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Haldane gap in a S=1 exchange model with long-range interactions

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Abstract. The ground-state properties of the $S = 1$ Haldane-Shastry model are studied using a modified Lanczos algorithm and diagonalizing exactly small chains. We find evidence that, as for the antiferromagnetic Heisenberg model, the spectrum shows a gap, in contrast to the $S = \frac{1}{2}$ case. The correlation functions $< S^z(0)S^z(m) >$ decay exponentially for large m. We find that the correlation functions for the Haldane-Shastry model decay faster than for the Heisenberg model. We estimate the infinite system limit for the ground-state energy, value of the gap and correlation functions.

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The $S = \frac{1}{2}$ Haldane-Shastry model [1,2] has attracted considerable attention since it is an integrable model that belongs to a class of systems with long-range interactions. The ground-state energy and correlation functions have been obtained [1-3] together with the thermodynamics [4]. The ground-state wave function is a spin singlet of the Jastrow-Gutzwiller form. The excitations are spin-$\frac{1}{2}$ spinons [4] that form a gas of a semionic nature [4,5]. 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 model solvable in greater detail than the short-range Heisenberg counterpart, solvable by the traditional Bethe ansatz method.

On the other hand, the similarities to the Heisenberg model lead to the interest in studying the model for higher values of the spin. In particular, the case of spin $S = 1$ (and in general the integer spin cases) are of interest since it has been established on general grounds and verified explicitly for short-range interactions, that these values are qualitatively different from the half-integer ones due to the Haldane gap [6].
The model Hamiltonian is a periodic version of $\frac{1}{r^2}$ exchange given by

$$H = J\phi^2 \sum_{i<j} \frac{\mathbf{S}_i.\mathbf{S}_j}{\sin^2[\phi(i-j)]} \tag{1}$$

where $\phi = \frac{\pi}{N}$ with N the number of lattice spins with lattice constant 1. We consider only the antiferromagnetic case $J = 1$.

In this paper we consider the $S = 1$ Haldane-Shastry model (HS) and study the ground-state properties. We use a modified Lanczos method [7,8] to obtain the ground-state and first excited state energies and the correlation functions for small systems of size up to 16 spins. We compare our results to those previously obtained for the Heisenberg case stressing the similarities and differences. We estimate the large system size limit of these quantities using the extrapolation method of Vanden Broeck and Schwartz (VBS) [9-11].

The exact energy spectrum has been obtained for the $S = \frac{1}{2}$ case [1-4]. The groundstate is a spin singlet with energy [2]

$$\frac{E}{NJ} = -\frac{\pi^2}{24}\left(1 + \frac{5}{N^2}\right) \tag{2}$$

with a $\frac{1}{N^2}$ correction like for the Heisenberg model [11]. The first excited state for N even and for the Heisenberg model is a $S_T = 1$ triplet where S_T is the total spin of a N-spin state. In the case of the HS model the first excited state is however a $S_T = 1$ quartet. (For N odd the groundstate is a quartet for both models). The full spectrum has been obtained [4] showing a supermultiplet structure such that the energies in units of $\frac{1}{4}\left(\frac{\pi}{N}\right)^2$ are integers [1]. A set of states with N_{sp} spin-$\frac{1}{2}$ spinon excitations with $S_T = S_T^z = \frac{N_{sp}}{2}$ (with $M = (N - N_{sp})/2$ reversed spins) generates the full energy spectrum [4].

The Hamiltonian (1) can be exactly diagonalized if we consider small chains [1]. For spin-S we have a basis of $(2S + 1)^N$ states which grows very fast as S and N grow. Taking $N \leq 8$ we have obtained the full spectrum for $S = 1$. For N even, the groundstate is again a singlet and the first excited state is a $S_T = 1$ triplet, as for the Heisenberg case. For N odd the groundstate is a singlet in both models.

Since the size of the matrices to diagonalize increases exponentially with the size of the chain, we used the modified Lanczos method [7] to obtain the groundstate and the

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first excited state energies, together with the groundstate correlation functions.

