Finite-lattice expansion for quantum spin chains

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We investigate the thermal properties of $s = \frac{1}{2}$ and 1 antiferromagnetic Heisenberg spin chains by an expansion in finite lattices. The expansion is based on expressing the quantity of interest, in the thermodynamic limit, as a sum over contributions from different length scales. The first few terms in the expansion, obtained by diagonalizing chains of length up to 13 for $s = \frac{1}{2}$ and length up to 9 for $s = 1$, provide an accurate estimate for the internal energy and specific heat for $T/J \geq 0.25$ and 0.35, respectively. At lower temperatures, by studying the exponential decay of the various terms in the expansion, we estimate the correlation length ξ. We get good estimates for ξ down to $T/J = 0.06$ for $s = \frac{1}{2}$ and $T/J = 0.02$ for $s = 1$. We find that for $s = 1$ ξ increases much more slowly than for $s = \frac{1}{2}$ and is consistent with a value of $\xi \approx 7$ at $T = 0$.

I. INTRODUCTION

Finite-size studies of quantum spin Hamiltonians have proved very valuable in extracting the thermodynamic properties of the system. At $T = 0$, they have been used to determine the ground-state energy, the excitation spectra, and various correlation functions of the spin chains, while at finite temperatures they have led to estimates for the internal energy, the specific heat, and other thermodynamic quantities.[1-3] Much of the extrapolation has relied on the assumption that an extensive quantity P_l, for a chain of length l, takes the form $P_l = lp + q$, where p is the bulk density in the thermodynamic limit and q is the contribution from the boundary. A plot of P_l versus l was used to estimate p. In this extrapolation scheme, the effects of correlations are ignored. Hence, the extrapolation becomes unreliable when the correlation length is comparable to the size of the largest system considered.

In this paper we consider a different scheme to obtain the thermodynamic quantities of interest by studying finite chains. It is based on a technique first developed in Ref. 4 and later in Ref. 5 for lattice gauge theories. The idea behind this scheme is to express the various thermodynamic quantities for the infinite chain as a sum over contributions associated with increasing length scales. The contribution to a given length scale l is obtained from the thermodynamic properties for chains with free boundary conditions up to length l ($l + 1$ spins) and it accounts for correlations of that length in the infinite system. This method enables a systematic study of the convergence of various thermodynamic quantities and also allows us to extract the correlation length.

For the $s = \frac{1}{2}$ chain, calculations are performed exactly up to $l = 13$ and for the $s = 1$ chain it is done up to $l = 9$. From this, 13 terms for $s = \frac{1}{2}$ and 9 terms for $s = 1$ are extracted in the above sum. The results for the infinite lattice are obtained by observing convergence in the sum. In particular, for the specific heat, we find excellent convergence for $T/J \geq 0.25$ for $s = \frac{1}{2}$ and $T/J \geq 0.35$ for $s = 1$. For the $s = \frac{1}{2}$ chain, there is a peak around $T/J \approx 0.45$ and for the $s = 1$ chain the peak is around $T/J \approx 0.8$. Thus, we have excellent convergence well

below the peak.

At low temperatures, where we do not observe good convergence, it is still possible to extract useful information. Since, the lth term in the sum is associated with correlations at length l, the sequence of terms will fall exponentially with l with the rate of decay being the correlation length ξ. The relationship of this correlation length to the usual spin-spin correlation length is not *a priori* obvious. To estimate ξ it is sufficient to study chains up to lengths $l \approx \xi$, while, to get an accurate estimate of the thermodynamic quantities, it is necessary to study chains up to lengths several times ξ. We calculate ξ down to a temperature of $T/J = 0.06$ for $s = \frac{1}{2}$ and $T/J = 0.02$ for the $s = 1$ chain. For $s = \frac{1}{2}$, the correlation length was calculated by Kamieniarz[6] by studying the spin-spin correlation function. We find that our estimates agree rather well with that of Kamieniarz. This agreement is quite interesting because our study does not involve any explicit calculation of correlation functions. It suggests that there is only one dominant length scale in the problem. We find that ξ, for the $s = 1$ chain, increases at a much slower rate compared to the $s = \frac{1}{2}$ chain. It is consistent with, and suggestive of, a finite correlation length at $T = 0$. This result is in agreement with Haldane's conjecture.[7]

The plan of the paper is as follows: In Sec. II we discuss the expansions for the thermodynamic properties in terms of finite lattices. The contribution from different length scale is defined. Section III deals with the appropriate calculations for the $s = \frac{1}{2}$ and 1 chains. In Sec. IV we calculate the thermodynamic properties including the internal energy and the specific heat. In Sec. V we analyze the contribution to the internal energy from different length scales and hence estimate the correlation length as a function of temperature. Finally, we present our conclusions in Sec. VI.

