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Finite-temperature correlation functions of the Haldane–Shastry model

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Abstract. Using numerical diagonalization of small systems we obtain the thermodynamics of the $S = \frac{1}{2}$ and $S = 1$ Haldane–Shastry (HS) model. We study the correlation functions and the susceptibility and compare them with the results for the Heisenberg (H) model. We find evidence that in the $S = 1$ case the low-T susceptibility decays exponentially to zero, indicating the existence of a gap, in agreement with our earlier study of the ground-state properties. The correlation functions $\langle S^z(0)S^z(m)\rangle$ for the HS model decay faster than for the Heisenberg case, with both m and temperature for both values of the spin. For large T all correlation functions for the HS model become negative.

1. Introduction

Exact solutions have provided a key understanding to quantum systems. In particular, low-dimensional systems have been solved exactly with techniques like the Bethe *ansatz* and conformal field theories. The Bethe *ansatz* generally applies to models involving local (contact) interactions. Another important class of integrable models involves long-range interactions of the $1/r^2$ type [1]. Among these, the lattice Haldane–Shastry [2, 3] model and its generalizations have attracted considerable interest. The model Hamiltonian is given by

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

where $\phi = \pi/N$, with N the number of lattice sites and with lattice constant 1. In the large-N limit the nearest-neighbour interaction is equal to the interaction in the Heisenberg model (for the same J).

In the $S = \frac{1}{2}$ case, the energy spectrum has been solved exactly [2–4]. The ground-state wavefunction 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 ground-state correlation functions have been obtained [2, 6] as well as the thermodynamics [4].

Higher values of the spin are also of interest. An exact solution is, however, not available for $S > \frac{1}{2}$. Another method that has been thoroughly used is numerical diagonalization of

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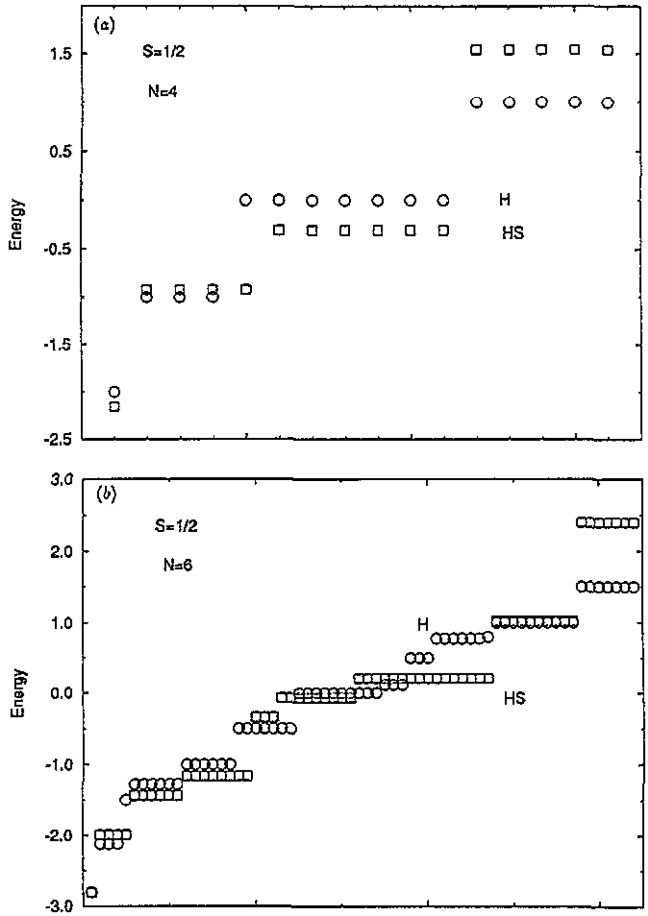


Figure 1. Set of energy values for $S = \frac{1}{2}$, (*a*) $N = 4$ and (*b*) $N = 6$ for the Heisenberg (H) and Haldane–Shastry (HS) models.

small systems. This method yields exact results for systems of increasing size, and the results for the infinite system can be estimated using standard extrapolation techniques [7].