The size of the vectors can be considerably reduced using the symmetries of the problem. The Hamiltonian commutes with the total spin operators $(\mathbf{S}_T)^2$ and S_T^z, with the translation operator T, the spin flip operator R and the reflection operator L ($i \to N+1-i, i = 1, \ldots, N$). 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.

The operators T and L commute with R, i.e. one has $[T, R] = [L, R] = 0$, but they do not commute with each other, since $LT = T^{-1}L$. The ground state eigenvalues are $r = l = 1$ and $t = 1$, corresponding to an wavevector $k = 0$. The first excited state has $r = l = -1$ and $t = -1$, corresponding to $k = \pi$ (for an even number of lattice points).

Although in general the operator L mixes k and $-k$ states, the ground state and the first excited state under consideration are simultaneous eigenvectors of the operators T, R and L.

The action of the local operators $S_i^{\pm}$ and S_i^z is simply given in the direct product basis $|m_1^z > \cdots |m_N^z >$. In general, these states are not eigenvectors of these additional symmetries. One forms then the classes of states which are closed under them. One starts with a state $|a>$, applies the translation operator T n_t times until one finds $T^{n_t}|a> = |a>$, where n_t is necessarily a divisor of N. One proceeds similarly with the operators R and L for which $n_r = 1, 2$ and $n_l = 1, 2$. The multiplicity of this class is $n_t n_r n_l$. The state $|a>$ is then the representative of this class. The other classes are formed proceeding in the same manner starting with other states, not already used, until the state space is exhausted. An eigenvector of the operator T (with eigenvalue t obeying to $t^{n_t} = 1$) is obtained applying to its representatives the symmetrization operator $\Omega_t' = (1 + t^{-1}T + (t^{-1}T)^2 + \cdots + (t^{-1}T)^{n_t - 1})$. For the states in this class we have $\Omega_t' = \frac{1}{s_t(a)}\Omega_t$, where the general operator $\Omega_t = (1 + t^{-1}T + (t^{-1}T)^2 + \cdots + (t^{-1}T)^{N-1})$ and $s_t(a) = N/n_t$ is the symmetry factor. The same applies to the operators R and L. As stated above, when $t = \pm 1$ it is possible to construct a simultaneous eigenvector of the operators T, R and L. In the cases in which the operator R or L does not introduce new states ($n_r = 1$ or $n_r = 1$) one should verify that the eigenvalues induced by the first operator(s) are compatible with those of the other operator(s). This allows to reduce even further the number of classes. Any eigenvector with these eigenvalues is completely defined by its projections on the representatives of the classes.

The method goes as follows [7]. To obtain an approximate ground state wave function we choose a trial wave function ψ_0 that can not be orthogonal to the true groundstate. We define a state ψ_1 as [7]

$$\psi_1 = \frac{\hat{H}\psi_0 - < H > \psi_0}{\left(< H^2 > - < H >^2\right)^{1/2}} \tag{3}$$

where $< \psi_1|\psi_1 > = 1$, $< \psi_1|\psi_0 > = 0$ and $< H^n > = < \psi_0|\hat{H}^n|\psi_0 >$. Defining a matrix of the Hamiltonian in the basis ψ_0, ψ_1 we can diagonalize it [7] obtaining a next order approximation for the energy ϵ_1, and ground state wavefunction $\tilde{\psi}_0$, with

$$\epsilon_1 = < H > + b\alpha \tag{4}$$

$$\tilde{\psi}_0 = \frac{\psi_0 + \alpha\psi_1}{\left(1 + \alpha^2\right)^{1/2}} \tag{5}$$

where

$$b = \left(< H^2 > - < H >^2\right)^{1/2} \tag{6}$$

$$\alpha = f - \left(f^2 + 1\right)^{1/2} \tag{7}$$

and

$$f = \frac{< H^3 > - 3 < H >< H^2 > + 2 < H >^3}{2\left(< H^2 > - < H >^2\right)^{3/2}}. \tag{8}$$

Taking $\tilde{\psi}_0$ as the new ψ_0 we can iterate the method to obtain a better estimate for the energy and ground state wave function.