II. FORMULATION OF THE EXPANSION

In this section an expansion is developed in terms of finite-size chains. The formulation exactly parallels Refs.

4 and 5. The Hamiltonian for the spin chain of length l and free boundary conditions is

$$\mathcal{H}_l = J \sum_{i=1}^{l} \mathbf{S}_i \cdot \mathbf{S}_{i+1} \ . \tag{2.1}$$

$\mathbf{S}_i$ is the spin operator at site i and it satisfies the following commutation relation:

$$[S_i^\alpha, S_j^\beta] = i\delta_{ij}\epsilon^{\alpha\beta\gamma}S_i^\gamma \ . \tag{2.2}$$

The superscripts denote the components of the spin vector. Let $\mathcal{P}_l$ denote a generic local operator summed over the whole chain. The expectation value of this operator on the finite spin chain is

$$P_l = \langle \mathcal{P}_l \rangle = \frac{\mathrm{Tr}\mathcal{P}_l \exp(-\beta\mathcal{H}_l)}{\mathrm{Tr}\exp(-\beta\mathcal{H}_l)} \ . \tag{2.3}$$

Note that positive values of J in (2.1) correspond to an antiferromagnet. The thermodynamic average density of this operator is

$$p = \lim_{l \to \infty} \frac{1}{l} P_l \ . \tag{2.4}$$

We now develop an expansion for p. The idea behind the expansion is to write the expectation value in the infinite chain as a sum of terms corresponding to correlations of a certain length contained in the chain. Toward that end we define another function $\hat{P}_l$ on a finite chain. $\hat{P}_l$ is the contribution to p that comes from a chain of length l that is not already present in any smaller chain:

$$\hat{P}_l = P_l - \sum_{m=1}^{l} (l-m+1)\hat{P}_m \ . \tag{2.5}$$

$(l-m+1)$ is the number of ways a chain of length m can be placed in a chain of length l. Equation (2.5), when substituted into (2.4), gives the following expansion for p:

$$p = \sum_{l=1}^{\infty} \hat{P}_l \ . \tag{2.6}$$

In the case of one dimension, there is a simplification which reduces (2.5) to

$$\hat{P}_l = P_l - 2P_{l-1} + P_{l-2} \tag{2.7}$$

and

$$p_l \equiv \sum_{i=1}^{l} \hat{P}_i = P_l - P_{l-1} \ . \tag{2.8}$$

As l gets larger, $\hat{P}_l$, accounts for contributions to p from longer-range correlations. Therefore, $\hat{P}_l$ is expected to get small quite fast as l increases, provided the calculation is not done near a critical point. In fact, at a fixed temperature, one expects $\hat{P}_l$ to fall off as $\exp(-l/\xi)$ for large l, and ξ is the correlation length at that temperature. This expansion scheme has two advantages. One is that it is possible to observe convergence in (2.6) by adding more and more terms. For small values of ξ, $\hat{P}_l$ falls rapidly and the convergence is very fast. Secondly, it is possible to extract ξ from $\hat{P}_l$, even in the temperature region where the convergence is not good.

III. DESCRIPTION OF THE CALCULATION ON A FINITE CHAIN

In this section we would like to outline our scheme for diagonalizing chains of finite length with free boundary conditions. A natural basis for the Hilbert space is the direct product of states denoted by

$$\otimes_i |s_i^z\rangle \ ,$$

where s_i^z take values $\pm\frac{1}{2}$ for spin-$\frac{1}{2}$ and 0 or ± 1 for spin-one chains. Each of these basis states will be called a pattern. Since the Hamiltonian commutes with the total spin operator, the Hilbert space naturally splits into sectors with different values of $S_t^z = \sum_i s_i^z$. It is enough to consider the sector of $S_t^z = 0$ (for spin-$\frac{1}{2}$ chains with an odd number of sites, the relevant sector is $S_t^z = \frac{1}{2}$), provided the total spin of each eigenstate can be evaluated. We shall discuss this point later.

