

Density matrix renormalization group study of critical behavior of the spin- $\frac{1}{2}$ alternating Heisenberg chain

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We investigate the critical behavior of the $S=1/2$ alternating Heisenberg chain using the density matrix renormalization group. The ground-state energy per spin, \tilde{e}_0 , and singlet-triplet energy gap $\tilde{\Delta}$ are determined for a range of alternations δ . Our results for the approach of \tilde{e}_0 to the uniform chain limit are well described by $c\delta^p$, with $p \approx 1.45$. The singlet-triplet gap is also well described by a power law, with $p \approx 0.73$, half of the \tilde{e}_0 power. The renormalization group predictions of power laws with logarithmic corrections can also accurately describe our data provided that a surprisingly large-scale parameter δ_0 is present in the logarithms.

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I. INTRODUCTION

The approach of quantum spin systems to criticality is an interesting and rather underexplored problem in computational physics. In this paper we consider the critical behavior of one of the simplest quasi-one-dimensional (quasi-1D) quantum spin systems, the alternating Heisenberg chain with spin $1/2$, as it approaches the uniform chain limit. This model is of special interest for the study of critical behavior, since much is known analytically about the gapless uniform-chain limit through the Bethe ansatz. This system is also important for studies of the magnetic spin-Peierls effect and gives a reasonably accurate description of magnetic interactions in many dimerized quasi-1D antiferromagnets.

The alternating Heisenberg antiferromagnet is a simple generalization of the uniform Heisenberg chain, with the nearest-neighbor exchange constant J replaced by two alternating values. The spin- $1/2$ system is defined by the Hamiltonian

$$H = \tilde{J} \sum_{i=1}^{L/2} [(1 + \delta) \vec{S}_{2i-1} \cdot \vec{S}_{2i} + (1 - \delta) \vec{S}_{2i} \cdot \vec{S}_{2i+1}] \quad (1)$$

and has a spin-singlet ground state with energy E_0 and a nonzero singlet-triplet gap $E_1 - E_0$ for any alternation¹ $0 < \delta < 1$.

For our study we introduce a finite-lattice, scaled ground-state energy per spin,

$$\tilde{e}_0(L, \delta) = E_0(L, \delta) / L\tilde{J}, \quad (2)$$

and a corresponding singlet-triplet gap

$$\tilde{\Delta}(L, \delta) = [E_1(L, \delta) - E_0(L, \delta)] / \tilde{J}. \quad (3)$$

The tilde indicates that these energies are scaled by \tilde{J} rather than $J \equiv (1 + \delta)\tilde{J}$, which would divide our results by a factor of $(1 + \delta)$ (*albeit* giving the same leading critical behavior). In addition, energies quoted with a single real argument and a tilde [e.g., $\tilde{e}_0(\delta)$] are bulk limits of the scaled alternating

chain, those with no tilde and a single integer argument [e.g., $e_0(L)$] are finite- L uniform chain results, and those with no arguments (e.g., e_0) are bulk limits of the uniform chain.

The uniform spin- $1/2$ Heisenberg antiferromagnetic chain, which we recover at $\delta=0$, is the best understood 1D critical quantum spin system. It has a ground-state energy per spin of $e_0 = 1/4 - \ln 2$ and a band of gapless spin-triplet excitations with dispersion relation $\omega(k)/J = \pi/2 |\sin(k)|$. The approach of noncritical models to this limiting case is not well established and has been the subject of surprisingly few theoretical and numerical studies.

Early analytical studies of the effect of a small alternation δ on the uniform chain were reported by Cross and Fisher² and Black and Emery.³ Cross and Fisher used a Jordan-Wigner transformation to map the original spin problem onto a pseudofermion Hamiltonian and approximated the latter by an exactly solvable Luttinger-Tomanaga model. This approach, which unfortunately involves uncontrolled approximations, yields critical exponents [defined by $f(\delta) \propto \delta^p$] of $p=4/3$ for the ground-state energy and $p=2/3$ for the singlet-triplet gap.

Black and Emery³ related the critical behavior of the alternating Heisenberg chain to the four-state Potts model and found logarithmic corrections to these power laws,

$$e_0 - \tilde{e}_0(\delta) \propto \delta^{4/3} / |\ln \delta|, \quad (4)$$

for the ground-state energy per spin, and

$$\tilde{\Delta}(\delta) \propto \delta^{2/3} / |\ln \delta|^{1/2}, \quad (5)$$

for the gap. Note that at this order the gap scales as the square root of the ground-state energy defect. More recent theoretical work by Affleck *et al.*⁴ has shown that Eqs. (4) and (5) are leading-order predictions of the renormalization group (RG). The overall constants in these results and implicit in the logarithms are nonuniversal and have not yet been determined analytically for this model.