For the first excited state we proceed in a similar manner, starting from a trivial wave function orthogonal to the true ground state (as guaranteed by some symmetry argument), but not orthogonal to the true first excited state. For small chains, where the use of the symmetries is not strictly necessary, one can look for the excited state with $S_T^z = 1$, which is necessarily orthogonal to the ground state. However, for larger chains one has to take into account the different symmetries, and with the additional eigenvalues one can still look for the $S_T^z = 0$ first excited state, as explained above.

Since the complete Hamiltonian commutes with the operators T, R and L only transitions to the classes constructed above are allowed, even if separate terms allow them. The action of the Hamiltonian on a state is obtained writing, within each class, $H\Omega'|a> = \frac{1}{s(a)}\Omega H|a>$, where Ω is the product of the three symmetry operators for T, R, and L. If $H|a> = \sum_b \alpha L^{p_l} R^{p_r} T^{p_t}|b>$, where $p_{l,r,t}$ are integers and $|b>$ is the representative of a class, one finally finds $< b|H\Omega'|a> = \sum_b \frac{s(b)}{s(a)}\alpha l^{p_l} r^{p_r} t^{p_t}$. One also has to take into account the multiplicity of the classes when normalizing states and making inner products of states.

The accuracy of the method was tested against the exact diagonalization of the full spectrum for sizes up to $N = 8$. We considered system sizes up to $N \leq 16$ (with N even).

This procedure gives the results for the several finite-size systems. We are however interested in the infinite system limit and standard extrapolation methods [9] have to be used like the VBS method [9,10]. In this method we want to estimate the limit of a finite sequence P_n ($n = 1, ..., N$). Defining

$$P_n^{(m+1)} = P_n^{(m)} + \frac{1}{Q_n^{(m)} - Q_{n-1}^{(m)}} \tag{9}$$

$$Q_n^{(m)} = \alpha_m Q_n^{(m-1)} + \frac{1}{P_{n+1}^{(m)} - P_n^{(m)}} \tag{10}$$

where $Q_n^{(-1)} = 0$, $P_n^{(0)} = P_n$ we obtain an estimate of the sequence iterating (like the recursive rule due to Wynn). If $\alpha_m = 0$ this is the Aitken-Shanks transformation which is adequate for exponential behavior. To generate the Padé-Shanks transformation we select $\alpha_m = 1$. A power law behavior is well fitted choosing the Hamer and Barber's transformation $\alpha_m = -[1 - (-1)^m]/2$. We get an estimate of the asymptotic value of the sequence P_n [9,10] selecting α_m appropriately.

Table 1. Groundstate energy and groundstate energy per spin as a function of N

N	$-E_N$	$-E_N/N$
4	6.168503	1.542126
6	8.270682	1.378447
8	10.59553	1.324441
10	13.00953	1.300953
12	15.46690	1.288908
14	17.94784	1.281988
16	20.44263	1.277664

Table 2. Extrapolated values for $-E_N/N$ for the Hamer-Barber (H-B), Padé-Shanks (P-S) and Aitken-Shanks (A-S) transformations (9,10)

$H-B$	$P-S$	$A-S$
1.263147	1.267894	1.265328

Table 3. Gap between the groundstate and the first excited state as a function of N

N	Gap	Gap/N
4	1.2337	0.30843
6	0.87226	0.14538
8	0.71962	0.08995
10	0.64551	0.06455
12	0.60678	0.05057
14	0.58550	0.04182
16	0.57333	0.03583

Table 4. Extrapolated values for the gap for the Hamer-Barber (H-B), Padé-Shanks (P-S) and Aitken-Shanks (A-S) transformations (9,10)