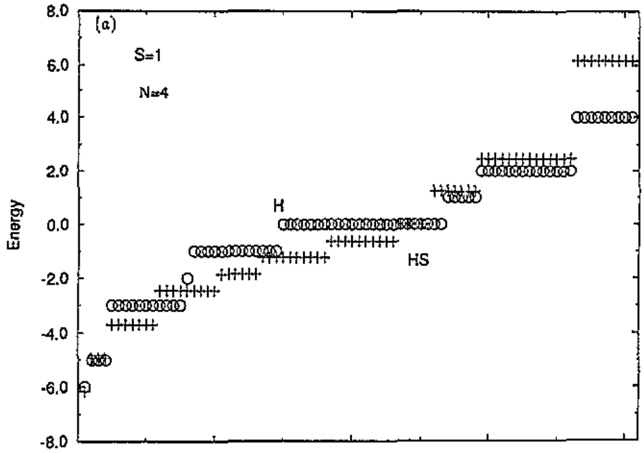
In this paper we exactly diagonalize small chains of sizes $N \leqslant 10$ for $S = \frac{1}{2}$ and $N \leqslant 8$ for $S = 1$. We obtain the full spectrum of energies and the wavefunctions, and study the thermodynamics. In particular, we calculate the correlation functions and the susceptibility, for both values of the spin.

The case of spin 1 is particularly interesting since, in contrast to the $S = \frac{1}{2}$ case, a Haldane gap is expected in the spectrum [8]. This result has now been confirmed by several authors for the case of short-range interactions and, recently, for the $S = 1$ Haldane–Shastry model [9], verifying that the ground-state correlation functions $\langle S^z(0)S^z(m)\rangle$ decay exponentially with m.

We want to calculate thermodynamic averages of the type

$$\langle \hat{A} \rangle = \frac{\mathrm{Tr}(\hat{A}\, \mathrm{e}^{-\beta \hat{H}})}{\mathrm{Tr}(\mathrm{e}^{-\beta \hat{H}})}. \tag{2}$$

Using a basis of states



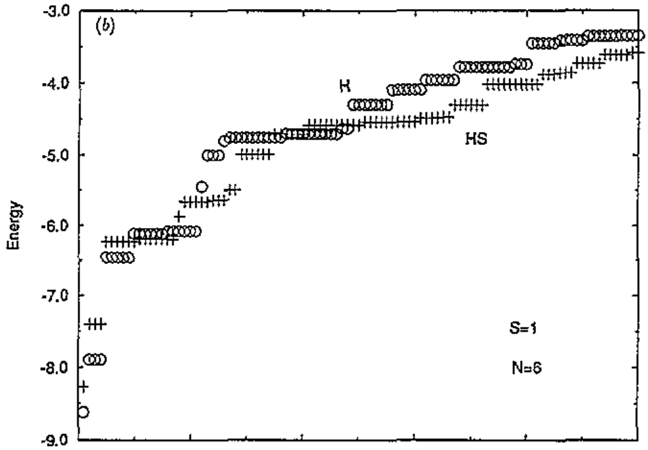


Figure 2. Set of energy values for (*a*) $S = 1$, $N = 4$ and (*b*) the first 100 levels for $N = 6$, $S = 1$ for the Heisenberg (H) and Haldane–Shastry (HS) models.

$$|l\rangle = |m_1, m_2, \ldots, m_N\rangle \tag{3}$$

where m_i are the S_i^z projections of the spin at site i ($i = 1, \ldots, N$), we can diagonalize the Hamiltonian matrix $\langle l|\hat{H}|l'\rangle$. Introducing $\hat{H}|m\rangle = E_m|m\rangle$, we can calculate the average (2) as

$$\langle \hat{A} \rangle = \frac{\sum_m \langle m|\hat{A}|m\rangle \mathrm{e}^{-\beta E_m}}{\sum_m \mathrm{e}^{-\beta E_m}} \tag{4}$$

with

$$\langle m|\hat{A}|m\rangle = \sum_{l,l'} \langle m|l\rangle \langle l|\hat{A}|l'\rangle \langle l'|m\rangle \tag{5}$$

or simply acting with the operator $\hat{A}$ on the states $|m\rangle$ expressed as a linear combination of the $|l\rangle$ states. In this way we calculate the susceptibility

$$\chi = \frac{\beta}{3N} \sum_{i,j} \langle S_i \cdot S_j \rangle \tag{6}$$

and the correlation functions

$$C_m = \frac{3}{N}\sum_{i=1}^{N}\frac{\langle S_i^z S_{i+m}^z\rangle}{S(S+1)}. \tag{7}$$

The matrix $\langle l|\hat{H}|l'\rangle$ can be block diagonalized using the symmetries of the Hamiltonian [10]. In particular, S_z and S^2 commute with the Hamiltonian, and this is translationally invariant.