Strong-coupling series have been derived to high order for the alternating chain and used to study critical behavior (see

Singh and Weihong⁵ and references cited therein). Singh and Weihong used Padé approximants to determine “effective” critical exponents for the ground-state energy defect, singlet-triplet gap, and other observables.

Several previous numerical studies have investigated the critical behavior of spin-1/2 alternating Heisenberg chains using bulk-limit extrapolations of exact diagonalization results on systems up to about $L=30$ in extent (see Barnes *et al.*⁶ and Yu and Haas⁷ and references cited therein). We shall see that important systematic errors can arise from extrapolations using these relatively small systems—for example, in estimates of critical exponents.

Studies of much larger spin-1/2 alternating Heisenberg chains have also been published using the density matrix RG (DMRG) algorithm, although there has been little systematic study of the critical behavior of the simple alternating chain model of Eq. (1) using the DMRG method. The single published reference on this topic is the work of Uhrig *et al.*,¹⁰ who estimate a gap critical exponent of 0.65. Their numerical energies, however, deviate systematically from this power law at small alternation δ (see Fig. 3 of Uhrig *et al.*¹⁰). In related work, Chitra *et al.*⁹ used the DMRG method to study the effects of dimerization and frustration on a generalized alternating chain model with next-nearest-neighbor couplings, and Lou *et al.*¹¹ studied the gap induced by a staggered magnetic field.

In this work we present a systematic DMRG study of the critical behavior of the original alternating spin-1/2 Heisenberg chain of Eq. (1) and compare the theoretical predictions, Eqs. (4) and (5), to numerical results for the ground-state energy per spin and singlet-triplet gap of this model, using systems up to $L=192$ in extent.

II. NUMERICAL METHOD

For our numerical study we employed the density matrix renormalization group algorithm,⁸ which is a very effective method for studying critical behavior in quasi-1D quantum spin systems. Numerical determination of the critical behavior of the alternating chain, or any similar quantum spin system, is a daunting computational task. One must accurately determine energy eigenvalues on quite large systems, since characteristic lengths typically diverge at critical points. An extrapolation through a series of fixed- L results is then required on sufficiently large lattices to ensure that one is in an asymptotic regime in which finite-size effects can be accurately parametrized and eliminated. The computer memory requirements for diagonalizing these large systems are such that the detailed critical behavior of relatively few quantum spin systems has been explored numerically.

The DMRG algorithm has previously been applied to various interacting fermion systems, including one-dimensional spin chains,⁸ lattice models,¹² quasilinear molecules,¹³ and nuclei.^{14,15} The essential concept in the DMRG method is to “grow” a small, finite system into a larger one by the iterative incorporation of new lattice sites. At each such iteration one retains only the m most relevant basis states for spanning the targeted energy eigenstate. (These basis states are chosen according to a density-matrix

weight.) This selective sampling of Hilbert space yields accurate energy eigenvalues on systems which are well beyond the limits of exact diagonalization. For details of the DMRG method we refer the reader to the original papers of White⁸ and to a series of lectures recently compiled by Peschel *et al.*¹²

Our numerical implementation proceeds as follows. We divide the spin chain into blocks A - a - B - b , where A and B denote the “system” and “environment” blocks and a and b are elementary blocks to be added to A and B , respectively. Blocks b and A are linked by periodic boundary conditions. We take spin dimers (two lattice sites of spin $s=1/2$ each) as our elementary blocks and use the infinite algorithm to grow the spin chain, while targeting the lowest-lying spin-0 or spin-1 state. In the case of the spin-0 ground state of the alternating Heisenberg chain, we found that subsequent sweeps with the finite algorithm do not lead to much improvement in the results of the infinite algorithm. In contrast, for the spin-1 state we found that sweeps with the finite algorithm were important for convergence. Our DMRG implementation uses large, sparse matrices, so the sparse matrix package ARPACK (Ref. 16) was employed. The time-consuming matrix-vector multiplications and the Arnoldi-Lanczos algorithm ARPACK were parallelized.

