Local spin correlations in Heisenberg antiferromagnets

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(Received 14 July 2000; revised manuscript received 27 October 2000; published 23 January 2001)

We use linked cluster series expansion methods to estimate the values of various short distance correlation functions in $S=1/2$ Heisenberg antiferromagnets at $T=0$, for dimension $d=1,2,3$. The method incorporates the possibility of spontaneous symmetry breaking, which is manifest in $d=2,3$. The results are important in providing a test for approximate theories of the antiferromagnetic ground state.

DOI: 10.1103/PhysRevB.63.064425 PACS number(s): 75.10.Jm, 75.40.Gb

I. INTRODUCTION

This paper deals with the problem of calculating correlation functions, at $T=0$, for the $S=1/2$ Heisenberg antiferromagnet

$$H=2J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j, \tag{1}$$

where the sum is over all nearest neighbor pairs. We consider explicitly the linear chain ($d=1$), the square lattice ($d=2$) and the simple cubic lattice ($d=3$). The correlation functions (correlators) are defined as

$$C(r)\equiv 4\langle \mathbf{S}_i\cdot\mathbf{S}_{i+r}\rangle_0 = C_l(r)+2C_t(r), \tag{2}$$

where the average is a ground state expectation value, r is the distance between sites in units of the lattice parameter, and the factor 4 is included for convenience. It is also convenient to separate the correlator into a longitudinal part $C_l(r)$ and a transverse part $C_t(r)$

$$C_l(r)\equiv 4\langle S_i^z S_{i+r}^z\rangle_0, \tag{3a}$$

$$C_t(r)\equiv 2\langle S_i^x S_{i+r}^x + S_i^y S_{i+r}^y\rangle_0 = \langle S_i^+ S_{i+r}^- + S_i^- S_{i+r}^+\rangle_0. \tag{3b}$$

C_l and C_t will differ if the Hamiltonian is generalized to include Ising anisotropy

$$H=2J\sum_{\langle ij\rangle}\left[S_i^z S_j^z+\lambda(S_i^x S_j^x+S_i^y S_j^y)\right] \tag{4}$$

as we shall do, or if the ground state of the isotropic Hamiltonian exhibits spontaneous symmetry breaking. We shall see that this occurs in dimension $d>1$.

The correlators characterize the nature of the ground state of the system, and hence an accurate knowledge of their values can be important for testing approximate analytic theories. Surprisingly, apart from the one-dimensional (1D) case, knowledge of their values is limited.

We use the method of linked cluster expansions in which the Hamiltonian is written as

$$H=H_0+\lambda V \tag{5}$$

with the Ising part taken as the unperturbed Hamiltonian and the remainder as a perturbation. To improve the convergence of the series and to check the reliability of the series extrapolation, we also include a local staggered field term $t\Sigma_i(-1)^i S_i^z$ in H_0, and subtract it from V, and adjust the strength t to get best convergence in the series. The basic idea of the method has been discussed before[1,2] so we only give brief details here. The ground state energy for a lattice of N sites can be written as a sum of contributions from all connected clusters as

$$E_0(\lambda)=\sum_\alpha C_\alpha^N \epsilon_\alpha(\lambda), \tag{6}$$

where C_α^N is the embedding constant for cluster α and $\epsilon_\alpha(\lambda)$ is a ''cumulant energy'' of cluster α, as defined below. The ground state energy for a finite cluster β can be written in a similar way, in terms of the cumulant energies of its subclusters,

$$E_0^\beta(\lambda)=\sum_\alpha C_\alpha^\beta \epsilon_\alpha(\lambda). \tag{7}$$

These equations allow the cumulant energies to be determined recursively. The cluster energies are obtained as perturbation series in λ through an efficient computerized Rayleigh-Schrödinger perturbation algorithm. To compute series for the correlator $C(r)$ in powers of λ we add a field term to H

$$H=H_0+\lambda V+h\sum_i \mathbf{S}_i\cdot\mathbf{S}_{i+r}, \tag{8}$$

compute the ground state energy in the form

TABLE I. Estimates of the total correlators $C(r)$ for the isotropic $S=\frac{1}{2}$ antiferromagnetic chain [Eq. (4) in text] from exact diagonalizations (Ref. 8) and series (the present work).

r	Exact diagonalization + finite size scaling (Ref. 8)	Series expansion evaluated at $\lambda=1$
1	-1.7724(6)	-1.773(2)
2	0.72795(6)	0.730(3)
3	-0.6027(3)	-0.588(15)
4	0.4158(10)	0.408(20)
5	-0.3705(10)	-0.38(3)
6	0.2946(12)	0.32(4)
7	-0.2697(20)	
8	0.2280(20)	

TABLE II. Coefficients of correlator series for the $S=\frac{1}{2}$ antiferromagnetic chain for $r=4$.