The Hamiltonian can be further block diagonalized by using additional symmetries. For the finite chain with free boundary conditions, we use two such symmetries.[8]

(1) Reflection about the midpoint of the chain. For a chain of length l this amounts to the transformation $s_i^z \to s_{l+2-i}^z$. Let R denote the operator which performs this transformation. Given a pattern $|a\rangle$, the pattern on reflection about the midpoint is $R|a\rangle$.

(2) Spin inversion. This amounts to the transformation $s_i^z \to -s_i^z$. We shall call the spin-inversion operator I. For a spin-$\frac{1}{2}$ chain with an odd number of sites, this symmetry is not useful.

It is obvious that both these operators have eigenvalues ± 1, and they commute with each other. The Hamiltonian in the $S_t^z = 0$ sector is therefore split into four sectors, denoted by $\alpha_r = \pm 1$ and $\alpha_i = \pm 1$, where α_r and α_i are the eigenvalues of R and I, respectively. Given a pattern $|a\rangle$, we can construct an eigenstate of the operator R and I by taking the linear combination

$$|\Psi_a\rangle = \frac{(1+\alpha_r R)(1+\alpha_i I)}{\mathcal{N}_a}|a\rangle \ . \tag{3.1}$$

$\mathcal{N}_a$ is the normalization factor. Let the number of distinct patterns in (3.1) be n_a (n_a takes values 1, 2, or 4). Then,

$$\mathcal{N}_a = \frac{4}{\sqrt{n_a}} \ . \tag{3.2}$$

By convention, only one of these patterns, viz., $|a\rangle$, will be called the generating pattern and the other distinct patterns obtained from $|a\rangle$ by operating with R, I, or RI will be called derived patterns. One should note that this state only contributes to n_a out of the four sectors. In the other sectors it vanishes identically. The number of generating patterns that contribute to a given sector is the dimension of the corresponding Hilbert space.

The next step involves the calculation of the Hamiltonian matrix in a given sector. We begin with the expression

$$\langle \Psi_a | \mathcal{H} | \Psi_b \rangle = \frac{1}{\mathcal{N}_a \mathcal{N}_b} \langle a | (1 + \alpha_r R)(1 + \alpha_i I) \mathcal{H} (1 + \alpha_r R)(1 + \alpha_i I) | b \rangle \ . \tag{3.3}$$

Since R and I commute with the Hamiltonian and $R^2 = I^2 = 1$, this leads to

$$\langle \Psi_a | \mathcal{H} | \Psi_b \rangle = \frac{4}{\mathcal{N}_a \mathcal{N}_b} \langle a | (1 + \alpha_r R)(1 + \alpha_i I) \mathcal{H} | b \rangle \ . \tag{3.4}$$

Since the states $|a\rangle$ and $|b\rangle$ are in the basis where the S_i^z operators are diagonal, it is natural to write

$$\mathbf{S}_i \cdot \mathbf{S}_j = S_i^z S_j^z + \tfrac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) \ , \tag{3.5}$$

where $S_i^{\pm}$ are the usual raising and lowering operators. The z part connects the state $|\Psi_b\rangle$ to itself, and is easily seen to be $\langle b | S_i^z S_j^z | b \rangle$. To evaluate the matrix element corresponding to the second term in (3.5), we first find all patterns $\{|b_p\rangle\}$ that are generated by that term acting on $|b\rangle$. For each $|b_p\rangle$ there is an associated generating pattern and this is one of the possible choices for $|a\rangle$ in (3.4). Note that $|a\rangle$ could quite well be $|b\rangle$. If the $|a\rangle$ so chosen does not contribute to the sector under consideration, i.e.,

$$(1 + \alpha_r R)(1 + \alpha_i I) | a \rangle = 0 \ ,$$

then it is discarded. In general, there could be more than one way to derive $|b_p\rangle$ from the generating pattern $|a\rangle$. Let the number of ways be N ($N \leq 4$), and one of the ways be $|b_p\rangle = R^m I^n |a\rangle$. Then the contribution to $\langle \Psi_a | \mathcal{H} | \Psi_b \rangle$ from $\tfrac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)$ is

$$\frac{4N}{\mathcal{N}_a \mathcal{N}_b} (\alpha_r)^m (\alpha_i)^n \langle b_p | \tfrac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) | a \rangle \ .$$

The Hamiltonian so constructed is diagonalized using standard procedures. Let the energy level be denoted by e_n and the corresponding eigenstate be $|n\rangle$.