$H-B$	$P-S$	$A-S$
0.55045	0.55439	0.55285

i) Ground-state wnergy

In Table 1 we show the values for the groundstate energy of the $S = 1$ Haldane-Shastry chain with sizes $N = 4$ to 16 (N even). A linear fit of the groundstate energy per spin as a function of $\frac{1}{N^2}$ yields (1.2568 ± 0.0016). Using the more accurate VBS method yields the results shown in Table 2. These results indicate that the behavior is not purely $\frac{1}{N^2}$ in contrast to the $S = \frac{1}{2}$ case. Other terms have to be included, particularly for small values of N. Since the spectrum has a gap (see below) we expect that the exponential behavior is more adequate [12,13]. It has been found for the Heisenberg model [13] that $\alpha_m = 1$ yields the best results. This has been found looking at the decay length at size N and requiring that

$$\xi(n,m) = \frac{2}{\ln\left(\frac{P_{n-1}^{(m-1)} - P_n^{(m-1)}}{P_n^{(m-1)} - P_{n+1}^{(m-1)}}\right)} \tag{11}$$

be such that

$$\xi(n,m) < \xi(n+1, m-1). \tag{12}$$

Only the Padé-Shanks transformation yielded consistent results [13]. In our case, however, all three cases yielded consistent tables and therefore we include the three choices.

ii) Gap

We consider now the gap (the difference in energy between the first excited state and the groundstate). In Table 3 we give the values of the gap as a function of N for the Haldane-Shastry model. In Fig. 1 we show the gap and the gap per spin as a function of N for the two models. The results seem to indicate that the gap is finite for both models in the $N \to \infty$ limit in agreement with Haldane's conjecture [6] and with previous results for the Heisenberg case. The VBS extrapolated values are shown in Table 4. In the case of the gap the Padé-Shanks yields once again consistent results but the other two do not obey (12) for the last iteration of (9,10). We recall that, for comparison, the value of the gap for the Heisenberg model is 0.41050 [13,14]. The extrapolated value of the gap per spin is close to but not zero due to the small number of points considered.

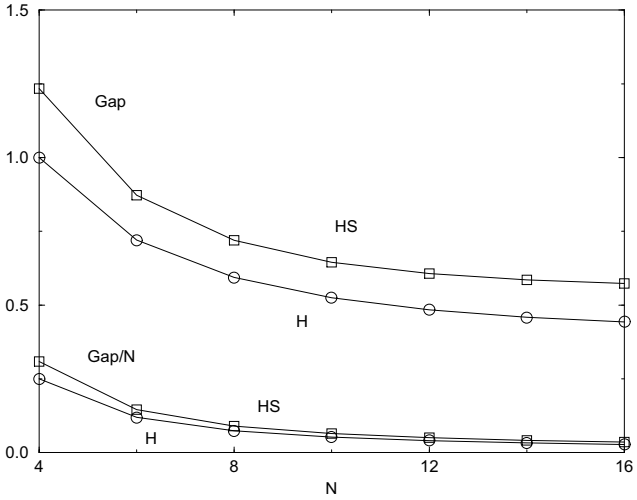

Fig. 1. Gap and gap per spin for both models, Heisenberg (H) and Haldane-Shastry (HS), as a function of N

iii) Correlation functions

The groundstate correlation functions are defined by

$$C_m(N) = \frac{3}{N} \sum_{i=1}^{N} \frac{< S_i^z S_{i+m}^z >}{S(S+1)} \tag{13}$$

In Table 5 we show them for the same set of system sizes and in Table 6 the VBS extrapolated values.

In Fig. 2 we compare the correlation functions with those for the Heisenberg model. For a finite system the energy scale of the two models is not the same. However, in the infinite system limit the nearest-neighbor interaction is the same. We feel therefore that it is worthwhile to compare the behavior for the two models. In Fig. 2a $|C_1|$ is displayed as a function of N; in Fig. 2b we show C_2 also as a function of N and in Fig. 2c we show C_m for $N = 16$ as a function of m. The general trend is that, in spite of the long-range nature of the interaction, the correlation functions for the Haldane-Shastry model decay faster (in the sense that the numerical values are smaller) than those for the Heisenberg model. A possible interpretation is that, similarly to the $S = \frac{1}{2}$ case, there may be an absence of interactions between the spinons.