Power of λ	$C(4)$	$C_l(4)$	$C_t(4)$
0	1.000000000	1.000000000	0.000000000
2	-2.000000000	-2.000000000	0.000000000
4	2.000000000	5.000000000×10^{-1}	7.500000000×10^{-1}
6	2.500000000×10^{-1}	2.375000000	-1.062500000
8	-1.265625000	-2.250000000	4.921875000×10^{-1}
10	3.281250000×10^{-1}	5.546875000×10^{-1}	$-1.132812500\times10^{-1}$
12	$-4.296875070\times10^{-2}$	$-1.865234375\times10^{-1}$	7.177734342×10^{-2}
14	1.225585910×10^{-1}	2.441406766×10^{-2}	4.907226169×10^{-2}
16	6.085209298×10^{-2}	7.099156584×10^{-2}	$-5.069736427\times10^{-3}$
18	5.311830238×10^{-3}	4.902810212×10^{-2}	$-2.185813594\times10^{-2}$
20	$-9.656318929\times10^{-3}$	2.493706992×10^{-2}	$-1.729669442\times10^{-2}$
22		7.884341059×10^{-3}	

$$\mathcal{E}_0(\lambda,h)=E_0(\lambda)+hNC(r)/4+O(h^2), \tag{9}$$

and hence extract series in λ for $C(r)$. For the longitudinal correlator the field term is $h\Sigma_i S_i^z S_{i+r}^z$. Examples are given in the following sections.

Two important questions are not addressed in this work: (i) the behavior of correlators at large distances, and the asymptotic behavior and associated critical exponents; (ii) correlators at finite temperature.

II. THE ONE-DIMENSIONAL CASE

The $S=\frac{1}{2}$ antiferromagnetic Heisenberg chain is exactly solvable by the Bethe ansatz,[3,4] and the ground state energy and elementary excitations are given by simple analytic expressions. However the wavefunction is sufficiently complex that little exact information is available on correlators. In fact only the first two are known exactly, and are

$$\langle \mathbf{S}_i\cdot\mathbf{S}_{i+1}\rangle=\frac{1}{4}(1-4\ln 2)=-0.443147\ldots, \tag{10}$$

$$\langle \mathbf{S}_i\cdot\mathbf{S}_{i+2}\rangle=\frac{1}{4}(1-16\ln 2+9\zeta(3))=0.182039\ldots.$$

The first result comes from the ground state energy,[5] while the second is obtained[6] via the strong coupling limit of the Hubbard model. There is no spontaneous symmetry breaking

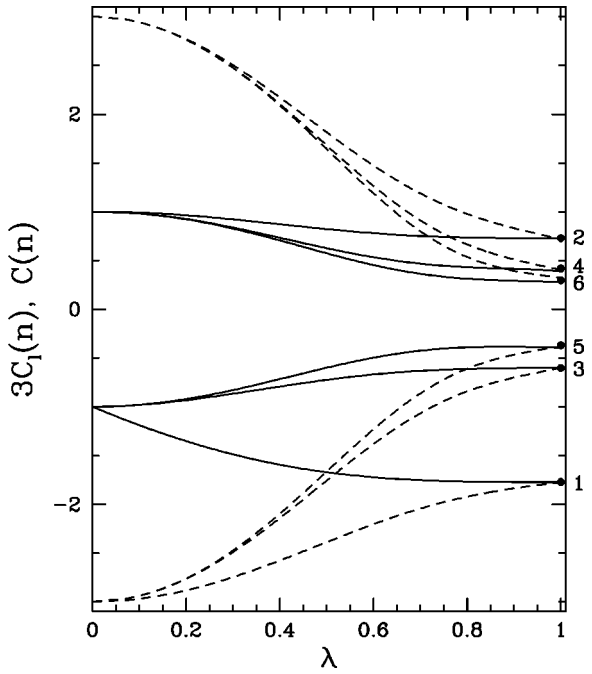

FIG. 1. Correlators $C(r)$ for the $S=\frac{1}{2}$ antiferromagnetic chain for $r=1,2,\ldots,6$. The full lines give the total correlator $C(r)$, the dashed lines give $3C_l(r)$. Curves for different r are labeled at the right hand edge. The circles at $\lambda=1$ are the values from the finite-lattice calculations (Ref. 8). Note that at the isotropic point $\lambda=1$ the longitudinal and transverse correlator are equal.

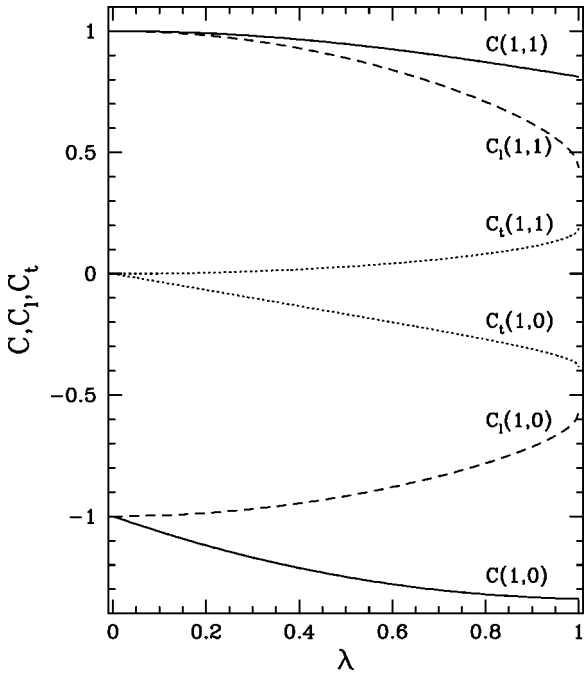

FIG. 2. Correlators for nearest and next-nearest neighbors for the square lattice, for varying anisotropy parameter λ. Full lines denote the total correlator $C(\mathbf{r})$, dashed lines the longitudinal correlator $C_l(\mathbf{r})$, and dotted lines the transverse correlator $C_t(\mathbf{r})$.

