	0.473 17
3			-0.556 77	-0.518 69	-0.503 16	-0.495 00	-0.490 08	-0.486 83
4				0.456 41	0.446 01	0.440 94	0.438 10	0.436 34
5					-0.479 88	-0.463 42	-0.454 58	-0.449 17
6						0.432 60	0.425 65	0.421 56
7							-0.446 04	-0.436 47
8								0.417 37

**Figure 6.** The correlation functions  $C(m)$  as functions of the temperature for the Haldane-Shastry model and for model (1) for  $N = 8$ .

the latter case). However, for  $m > 1$  the correlation functions  $C_{alt}(m)$  are considerably larger and reach their extrapolated values for much smaller system sizes. We estimate the correlation function exponent taking  $C(N/2) \sim (-1)^{N/2} 1/N^\eta$  [8] since for the system sizes considered it yields better results than a plot of  $C(m)$  as a function of  $m$  for fixed  $N$  [8]. We estimate  $\eta = 0.16, 0.24, 0.49$ , for  $\alpha = 1.01, 2, 3$ , respectively (taking a fit using the system sizes up to  $N = 16$  and excluding the  $N = 4$  point). Besides the alternating signal, the correlation functions are modulated by an oscillatory function that decreases in amplitude as  $N$  grows. Note that  $|C_{alt}(2m + 1)| > |C_{alt}(2m)|$  for  $m \geq 1$  due to the oscillatory nature



**Figure 7.** The correlation function  $C(N/2)$  as a function of the temperature for  $N = 8$  and  $\alpha = 1.01, 2, 3$ .

of the interaction (in figure 4(b) this is explicitly shown for  $|C(3)| > C(2)$ ).

In figure 5 we show the susceptibility as a function of temperature for  $\alpha = 2$ . For  $N$  even, the ground state is a singlet, but for  $N$  odd, is degenerate (a triplet) (as for the  $S = 1/2$  Heisenberg model). Therefore  $\chi$  alternates between zero and very large values at small  $T$ . Comparing with results obtained for other models (like the Heisenberg and the Haldane–Shastry models for integer and half-integer spins) this alternation suggests a gapless spectrum (in the case of a gap both the even and odd system sizes give a vanishing susceptibility at zero temperature). This would imply a finite value for the susceptibility (the extrapolation error is large and we do not estimate the zero- $T$  susceptibility). As  $\alpha \rightarrow 3$  we find the same type of behaviour indicating that there is no true gap and that the extrapolated results are a consequence of the finiteness of the systems studied. The reason for this is that the decay of the interaction is faster (and therefore the transition to gapless behaviour is slower) and the finite sizes considered are not large enough to correctly extrapolate to zero.

In figure 6 we show the correlation functions as functions of  $T$  for the positive case and the alternating case for  $\alpha = 2$ . Consistently with the ground-state results, the correlation functions also decay much more slowly with temperature in the alternating case. In figure 7 we show  $C(N/2)$  for  $N = 8$  for several values of  $\alpha$ .

In summary, we have identified a new class of integer spin chains that are gapless. The interaction is long ranged and non-frustrating. Indeed, the stabilizing ferromagnetic next-nearest-neighbour interaction changes the behaviour of the system qualitatively with

respect to an antiferromagnetic frustrating nnn interaction [10, 11]. We calculated the gap (for  $S = 1$ ) using a modified Lanczos method, finding a vanishing value in the extrapolated limit. We also found that the correlation functions have a considerably larger range both with distance and as a function of temperature. The results obtained may be useful for studying  $S = 1$  impurity spins embedded in a half-filled conduction electron matrix and coupled via a RKKY interaction.

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- [26] For  $\alpha < \alpha_s$  the energy per spin increases with the system size and for  $\alpha > \alpha_s$  it decreases, where  $\alpha_s \sim 1.693$ .