It has been argued that the behavior of the correlation functions $C_{N/2}$ when $N \to \infty$ reflects their behavior with

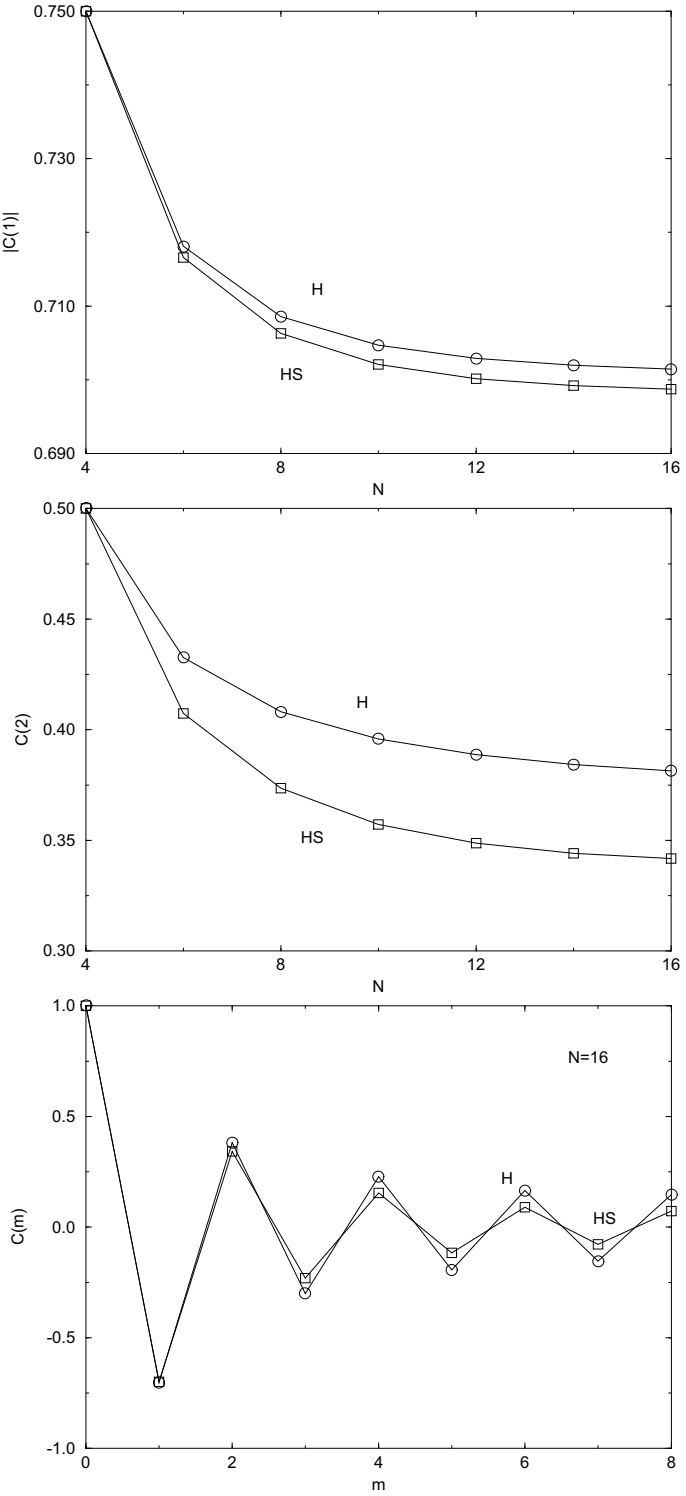

Fig. 2a–c. Correlation functions for the Heisenberg (H) and Haldane-Shastry (HS) models for **a** $|C_1|$, **b** C_2 as a function of N and **c** C_m for $N = 16$ vs. m

distance in the infinite system [15,8]. If there is a gap in the spectrum it is expected that

$$\lim_{m\to\infty} |C_m| \sim Be^{-\frac{m}{\xi}} \tag{14}$$

instead of the power-law behavior observed in the $S = \frac{1}{2}$ case (in both models). In Fig. 3 we plot $\ln|C_{N/2}|$ vs. N