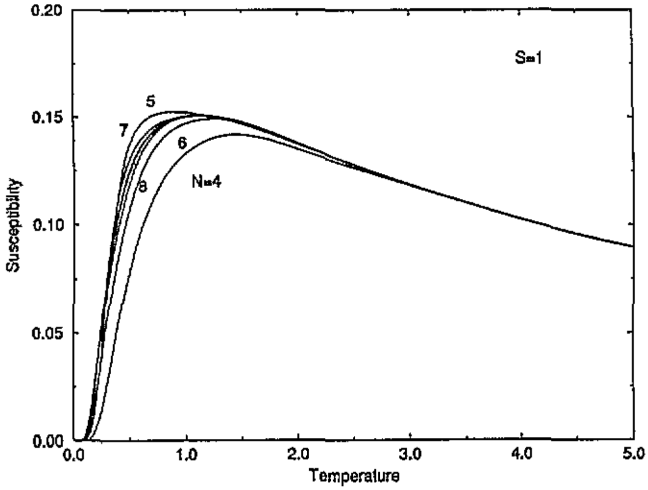


Figure 3. Susceptibility against T for the $S = 1$ Haldane–Shastry model for the set of values $N = 4, 5, 6, 7, 8$, together with the extrapolated value.

2. Energy spectrum

The exact energy spectrum has been obtained for the $S = \frac{1}{2}$ case [2, 4]. The ground state is a spin singlet with energy [3]

$$\frac{E}{NJ} = -\frac{\pi^2}{24}\left(1 + \frac{5}{N^2}\right). \tag{8}$$

In figure 1 we show the energy spectrum for $S = \frac{1}{2}$, (*a*) $N = 4$ and (*b*) $N = 6$ for the Heisenberg and Haldane–Shastry models. The ground state is a spin singlet in both models. However, the first excited state is an $S_T = 1$ triplet in the Heisenberg case but an $S_T = 1$ quartet in the Haldane–Shastry case, where S_T is the total spin of an N-spin state. Also, it is clearly seen for $N = 6$ (and higher values) that the Haldane–Shastry spectrum displays a supermultiplet structure [2, 4] with the feature that the energies in units of $\frac{1}{4}(\pi/N)^2$ are integers [2]. The sets of integers are $-14, -6, -2, 10$ for $N = 4$ and $-41, -29, -21, -17, -5, -1, 3, 15, 35$ for $N = 6$, for instance. In figure 2(*a*) we show the spectra for $S = 1$ and $N = 4$ and in figure 2(*b*) the first 100 levels for $S = 1$ and $N = 6$, again for both models. In this case the two spectra are more similar. The ground state is

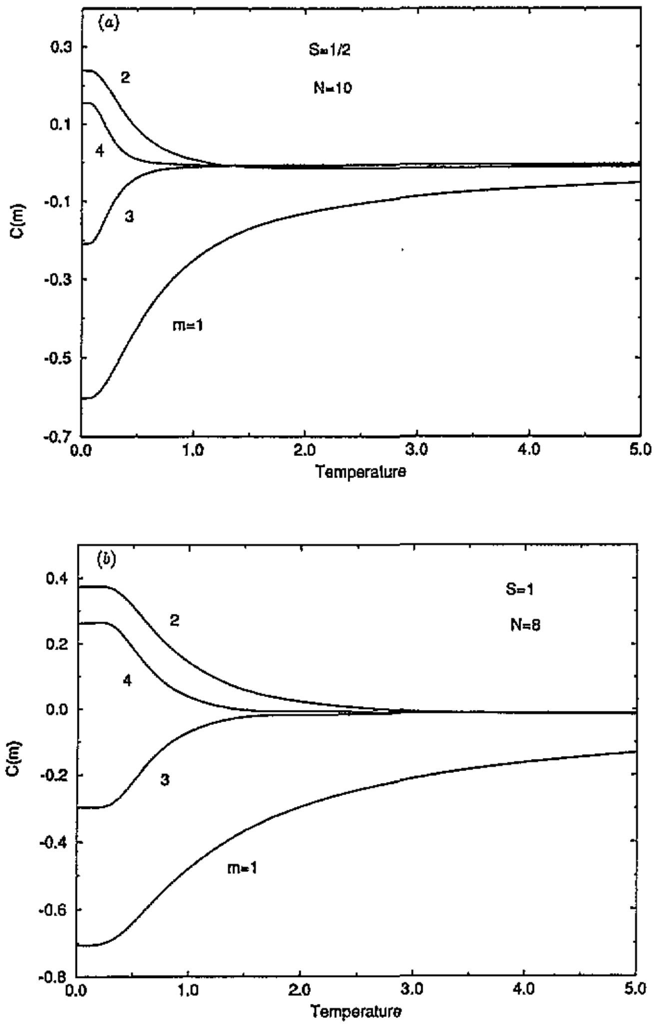
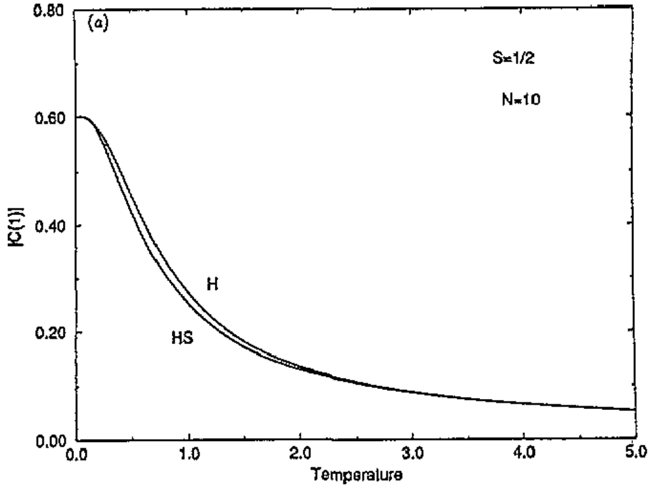