TABLE III. Nonzero coefficients of various correlator series for the $S=\frac{1}{2}$ antiferromagnet on the square lattice ($t=0$).

Power of λ	$C(\mathbf{r})$	$C_l(\mathbf{r})$	$C_t(\mathbf{r})$
		$\mathbf{r}=(1,0)$	
0	-1.000000000	-1.000000000	0.000000000
1	$-6.666666667\times10^{-1}$	0.000000000	$-3.333333333\times10^{-1}$
2	3.333333333×10^{-1}	3.333333333×10^{-1}	0.000000000
3	7.407407407×10^{-3}	0.000000000	3.703703704×10^{-3}
4	$-5.555555556\times10^{-3}$	$-5.555555556\times10^{-3}$	0.000000000
5	$-1.897883598\times10^{-2}$	0.000000000	$-9.489417989\times10^{-3}$
6	1.581569665×10^{-2}	1.581569665×10^{-2}	0.000000000
7	$-1.320340554\times10^{-2}$	0.000000000	$-6.601702770\times10^{-3}$
8	1.155297985×10^{-2}	1.155297985×10^{-2}	0.000000000
9	$-6.237012985\times10^{-3}$	0.000000000	$-3.118506492\times10^{-3}$
10	5.613311689×10^{-3}	5.613311689×10^{-3}	0.000000000
11	$-5.806609913\times10^{-3}$	0.000000000	$-2.903304957\times10^{-3}$
12	5.322725757×10^{-3}	5.322725757×10^{-3}	0.000000000
13	$-4.231435003\times10^{-3}$	0.000000000	$-2.115717502\times10^{-3}$
14	3.929189659×10^{-3}	3.929189659×10^{-3}	0.000000000
		$\mathbf{r}=(1,1)$	
0	1.000000000	1.000000000	0.000000000
2	$-2.222222222\times10^{-1}$	$-4.444444444\times10^{-1}$	1.111111111×10^{-1}
4	3.444444444×10^{-2}	4.567901235×10^{-3}	1.493827160×10^{-2}
6	7.314352902×10^{-4}	$-1.979035301\times10^{-2}$	1.026089415×10^{-2}
8	$-1.582060575\times10^{-3}$	$-1.475015802\times10^{-2}$	6.584048724×10^{-3}
		$\mathbf{r}=(2,0)$	
0	1.000000000	1.000000000	0.000000000
2	$-3.333333333\times10^{-1}$	$-4.444444444\times10^{-1}$	5.555555556×10^{-2}
4	4.246913580×10^{-2}	$-1.666666667\times10^{-2}$	2.956790123×10^{-2}
6	3.666832535×10^{-3}	$-1.353930181\times10^{-2}$	8.603067173×10^{-3}
8	$-3.706741518\times10^{-3}$	$-1.786067634\times10^{-2}$	7.076967412×10^{-3}
		$\mathbf{r}=(3,0)$	
0	-1.000000000	-1.000000000	0.000000000
1	0.000000000	0.000000000	0.000000000
2	4.444444444×10^{-1}	4.444444444×10^{-1}	0.000000000
3	$-3.888888889\times10^{-2}$	0.000000000	$-1.944444444\times10^{-2}$
4	2.037037037×10^{-2}	2.037037037×10^{-2}	0.000000000
5	$-4.035089653\times10^{-2}$	0.000000000	$-2.017544827\times10^{-2}$
6	2.054058327×10^{-2}	2.054058327×10^{-2}	0.000000000
7	$-1.401574252\times10^{-2}$	0.000000000	$-7.007871260\times10^{-3}$
8	1.785822451×10^{-2}	1.785822451×10^{-2}	0.000000000
		$\mathbf{r}=(4,0)$	
0	1.000000000	1.000000000	0.000000000
2	$-4.444444444\times10^{-1}$	$-4.444444444\times10^{-1}$	0.000000000
4	$-1.172839506\times10^{-2}$	$-2.172839506\times10^{-2}$	5.000000000×10^{-3}
6	$-1.337086028\times10^{-3}$	$-2.198640296\times10^{-2}$	1.032465846×10^{-2}

in the ground state of the isotropic spin chain, and hence longitudinal and transverse correlators are equal, and obtainable directly from Eq. (2).