The next step is to find the total spin eigenvalue of these energy eigenstates. To this end we calculate the matrix

$$\langle m | \mathbf{S}_t \cdot \mathbf{S}_t | n \rangle \ ,$$

where $\mathbf{S}_t = \sum_i \mathbf{S}_i$ is the total spin operator. If there are no accidental degeneracies of the Hamiltonian, then this should be a diagonal matrix with eigenvalues $s(s+1)$, where $s = 0, 1, 2, \ldots$. We do find occasional degeneracies and then the spin matrix in that subspace is diagonalized to obtain the corresponding eigenvalues. That the eigenvalues of this matrix agree with some $s(s+1)$ and the total number of states in each spin sector come out as expected, serves as a check on our calculations.

The result of this calculation is a set of eigenstates labeled by the total spin s_n and energy e_n. It is now straightforward to calculate the thermodynamic quantities such as free energy, internal energy, and specific heat.

IV. THERMODYNAMIC PROPERTIES

In this section we analyze the internal energy and the specific heat for the antiferromagnetic $s = \tfrac{1}{2}$ and 1 chain. These quantities are defined as

$$E = \lim_{l \to \infty} \frac{1}{l} \langle \mathcal{H}_l \rangle \ , \tag{4.1}$$

$$C = \frac{dE}{dT} \ . \tag{4.2}$$

As in (2.5), let $\hat{E}_l$ and $\hat{C}_l$ denote the contribution to the total quantity arising from the chain of length l. We find that the contributions from the chains of odd and even lengths are opposite in sign. To account for this odd-even alternation, we define

$$\tilde{E}_l = \tfrac{1}{2} \hat{E}_1 + \sum_{m=2}^{l} \frac{\hat{E}_m + \hat{E}_{m-1}}{2}$$

and a similar definition can be given for $\tilde{C}_n$. Note that, from (2.6), $E = \lim_{l \to \infty} \tilde{E}_l$ and a similar limit holds for C.

In Fig. 1, $\tilde{E}_l$, $l = 10, 11, 12, 13$ for the $s = \tfrac{1}{2}$ chain is plotted. We find excellent convergence for $T/J \geq 0.2$. The asterisk denotes the correct answer at zero temperature and is bracketed by $\tilde{E}_l$ even from below and for l odd from above.

In Fig. 2, $\tilde{C}_l$, $l = 10, 11, 12, 13$ for the $s = \tfrac{1}{2}$ chain is plotted. We find excellent convergence for $T/J \geq 0.25$. Note that the convergence is weaker in the specific heat than in the internal energy. However, there is good convergence well beyond the peak in the specific heat which occurs at $T/J \approx 0.45$. The results of previous finite-size extrapolations by Blöte[3] are shown by an asterisk. We find that his results are close to ours; however, there is deviation even at T/J as large as 2.0. Since our results do not show any noticable change when going from $l = 10$ to 13 for $T/J \geq 0.4$, it is a more accurate estimate
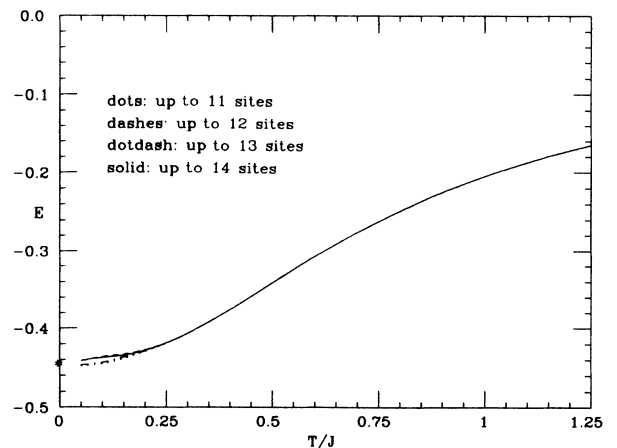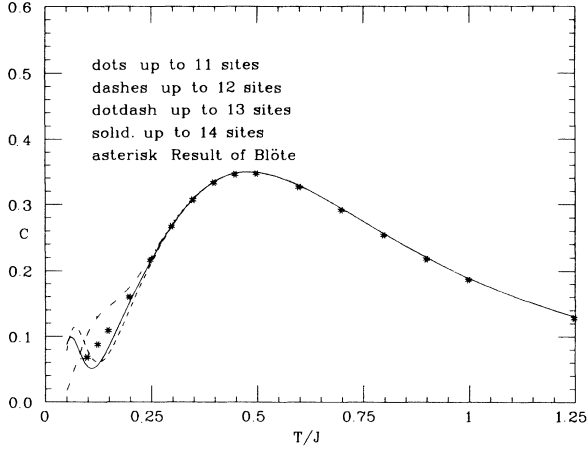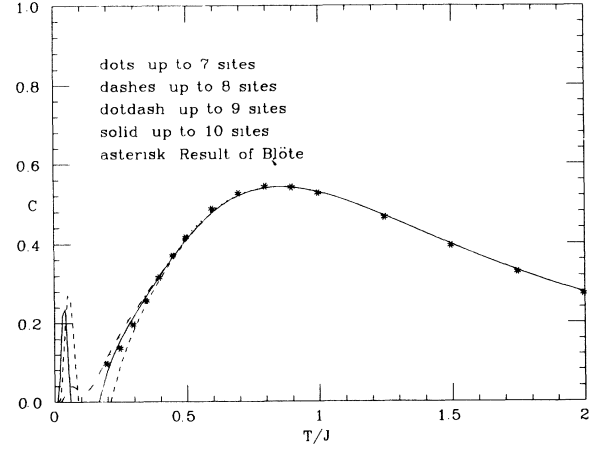