Figure 4. Correlation functions C_m against T for (a) the $S = \frac{1}{2}$ and $N = 10$ and (b) the $S = 1$ and $N = 8$ Haldane–Shastry model.

still a singlet and the first excited state is a triplet in both models. In [9] it was shown that, for the Haldane–Shastry model, the infinite-system estimate for the gap is finite, as for the Heisenberg case [8, 11]. This result was obtained studying systems of sizes up to $N = 12$ using the modified Lanczos method [12] and a Vanden Broeck and Schwartz extrapolation algorithm (VBS) [7, 13].

3. Susceptibility

Let us consider now the $S = \frac{1}{2}$ susceptibility. An exact solution has been found for both models. For the Heisenberg case the zero-T result was obtained by the Bethe *ansatz* [14] and the temperature dependence by diagonalization of small systems [10] and by the numerical solution of the thermodynamic Bethe *ansatz* equations [15]. The Haldane–Shastry case was



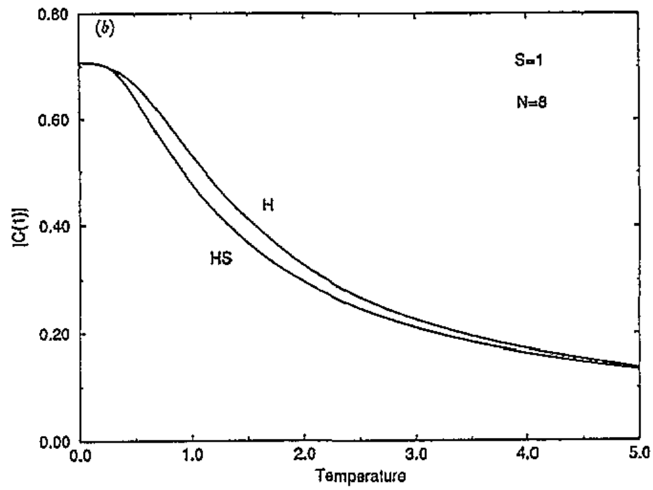


Figure 5. Correlation function C_1 against T for (a) $S = \frac{1}{2}$, $N = 10$ and (b) $S = 1$, $N = 8$ for the Heisenberg (H) and Haldane–Shastry (HS) models.

solved analytically yielding the simple result [4]

$$\chi = \frac{\beta}{2\pi} \int_0^{\pi/2} \mathrm{d}v\, \mathrm{e}^{2\beta J f} \tag{9}$$

where $f(v) = [v^2 - (\pi/2)^2]/4$. The zero-$T$ value is [3]

$$\chi(T = 0) = \frac{1}{\pi^2} \tag{10}$$

as for the Heisenberg model.