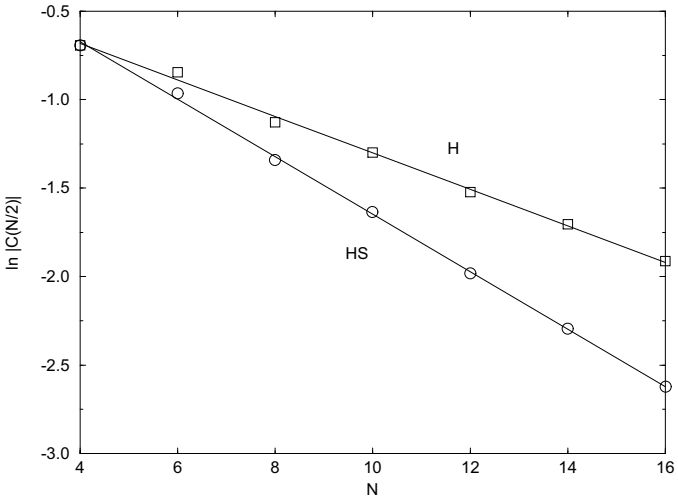

Fig. 3. The logarithm of the correlation function $C_{N/2}$ as a function of N for the Heisenberg (H) and Haldane-Shastry (HS) models. The solid line is the linear fit showing the exponential behavior

for both models. A linear fit yields for the Haldane-Shastry model

$$\ln|C_{N/2}| = (-0.02 \pm 0.02) - (0.162 \pm 0.0019)N \tag{15}$$

which corresponds to a correlation length of the order of $\xi = 3.1$. A similar analysis for the Heisenberg model gives ξ_H of the order of 4.9. The quality of the fits is similar for both models. However, the correlation length for the Heisenberg model has been estimated to be $\xi_H = 6.03$ [14] obtained from a fit to the large distance limit of the Bessel function $K_0(r/\xi)$, which asymptotically behaves as $\sim (\xi/r)^{1/2}e^{-r/\xi}$, and, therefore, a plot like in Fig. 3 underestimates the correlation length for the Heisenberg model.

In Fig. 4a we show $\ln|C(m)|$ as a function of m for $N = 16$. At large m we expect an exponential decay of the form of (14) with possible corrections. It is clear that the exponential behavior has not been fully reached. The exponential behavior is probably, as for the Heisenberg model, only to leading order. We have tried several functional forms like those for the Heisenberg model. In Fig. 4b we plot $F(m) = \ln(|C(m)|m^{1/2})$ as a function of m for $N = 16$. It is clear that for these system sizes the fit is poor even for the Heisenberg model. One requires larger systems to reach the limiting behavior. Note, however, that the functional form for the Haldane-Shastry has not been determined and therefore the numerical results are not conclusive to extrapolate to the large N limit. On the other hand, the linear fit of Fig. 3 is quite good for both models. We take the value obtained for ξ for the Haldane-Shastry model to be the estimate obtained by this fit.

Larger system sizes and the appropriate functional form are therefore required to more accurately determine the correlation length for the Haldane-Shastry model.

In summary, in this work we have studied the ground-state of the $S = 1$ Haldane-Shastry model, which has been recently presented [1,2] and solved exactly for $S = \frac{1}{2}$. The importance of the model lies on the fact that it belongs to a new class [5] of integrable systems. We have confirmed that, according to arguments by Haldane, the model shows a finite gap in the energy spectrum. We based our result on the

Table 5. Correlation functions C_m for the set of values N = 4 to 16 with N even

N	4	6	8	10	12	14	16
m							
1	−0.75000	−0.71660	−0.70630	−0.70210	−0.70017	−0.69923	−0.69876
2	0.50000	0.40744	0.37357	0.35722	0.34872	0.34420	0.34177
3		−0.38168	−0.29832	−0.26270	−0.24504	−0.23586	−0.23099
4			0.26209	0.20479	0.17697	0.16261	0.15501
5				−0.19443	−0.14946	−0.12729	−0.11582
6					0.13797	0.10601	0.08972
7						−0.10088	−0.07720
8							0.07251