FIG. 1. Internal energy for the $s = \tfrac{1}{2}$ chain.

FIG. 2. Specific heat for the $s = \frac{1}{2}$ chain.

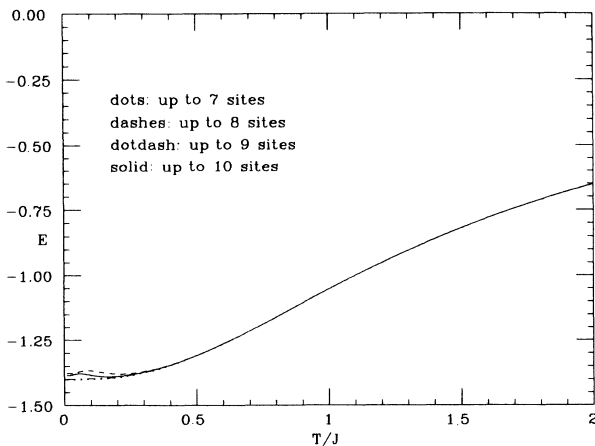

FIG. 4. Specific heat for the $s = 1$ chain.

of the quantity in the thermodynamic limit. From the finite-temperature Bethe ansatz,[9,10] the specific heat is known to be linear at low temperature with deviations expected above $T/J = 0.1$. Since we have convergence only up to $T/J = 0.25$, we cannot trivially extrapolate the result here to match with a linear plot for small T/J.

In Fig. 3, $\tilde{E}_l$, $l = 6,7,8,9$ for the $s = 1$ chain is plotted. We find excellent convergence for $T/J \geq 0.3$. By analogy with the $s = \frac{1}{2}$ chain, we expect E_l for l even to bound the ground-state energy e_0 from below and for l odd from above. This would imply that $-1.3992 \leq e_0 \leq -1.3850$. Judging from the pattern of convergence, we expect the number to be closer to the lower bound. However, the earlier estimates for the ground-state energy[2] have been approximately -1.402 and are outside the bracketed region.

In Fig. 4, $\tilde{C}_l$, $l = 6,7,8,9$ for the $s = 1$ chain is plotted. We find excellent convergence for $T/J \geq 0.35$. Note again that the convergence is weaker in the specific heat than in the internal energy but extends beyond the peak

which occurs at $T/J \approx 0.8$. The behavior of the specific heat is quite similar to the $s = \frac{1}{2}$ chain in the temperature region where we have good convergence. Here again the results of Blöte are shown by an asterisk. The convergence properties are similar to the $s = \frac{1}{2}$ case. Assumption of a gap implies that $C \sim \exp(-\Delta/T)$ with a temperature-dependent prefactor. Any fit of our results in the region around $T/J \approx 0.4$ seems to be quite sensitive to the choice of the prefactor. If we do not choose any prefactor, then we get a gap that is consistent with the zero-temperature estimates of $0.4J$.