The first serious attempts to obtain further results for the antiferromagnetic chain were by Bonner and Fisher,[7] who used exact diagonalizations for systems up to $N=10$ spins, and by Kaplan and co-workers[8] who extended this to $N=18$. These results suffer from large finite-size effects, and need to be extrapolated to the therodynamic limit via a finite-size scaling ansatz. In this way Kaplan *et al.* estimated the value of correlators up to 8th neighbors, with confidence limits of about 1% in $C(8)$. We show these values in Table I. Subsequently Lin and Campell[9] extended the exact diagonalizations to $N=30$. By use of the empirical scaling relation

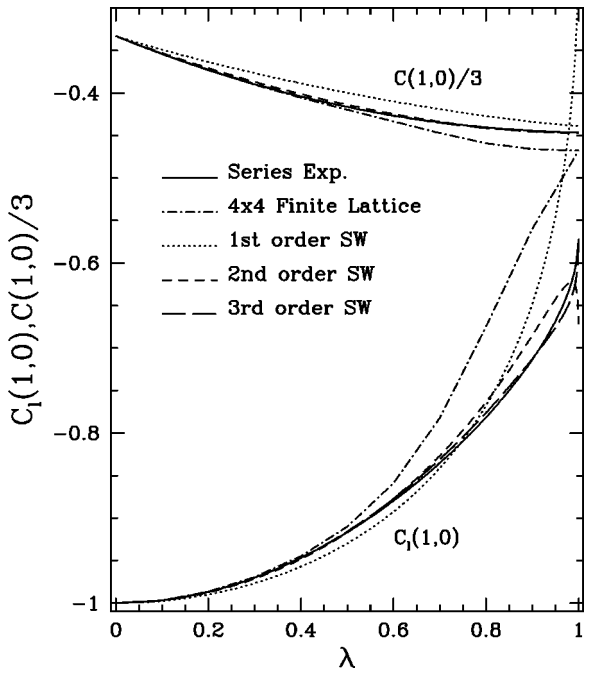

FIG. 3. Comparison between series (this work) and other estimates of the nearest neighbor correlator for the square lattice, for varying anisotropy parameter λ.

$$C_N(r) = C_\infty(r) f(r/N) \tag{11}$$

with

$$f(y) = [1 + 0.28822 \sinh^2(1.673y)]^{1.75}, \tag{12}$$

they estimated correlators up to $r=15$, i.e., 15th neighbors. However the accuracy of this scaling is perhaps doubtful since it is known that there are logarithmic terms which slow convergence.[10]

The development of the density matrix renormalization group (DMRG) method[11] allows much longer chains to be treated with high numerical accuracy. Hallberg *et al.*[12] have used DMRG to compute correlators for Heisenberg chains up to $N=70$ spins, with a scaling function similar to Eq. (11) used to extrapolate to the thermodynamic limit. The data were shown to be consistent with the asymptotic behavior

$$C(r) \sim (-1)^r (\ln r)^{1/2}/r \tag{13}$$

predicted by field theory.[10]

We have described the series method briefly in the Introduction. Using this approach we have computed expansions in λ, for both the total and longitudinal correlators for distances $r=1,2,\ldots,10$. The maximum order is λ^{24} for $r=1$ and λ^{16} for $r=10$. We note that the longitudinal correlators, and the total correlators for r even, contain only even powers of λ. We also note that the series are rather erratic, both in sign and magnitude of the coefficients. This had already been noted by Walker[13] who expanded the ground state energy, and hence $C(1)$, to order λ.[14] Rather than quote all series here we will make them available to any reader on request. Table II shows the coefficients for the series for $C(4)$, $C_l(4)$, and $C_t(4)$. We note that, as expected, the series for the transverse correlator $C_t(r)$ starts with a term λ^r.

The series have been evaluated for fixed λ by means of integrated differential approximants,[14] and the values of correlators for $r=1,2,\ldots,6$ are shown in Fig. 1. The analysis becomes less precise as the weakly singular point $\lambda=1$ is approached. We also show in Fig. 1 the extrapolated exact diagonalization results. As can be seen from the figure, and from Table I, the agreement is very good. It is clear that in one dimension the series method is not able to match the precision of either scaled finite lattice or DMRG results, but in higher dimension these latter methods are not competitive. Furthermore, as we shall show, the series analysis can be made more precise in $d \geqslant 2$ because the stronger singularity at $\lambda=1$ can be removed by a transformation, and the Ising expansions used here are more suitable for $d \geqslant 2$, where the ground state has long range Neél order.

We should mention here also the work of Singh *et al.*[15] who used exactly the same method as ours to compute the structure factors

$$S_{zz} = \frac{1}{4} \sum_{r=-\infty}^{\infty} [(-1)^r C_l(r) - 4\langle S_0^z \rangle^2] \tag{14}$$

and

$$S_{+-} = \frac{1}{2} \sum_{r=-\infty}^{\infty} (-1)^r C_t(r) \tag{15}$$

for the $S=\frac{1}{2}$ antiferromagnetic chain. Our correlator series, when summed, agree with their results.