The infinite-system extrapolation using the numerical diagonalization technique is somewhat difficult. For N even, the ground state is a singlet and for any finite N there is a finite gap to the first excited state rendering the zero-T susceptibility null. On the

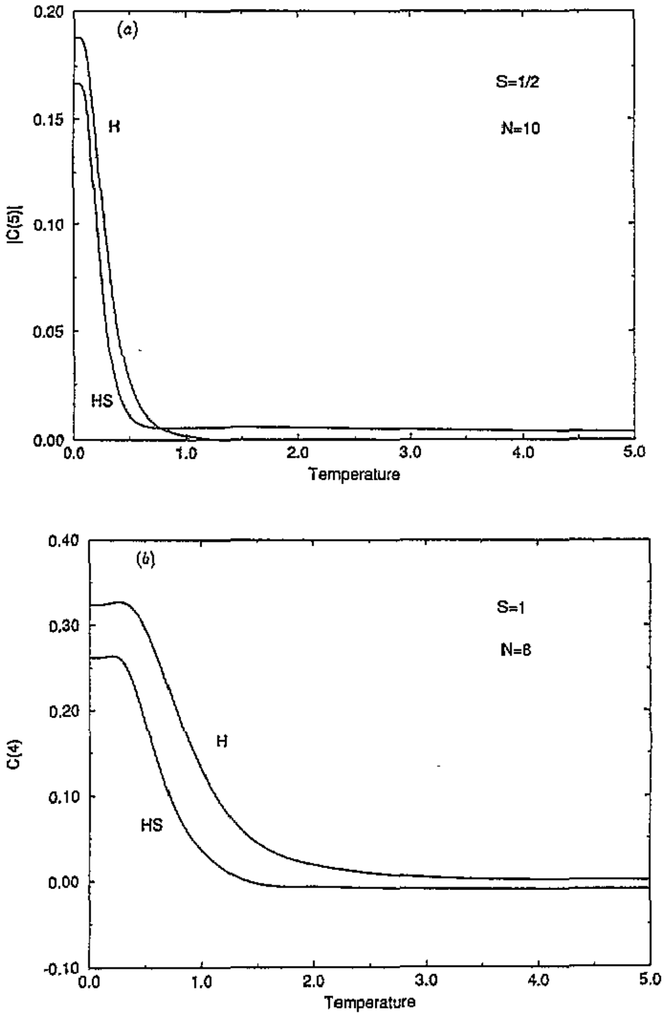


Figure 6. Comparison of $C_{N/2}$ for the Heisenberg (H) and Haldane–Shastry (HS) models for (*a*) $S = \frac{1}{2}$, $N = 10$ and (*b*) $S = 1$, $N = 8$.

other hand, for N odd the ground state is a quartet, which implies a diverging zero-T susceptibility. Since the correct limit is finite (equation (9)) the extrapolation is somewhat difficult [10]. This holds true for both models.

There is no exact solution in the $S = 1$ case for any of these models. On the other hand, both the N even and the N odd ground states are singlets (for both models). Since there is a finite gap (for finite and for infinite systems [9]) the zero-T susceptibility is zero for all values of N.

In figure 3 we show the susceptibility for the $S = 1$ Haldane–Shastry model for the values of $N = 4, 5, 6, 7, 8$. As N grows the convergence is fast. We can therefore estimate the infinite-size curve taking the average of the $N = 7$ and the $N = 8$ curves [10]. The low-T susceptibility is exponentially small, indicative of a finite gap, confirming our previous result [9].