The specific heat of the quasi-one-dimensional (1D) $s = 1$ chain CsNiCl$_3$ has also been studied experimentally.[11] This system has $J/k_B \approx 27$ K and Néel temperature for three-dimensional ordering of 4.8 K. Therefore, a comparison with the experiment can be done only for $T/J \geq 0.2$. In the experiments, the magnetic contribution to the specific heat was separated and a comparison was done with Blöte's results. The low-temperature data were fitted to a linear T dependence as expected for a gapless system. Our studies here suggest that, to distinguish between the presence or absence of a gap, the specific heat of a quasi-1 D chain should be measured at temperatures at least as low as $T \approx 0.1J$.

V. ANALYSIS OF THE CORRELATION LENGTH

In the previous section the analysis of internal energy and specific heat did not show good convergence at low values of T/J. This is because the correlation length in the system is getting large and longer chains have a significant contribution. Even though the convergence for the thermodynamic quantities is not good, it is still possible to extract a correlation length.

We concentrate on $\hat{E}_l$ and view it as function of l at a fixed T/J. We expect it to have an exponential decay, and in view of this, $\ln_{10}|\hat{E}_l|$ is plotted as function of l. The magnitude is to take the alternating sign into account.

In Figs. 5(a) and 5(b), we find a good straight line fit for large l. The negative of the slope of the line is the inverse

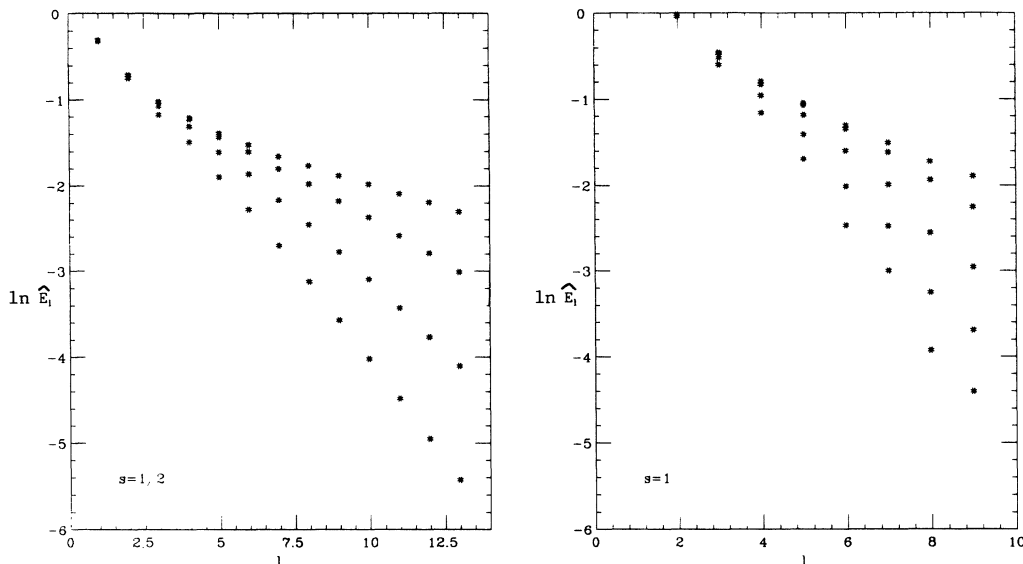FIG. 3. Internal energy for the $s = 1$ chain.

FIG. 5. $\ln_{10}|\hat{E}_l|$ vs l for the $s = \frac{1}{2}$ and 1 chains.

of the correlation length. This analysis is not relevant at large T/J since the correlation length is very small. The analysis will not give reliable results below a certain T/J since the correlation length is large and we have not gone to long enough chains. But we get good estimates in the range $0.06 \le T/J \le 0.2$ for $s = \frac{1}{2}$ and in the range $0.02 \le T/J \le 0.2$ for $s = 1$. This is the region where the thermodynamic quantities analyzed in the previous section did not show good convergence. This is because the correlation length is above two or three lattice spacings and so chains of length not considered in the calculation here will have a significant contribution.