TABLE IV. Values of correlators for the isotropic $S=\frac{1}{2}$ Heisenberg antiferromagnet on the square lattice.

r	Series (this work)			Finite lattice[b]	Linear spin wave theory[a]		
	$C(\mathbf{r})$	$C_l(\mathbf{r})$	$C_t(\mathbf{r})$	$C(\mathbf{r})$	$C(\mathbf{r})$	$C_l(\mathbf{r})$	$C_t(\mathbf{r})$
(1,0)	-1.3386(2)	-0.572(4)	-0.383	-1.344, −	-1.316	-0.2136	-0.551
(1,1)	0.812(6)	0.430(6)	0.191	0.765, 0.82	0.795	0.2136	0.291
(2,0)	0.712(10)	0.408(10)	0.152	0.84, 0.71	0.673	0.2136	0.230
(3,0)	-0.60(2)	-0.386(10)	-0.11	-0.75, -0.60	-0.526	-0.2136	-0.156
(4,0)	0.54(3)	0.376(20)	0.08	−, 0.53	0.440	0.2136	0.113

[a]From exact diagonalizations, $N=26$ (Ref. 17), and projector Monte Carlo (Ref. 20).

[b]For $\mathbf{r}=(1,0)$ we also have results from second and third order spin-wave theory (Ref. 27), which give for C, C_l and C_t respectively $-1.3408, -0.672, -0.334$ (second order) and -1.3400, -0.575, -0.383 (third order).

TABLE V. Nonzero coefficients of various correlator series for the $S=\frac{1}{2}$ antiferromagnet on the simple cubic lattice ($t=0$).

Power of λ	$C(\mathbf{r})$	$C_l(\mathbf{r})$	$C_t(\mathbf{r})$
		$\mathbf{r}=(1,0,0)$	
0	-1.000000000	-1.000000000	0.000000000
1	$-4.000000000\times10^{-1}$	0.000000000	$-2.000000000\times10^{-1}$
2	2.000000000×10^{-1}	2.000000000×10^{-1}	0.000000000
3	2.666666667×10^{-3}	0.000000000	1.333333333×10^{-3}
4	$-2.000000000\times10^{-3}$	$-2.000000000\times10^{-3}$	0.000000000
5	$-1.252256756\times10^{-2}$	0.000000000	$-6.261283778\times10^{-3}$
6	1.043547296×10^{-2}	1.043547296×10^{-2}	0.000000000
7	$-5.018108039\times10^{-3}$	0.000000000	$-2.509054019\times10^{-3}$
8	4.390844534×10^{-3}	4.390844534×10^{-3}	0.000000000
9	$-3.490020757\times10^{-3}$	0.000000000	$-1.745010379\times10^{-3}$
10	3.141018683×10^{-3}	3.141018683×10^{-3}	0.000000000
11	$-2.400011436\times10^{-3}$	0.000000000	$-1.200005718\times10^{-3}$
12	2.200010484×10^{-3}	2.200010484×10^{-3}	0.000000000
		$\mathbf{r}=(1,1,0)$	
0	1.000000000	1.000000000	0.000000000
2	$-1.600000000\times10^{-1}$	$-2.400000000\times10^{-1}$	4.000000000×10^{-2}
4	1.766543210×10^{-2}	7.567901234×10^{-4}	8.454320988×10^{-3}
6	$-3.636588526\times10^{-3}$	$-1.226438856\times10^{-2}$	4.313900018×10^{-3}
		$\mathbf{r}=(2,0,0)$	
0	1.000000000	1.000000000	0.000000000
2	$-2.000000000\times10^{-1}$	$-2.400000000\times10^{-1}$	2.000000000×10^{-2}
4	1.251358025×10^{-2}	$-1.106172840\times10^{-3}$	6.809876543×10^{-3}
6	$-4.632761555\times10^{-3}$	$-1.262448646\times10^{-2}$	3.995862454×10^{-3}
8	$-9.042568955\times10^{-4}$	$-5.558061905\times10^{-3}$	2.326902505×10^{-3}
		$\mathbf{r}=(3,0,0)$	
0	-1.000000000	-1.000000000	0.000000000
1	0.000000000	0.000000000	0.000000000
2	2.400000000×10^{-1}	2.400000000×10^{-1}	0.000000000
3	$-8.148148148\times10^{-3}$	0.000000000	$-4.074074074\times10^{-3}$
4	1.550617284×10^{-3}	1.550617284×10^{-3}	0.000000000
5	$-5.458926876\times10^{-3}$	0.000000000	$-2.729463438\times10^{-3}$
6	1.292980049×10^{-2}	1.292980049×10^{-2}	0.000000000
7	$-4.261178891\times10^{-3}$	0.000000000	$-2.130589445\times10^{-3}$
		$\mathbf{r}=(4,0,0)$	
0	1.000000000	1.000000000	0.000000000
2	$-2.400000000\times10^{-1}$	$-2.400000000\times10^{-1}$	0.000000000
4	$-4.098765432\times10^{-4}$	$-1.644444444\times10^{-3}$	6.172839506×10^{-4}
6	$-1.131207676\times10^{-2}$	$-1.297046176\times10^{-2}$	8.291924985×10^{-4}