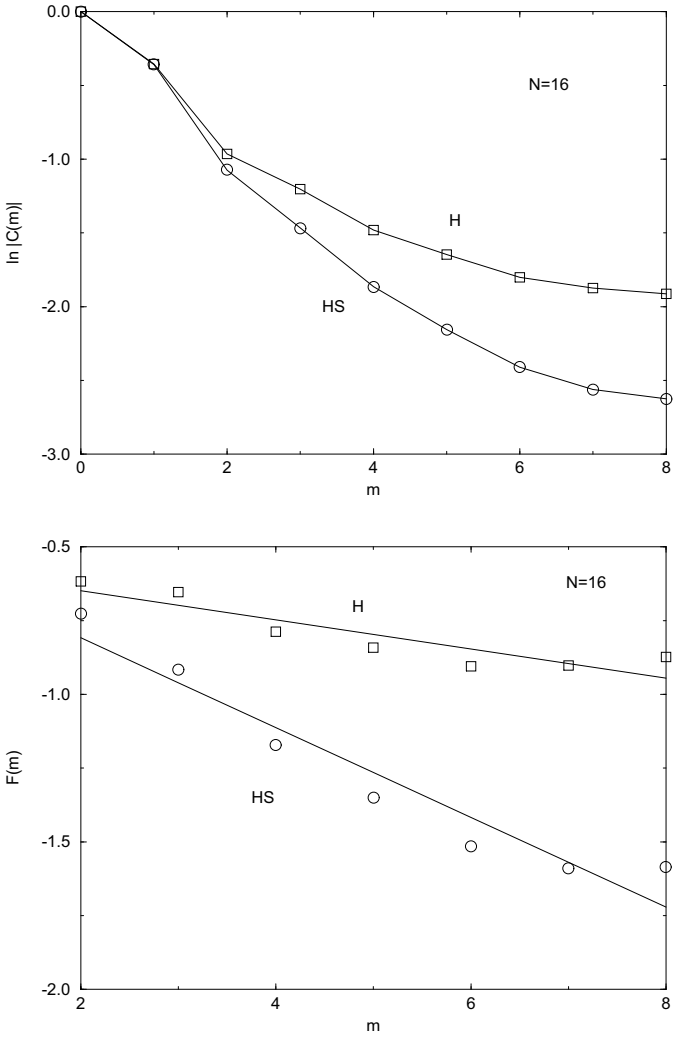

Fig. 4. a The logarithm of the correlation functions $|C(m)|$ and **b** $F(m) = \ln(|C(m)|m^{1/2})$ as a function of m for N = 16 for the Heisenberg (H) and Haldane-Shastry (HS) models

Table 6. Extrapolated values for the correlation functions C_m for the same set of values of N using the Hamer-Barber (H-B), Padé-Shanks (P-S) and Aitken-Shanks (A-S) transformations (9,10)

m	$H-B$	$P-S$	$A-S$
1	−0.69829	−0.69828	−0.69827
2	0.33890	0.33887	0.33893
3	−0.22531	−0.22559	−0.22546
	−0.22533	−0.22536	−0.22534
4	0.14616	0.14624	0.14620
5	−0.10573	−0.10573	−0.10573
	−0.10352	−0.10352	−0.10352
6	0.07279	0.07279	0.07279

extrapolated value of the calculated gap for various small chains and on the exponential behavior of the correlation function $C_{N/2}$ with N. We have also obtained, by comparison to the Heisenberg case, that the correlation functions for the Haldane-Shastry model decay faster as a function of both m and N. The same happens in the $S = 1/2$ case where the spectrum is gapless. This is due to the oscillatory nature of the (positive) interaction in this model. The estimated correlation length is smaller for the Haldane-Shastry model and the value of the gap is larger than for the Heisenberg model. These exact numerical results further extend the similarities and differences between the two models for a case (S = 1) which is not exactly solvable, in contrast to the $S = \frac{1}{2}$ case.

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