In Fig. 6 we plot the results of our analysis. The correlation length for $s = \frac{1}{2}$ was calculated previously by Kamieniarz[6] through the second moment of the spin-spin correlation function. His estimates are shown by squares. We find that our results agree quite well with his, suggesting that there is a single dominant length in the prob-
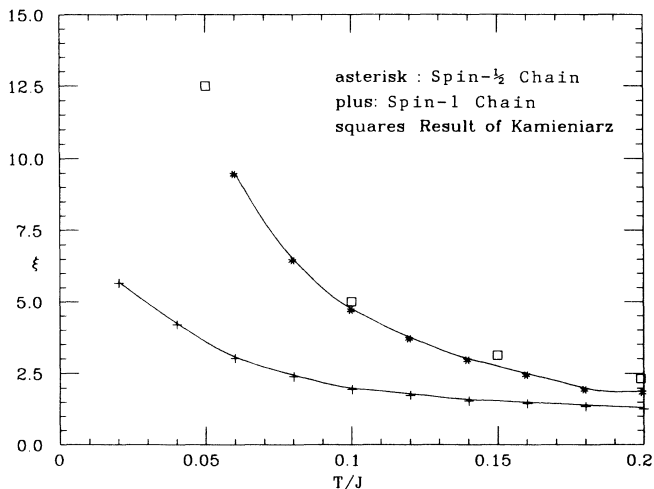
lem. We are not aware of any calculation of the correlation length for the $s = 1$ chain at finite temperatures. We find that, for $s = 1$, the correlation length rises much more slowly as T/J decreases when compared to the $s = \frac{1}{2}$ chain. A crude estimate for the zero-temperature value is approximately 7 which is in agreement with other numerical studies at $T = 0$.[8] This the only clear difference between the $s = \frac{1}{2}$ and 1 chains in our study. It also seems to indicate that it is easier to observe the effect of the gap in the spin-spin correlation function than in the specific heat.

VI. CONCLUSIONS

In this paper we have developed an expansion for the thermodynamic quantities of the Heisenberg spin chains. Each term in the expansion is obtained from an exact diagonalization of a finite chain with free boundary conditions. It accounts for the contribution to the infinite system from that particular finite chain which has not been accounted for by any smaller chain. This enables a systematic study of the contributions from various length scales. We have fully diagonalized all spin chains up to $l = 13$ for $s = \frac{1}{2}$ and $l = 9$ for $s = 1$. From these results we get 13 terms in the expansion for $s = \frac{1}{2}$ and 9 terms in the expansion for $s = 1$. Our calculation of the specific heat shows excellent convergence for $T/J \ge 0.25$ and $T/J \ge 0.35$ for $s = \frac{1}{2}$ and 1, respectively. Our expansion procedure enables us to extract the correlation length even in the region where we do not get good convergence. Analysis shows that the correlation length rises sharply in the case of $s = \frac{1}{2}$ as the temperature decreases, consistent with an infinite correlation length at zero temperature. For the $s = 1$ chain, the increase in the correlation length with decrease in temperature is less dramatic and is consistent with a finite correlation length at zero temperature. These conclusions are in agreement with Haldane's conjecture.

FIG. 6. Correlation lengths for the $s = \frac{1}{2}$ and 1 chains.

[1] Pioneering work for the $s = \frac{1}{2}$ chain was done by J. C. Bonner and M. E. Fisher, Phys. Rev. A **135**, 640 (1964). For an early set of references see E. H. Lieb and D. C. Mattis, *Mathematical Physics in One Dimension* (Academic, New York, 1966).

[2] For numerical work on the $s = 1$ chain, see R. Botet, R. Jullien, and M. Kolb, Phys. Rev. B **28**, 3914 (1983); M. P. Nightingale and H. W. J. Blote, *ibid.* **33**, 659 (1986).

[3] H. W. J. Blöte, Physica **79B**, 427 (1975).

[4] H. Arisue and T. Fujiwara, Prog. Theor. Phys. **72**, 1176 (1984); (unpublished).

[5] R. Narayanan and P. Vranas, Nucl. Phys. **B330**, 608 (1990).

[6] G. Kamieniarz, Phys. Rev. B **38**, 4873 (1988).

[7] F. D. M. Haldane, Phys. Lett. **93A**, 464 (1983); see also, I. Affleck, Nucl. Phys. **B265**, 409 (1986).

[8] T. Kennedy, J. Phys. Condens. Matter **2**, 5737 (1990).

[9] M. Gaudin, Phys. Rev. Lett. **26**, 1301 (1971).

[10] M. Takahashi, Prog. Theor. Phys. **50**, 1519 (1973).

[11] D. Moses, H. Shechter, E. Ehrenfreund, and J. Makovsky, J. Phys. C **10**, 433 (1977).