III. THE TWO-DIMENSIONAL CASE

There has been much interest, in recent years, in the nature of the ground state of the Heisenberg antiferromagnet on the square lattice. There is considerable evidence, from exact diagonalizations[16–18] and quantum Monte Carlo calculations[19–21] that the ground state breaks rotational symmetry, giving rise to a staggered magnetization in some direction. This is generally referred to as a quantum Néel state, with Néel type order reduced to ~60% of its classical value by quantum fluctuations. The situation is summarized in recent reviews.[22,23] The focus has generally been on the ground state energy and staggered magnetization, although some short range correlators have also been computed.

In any finite system there can be no spontaneous symmetry breaking and hence the exact diagonalization and Monte Carlo studies cannot distinguish between the longitudinal and transverse correlators for the isotropic case. Furthermore if C_l or C_t are computed by these methods the values will not yield correct results for the thermodynamic limit, where $C_l \neq C_t$.

Other approaches, such as spin wave (SW) theory,[24–27]

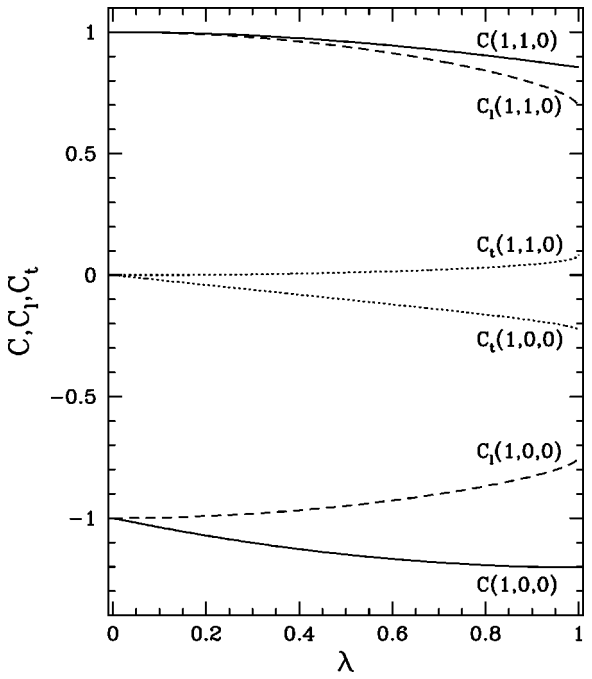

FIG. 4. Correlators for nearest and next-nearest neighbors for the simple cubic lattice. Full, dashed, and dotted lines represent total, longitudinal, and transverse correlators, respectively.

variational methods,[28] or perturbation series about the Ising limit[27,29] start from a broken symmetry state, which is preserved during the calculation. It seems highly likely, although we know of no proof, that these approaches will yield the correct symmetry-broken state of the infinite isotropic system.

We have computed series expansions for a number of local correlators for the square lattice $S=\frac{1}{2}$ antiferromagnet. The expansions start from the Ising limit and are carried through order 14,9,9,9,7 for $C(\mathbf{r})$, $C_l(\mathbf{r})$ with $\mathbf{r}=(0,1)$, (1,1), (2,0), (3,0), (4,0). The series coefficients (for $t=0$) are given Table III.

In analyzing the series it is advantageous to transform to a new variable

$$\delta=1-(1-\lambda)^{1/2}, \tag{16}$$

to remove the singularity at $\lambda=1$. Spin wave theory predicts a square root singularity of this type. This transformation was first proposed by Huse[30] and was also used in earlier work on the square lattice case.[27] We then use both integrated first-order inhomogeneous differential approximants[14] and Padé approximants to extrapolate the series to the isotropic point $\delta=1$ ($\lambda=1$). In the Appendix, we give a brief summary of the analysis method, with an example. The results are shown as functions of λ in Fig. 2 for $\mathbf{r}=(1,0)$, (1,1). We also show the transverse correlator, obtained from Eq. (3b). In the Ising limit the total and longitudinal correlators are equal and the transverse correlator is zero. As we increase the transverse coupling, the longitudinal correlators decrease in magnitude while, as expected, the transverse correlators increase, while the total correlator increases in magnitude for nearest neighbors, but is reduced for second neighbors. The behavior of further correlators is similar, and is not shown. It is also noteworthy that at $\lambda=1$ the longitudinal and transverse correlators remain unequal, reflecting the symmetry broken ground state. In Fig. 3 we show a comparison between our series results and other methods for the nearest neighbor correlators. For small λ all methods are in close agreement, but near the isotropic point linear spin wave theory become poor for longitudinal (and transverse) correlators, whereas exact finite lattice diagonalizations have longitudinal and transverse correlators equal at $\lambda=1$. Third order spin-wave theory is much better, being almost indistinguishable from the series results over the whole range of λ.