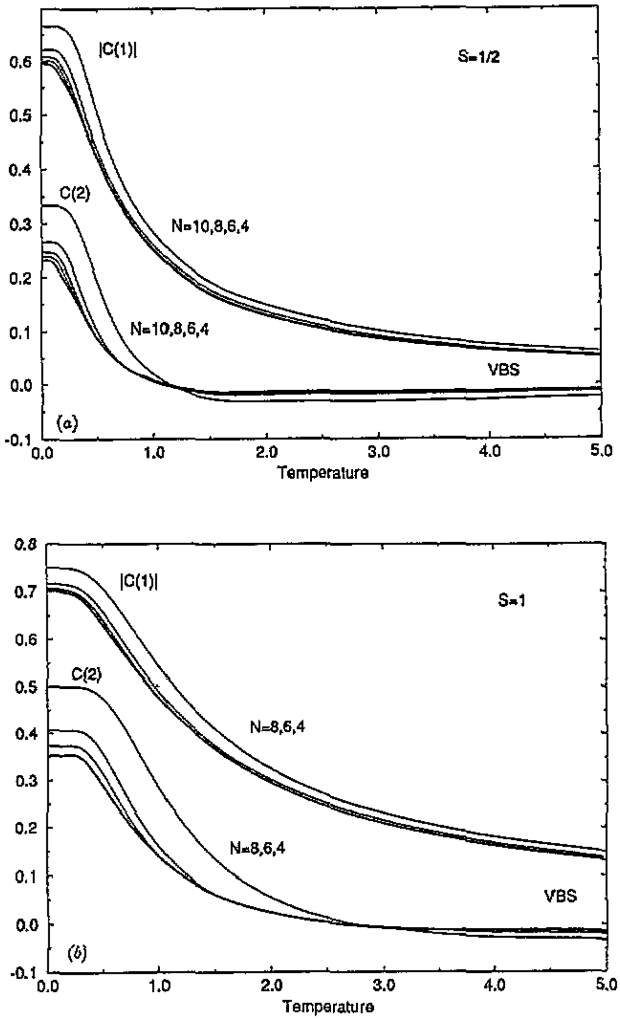


Figure 7. Correlation functions $|C_1|$ and C_2 against T for the Haldane–Shastry model for the set of values (*a*) $S = \frac{1}{2}$, $N = 4, 6, 8, 10$ and the VBS extrapolated curve and (*b*) $S = 1$, $N = 4, 6, 8$ and the VBS result.

4. Correlation functions

We consider now the correlation functions for the Haldane–Shastry model. The ground-state correlation functions have been obtained analytically for $S = \frac{1}{2}$ [2, 6] and numerically for the $S = 1$ case [9]. In figure 4 we show the correlation functions as a function of temperature for (*a*) $S = \frac{1}{2}$, $N = 10$ and (*b*) $S = 1$, $N = 8$. Note that as T grows all the correlation functions for both spin values become negative, in contrast to the Heisenberg case.

In figures 5(*a*) and 5(*b*) we compare the C_1 correlation function for both models for the $S = \frac{1}{2}$ and $S = 1$ cases, respectively. Note that the zero-T result is the same for both models for both values of the spin. It is seen that the correlation functions decay faster with T for the Haldane–Shastry model even though the interactions are long ranged (as found for the ground-state dependence on N [9]). This can be interpreted due to an absence of interactions between the spinons in the Haldane–Shastry case, as shown by the absence of logarithmic corrections to the $S = \frac{1}{2}$ ground-state correlation function exponent [2, 3, 6].

In figures 6(*a*) and 6(*b*) we show the $C_{N/2}$ correlation function for both models for $S = \frac{1}{2}$ and $S = 1$, respectively. Once again, the decay with T is faster for the Haldane–Shastry model. Note however that for $S = \frac{1}{2}$ as $T \geqslant 1$ the Heisenberg correlation function decays faster to zero. Note also that for $S = 1$ the correlation function goes through a maximum for both models, in contrast to the $S = \frac{1}{2}$ case. Once again, the Haldane–Shastry correlation functions become negative for large T. If we were to plot for $S = 1$ the absolute value of $C(4)$ we could see, similarly to the $S = \frac{1}{2}$ case, that $|C(4)|$ decays faster to zero for the Heisenberg model than for the Haldane–Shastry model. For the cases we have considered, we found that for $m \geqslant 3$ and odd, and for both values of the spin, the trend is like the one shown in figure 6(*a*). Also, for m even and, once again, for both values of the spin, the behaviour is similar to figure 6(*b*), since the correlation functions for the HS model become negative, in contrast to the Heisenberg case.

In figure 7 we show the correlation functions C_1 and C_2 against T for the spin values (*a*) $S = \frac{1}{2}$ and (*b*) $S = 1$. We show the convergence as N grows and we have included the extrapolated curves to the infinite system size using the VBS method [7, 13]. The convergence is fast, particularly for C_1.

In summary, we have studied the finite-temperature behaviour of the correlation functions of the Haldane–Shastry model, extending the results previously obtained for the ground state for $S = \frac{1}{2}$ [2, 3, 6] and $S = 1$ [9]. We also studied the $S = 1$ susceptibility and found that it is vanishingly small at low T, confirming that there is a finite gap in agreement with the results previously obtained [9], as shown by the exponentially decaying behaviour of the ground-state correlation function and the extrapolated value for the gap, obtained by the Lanczos algorithm for small chains. In the large-N limit the interactions between nearest neighbours in both models have the same scale. We have therefore compared results for both models, even though we studied finite systems. We have confirmed that the correlation functions for the Haldane–Shastry model decay faster with T than those for the Heisenberg model, as obtained previously [9] for the ground-state values as a function of system size and distance. This holds for both values of the spin.

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