TABLE VI. Values of correlators for the isotropic $S=\frac{1}{2}$ Heisenberg antiferromagnet on the simple cubic lattice.

r	Series (this work)			Linear spin wave theory[a]		
	$C(\mathbf{r})$	$C_l(\mathbf{r})$	$C_t(\mathbf{r})$	$C(\mathbf{r})$	$C_l(\mathbf{r})$	$C_t(\mathbf{r})$
(1,0,0)	-1.2028(3)	-0.775(3)	-0.214	-1.1943	-0.6866	-0.2539
(1,1,0)	0.857(2)	0.683(8)	0.087	0.8440	0.6866	0.0787
(2,0,0)	0.807(2)	0.684(8)	0.061	0.7900	0.6866	0.0517
(3,0,0)	-0.768(8)	-0.676(8)	-0.046	-0.7317	-0.6866	-0.0226
(4,0,0)	0.755(8)	0.672(8)	0.041	0.7097	0.6866	0.0116

[a]For $\mathbf{r}=(1,0,0)$ we also have results from second and third order spin-wave theory (Ref. 27), which give for C, C_l, and C_t respectively $-1.2038, -0.7756, -0.2141$ (second order) and -1.2033, -0.770(2), -0.2165(9) (third order).

In Table IV we give numerical estimates of all the correlators at the isotropic point, obtained by our series method and by exact diagonalization–Monte Carlo on finite lattices[17,20] and linear spin wave theory.[6] We believe that the expressions in Ref. 6 contain minor errors, and should read, for 0 and **r** on the same sublattice

$$\langle \mathbf{S}_0\cdot\mathbf{S}_r\rangle = S^2+S\left(1-\frac{2}{N}\sum_{\mathbf{k}}\frac{1-\cos\mathbf{k}\cdot\mathbf{r}}{\sqrt{1-\lambda^2\gamma_k^2}}\right)+\cdots, \tag{17}$$

$$\langle S_0^z S_r^z\rangle = S^2+S\left(1-\frac{2}{N}\sum_{\mathbf{k}}\frac{1}{\sqrt{1-\lambda^2\gamma_k^2}}\right)+\cdots,$$

while for 0 and **r** on different sublattices

$$\langle \mathbf{S}_0\cdot\mathbf{S}_r\rangle = -S^2-S\left(1-\frac{2}{N}\sum_{\mathbf{k}}\frac{1-\lambda\gamma_k\cos\mathbf{k}\cdot\mathbf{r}}{\sqrt{1-\lambda^2\gamma_k^2}}\right)+\cdots, \tag{18}$$

$$\langle S_0^z S_r^z\rangle = S^2+S\left(1-\frac{2}{N}\sum_{\mathbf{k}}\frac{1}{\sqrt{1-\lambda^2\gamma_k^2}}\right)+\cdots,$$

where the notation is as in Ref. 6, and λ is the anisotropy parameter.

We note from Eqs. (17) and (18) and Table IV that first order spin-wave theory gives a longitudinal correlator which is independent of distance, clearly an artifact of the approximation. The total correlator is however consistent with the series results. The picture is considerably improved in higher

TABLE VII. The results of $\{m/n/l\}$ integrated differential approximants to the series in δ for $C_l(\mathbf{r})$ in the square lattice with $\mathbf{r}=(1,1)$ and the strength of local staggered field $t=0$ and 0.5. An asterisk denotes a defective approximant.

n	$\{(n-2)/n/l\}$	$\{(n-1)/n/l\}$	$\{n/n/l\}$	$\{(n+1)/n/l\}$	$\{(n+2)/n/l\}$
			$l=0$ and $t=0$		
$n=1$		0.43718	0.44015	0.43989	
$n=2$	0.43979	0.43758			
$n=3$					
			$l=1$ and $t=0$		
$n=1$		0.44040	*		
$n=2$	0.43017				
			$l=0$ and $t=0.5$		
$n=1$			0.36788	*	0.46865
$n=2$		0.47864*	0.44338	0.43180	0.43299
$n=3$	0.41540	0.41979	0.43291	0.43341	0.43303
$n=4$	*	0.43326	0.43296		
$n=5$	0.43131				
			$l=1$ and $t=0.5$		
$n=1$					0.05032*
$n=2$		0.42988	0.40929	0.43366	0.43336
$n=3$	0.41873	*	0.43335	0.43323	
$n=4$		0.42953			
			$l=2$ and $t=0.5$		
$n=1$			0.47279	0.21519*	0.49440
$n=2$	0.38870	0.41838	0.43031	0.43313	0.43151
$n=3$	0.41813	0.43194	0.43094		
$n=4$	0.43053				
			$l=3$ and $t=0.5$		
$n=1$				0.42163	0.46727*
$n=2$	0.50773*	0.43001	0.43036	0.43108	
$n=3$	0.43944	0.43105			

order spin-wave theory where, for example, third order spin wave theory[27] gives 3-figure agreement with series for all of C, C_l, and C_t for nearest neighbors. We have not attempted to carry this out for further neighbors, and are unaware of any work along these lines.

IV. THE THREE-DIMENSIONAL CASE

We have used the same series approach to calculate correlators for the $S=\frac{1}{2}$ antiferromagnet on the simple cubic lattice. The magnetically ordered ground state will again be reflected in a difference between longitudinal and transverse correlators at the isotropic limit.

Expansions, starting from the Ising limit, have been obtained for $C(\mathbf{r})$, $C_l(\mathbf{r})$ for the five cases $\mathbf{r}=(1,0,0)$, (1,1,0), (2,0,0), (3,0,0), (4,0,0) to order 12,7,9,7,7 respectively. We have again used a staggered field term $t\Sigma_i(-1)^i S_i^z$ to improve convergence. The series coefficients (for $t=0$) are given in Table V. The series is extrapolated in a similar way as that for the square lattice. Figure 4 shows the nearest and next-nearest neighbor correlators as functions of the anisotropy parameters. This is qualitatively similar to Fig. 2, but clearly shows that in 3-dimensions transverse correlators are reduced and the difference between transverse and longitudinal correlators is increased for all values of the anisotropy parameter.

In Table VI we give numerical estimates of all correlators at the isotropic point, and a comparison with first order spin-wave theory. It is apparent that the correlators fall off more slowly with distance than in the two-dimensional case, reflecting the greater stability of antiferromagnetic long-range order in the ground state in 3-dimensions. It is also apparent that the transverse correlators are, relatively, much weaker in 3-dimensions, consistent with weaker quantum fluctuations. Linear spin-wave theory gives reasonable results for the total correlators, but again suffers from the defect of having longitudinal correlators independent of distance. Third-order spin-wave theory gives results for nearest neighbor correlators in excellent agreement with the series results.

V. CONCLUSIONS

We have used series methods to obtain numerical estimates for short-distance ground state correlation functions for the $S=\frac{1}{2}$ Heisenberg antiferromagnet on square and simple cubic lattices. Despite their importance in characteris-

ing the nature of the antiferromagnetic ground state, there appears to have been little previous work on the subject.

The series approach is able to provide rather precise estimates for correlators up to at least 4 lattice spacings. The results reflect the known breaking of rotational symmetry in the ground state, in that longitudinal and transverse correlators remain unequal even in the isotropic Hamiltonian limit. Exact diagonalizations and Monte Carlo calculations on finite lattices are unable to account for this and hence will not yield correct estimates for longitudinal and transverse correlators separately. In 3-dimensions no results are available from diagonalizations or quantum Monte Carlo, beyond nearest neighbors.

We have shown that first-order spin wave theory gives rather poor estimates but second and third order spin wave theory gives excellent agreement with series results for nearest-neighbor correlators. Higher order spin wave results have not been obtained for further correlators, to our knowledge.

As a test of the method we also computed correlation series for the one-dimensional case. The results were quantitatively accurate, but less precise than the DMRG method.

This approach can also be used to calculate correlators for more complex models involving competing interactions. For example, we have studied the J_1-J_2 model,[31] which has a quantum critical point at $J_2/J_1\simeq 0.38$, where the Néel order is destroyed and the system enters a magnetically disordered spin-liquid phase. We find that the difference between longitudinal and transverse correlators remains nonzero in the Neél phase, but vanishes at the quantum critical point, indicating a restoration of full rotational symmetry in the ground state at that point. We expect this method to prove useful in other problems of this type.

ACKNOWLEDGMENTS

This work forms part of a research project supported by a grant from the Australian Research Council. We thank Dr. Oleg Sushkov for stimulating our interest in this problem. The computation has been performed on Silicon Graphics Power Challenge and Convex machines. We thank the New South Wales Centre for Parallel Computing for facilities and assistance with the calculations.

APPENDIX: SOME DETAILS OF SERIES ANALYSIS

For the reader who is not familar with series analysis techniques, we give here a brief summary.

We have employed the standard techniques of integrated differential approximants and naive Padé approximants[14] to extrapolate the series. The integrated differential approximants are a natural generalization of the Padé approximant, and can approximate more general types of singularities.[14] The $\{m/n/l\}$ first-order inhomogeneous differential approximant to a function

$$f(\lambda)=\sum_{n\geqslant 0} a_n\lambda^n$$

is a function of polynomials P_n, Q_m and R_l of degree n, m, and l respectively, satisfying the differential equation:

$$P_n(\lambda)\frac{df(\lambda)}{d\lambda}+Q_m(\lambda)f(\lambda)+R_l(\lambda)=0(\lambda^{n+m+l+2}). \tag{A1}$$

Once P_n, Q_m and R_l are determined order-by-order from Eq. (A1), the approximant is the function which satisfies Eq. (A1) with the right-hand side replaced by zero. It may be found by numerical integration.

The results of integrated differential approximants for series $C_l(\mathbf{r})$ in square lattice with $\mathbf{r}=(1,1)$ and strength of local staggered field $t=0$ and 0.5 are given in Table VII. Disregarding the outlying approximants we estimate $C_l(1,1)=0.430\pm 0.006$, where the error is an estimated confidence limit.

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