The ground-state energy per spin $\tilde{e}_0(L, \delta)$ of a spin chain of length L and alternation δ is of special interest for our study of critical behavior [see Eq. (2)]. The DMRG method yields approximate values $\tilde{e}_0(m; L, \delta)$ that typically converge exponentially fast from above as one increases the number m of states retained.^{8,12} We also observed this behavior in the present study. We computed $\tilde{e}_0(m; L, \delta)$ numerically using the DMRG method on chains of length $L=28, 48, 96, 144$, and 192 and alternation $\delta=2^{-3}, 2^{-4}, 2^{-5}, \dots, 2^{-10}$. At each L and δ we increased m in steps of 10 starting at $m=30$ until a fit of the form $\tilde{e}_0(m; L, \delta) = \tilde{e}_0(L, \delta) + c_1 \exp(-c_2 m)$ gave sufficiently stable coefficients for our desired accuracy; this m extrapolation yielded our DMRG energy estimate $\tilde{e}_0(L, \delta)$. We found that the maximum m needed for convergence to a given accuracy increases with increasing chain length L and decreasing alternation δ . For our extreme case $L=192$ and $\delta=2^{-10}$, adequate convergence was not achieved until $m=150$, and we retained the maximum of $m=170$ states in this case. This resulted in a sparse matrix problem of dimension $\approx 9 \times 10^4$ at each DMRG iteration. Finally, we also confirmed recovery of exact $L=28$ alternating chain results on allowing our DMRG code to iterate to the full Hilbert space. Figure 1 shows the m -dependent DMRG results for two computationally challenging sets of parameters ($L=144, 192, \delta=2^{-10}$) for the spin-0 ground-state energy (left panel) and the spin-1 ground-state energy (right panel). The exponential fits shown evidently describe the large- m data points quite well.

III. RESULTS

Table I gives our DMRG results for the ground-state energy per spin for different alternations δ and chain lengths L . For the rather large alternations $\delta=2^{-3}$ and 2^{-4} we con-

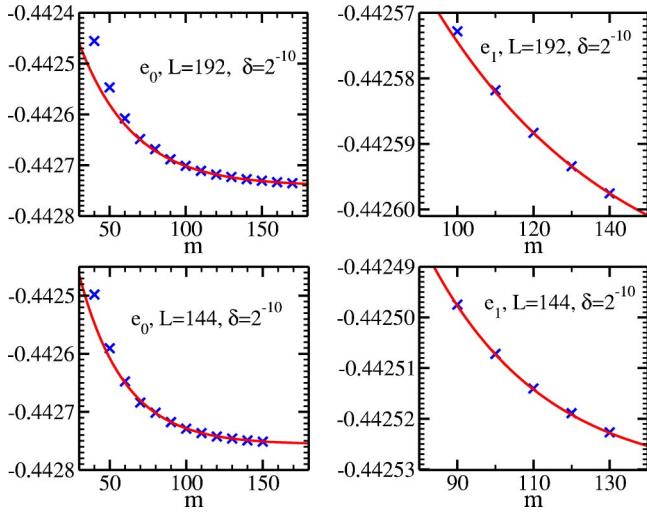


FIG. 1. Left panel: m -dependent DMRG results (data points) for the spin-0 ground-state energy e_0 and alternation $\delta=2^{-10}$ for spin chains of length $L=144$ (bottom) and $L=192$ (top) and exponential fits to the high- m data points (solid lines). Right panel: same as left panel, but for the spin-1 ground-state energy e_1 .

firmed convergence to accurately known energies with increasing basis state number m , as well as convergence with increasing chain length L . Finite-size effects were more pronounced at smaller δ , as expected since the system is closer to criticality. We estimate that the energy errors in Table I are a few units in the last digit, based on the difference between the maximum- m DMRG result and the exponential $m \rightarrow \infty$ extrapolation which we quote.

Figure 2 shows the approach of $\tilde{e}_0(L, \delta)$ to the limit $e_0 = 1/4 - \ln 2$ as a function of alternation δ for spin chains of increasing length, $L=28, 48, 96, 144$, and 192 . Finite-size effects are evident for sufficiently small δ even for the largest system size considered in this work. However, the asymptotic large- L envelope evident in this figure for $\delta \gtrsim 2^{-8}$ clearly shows the bulk limit. The dashed line is a power-law fit $c_0 \delta^p$ to this envelope, which gives $c_0=0.39$ and exponent $p=1.45$. The renormalization group prediction $p=4/3$ from Eq. (4) (without the logarithmic factor) is also shown, displaced for clarity of presentation. Clearly this gives an inferior description of the DMRG data over the range considered here.

Figure 3 shows the singlet-triplet gap $\tilde{\Delta}(L, \delta)$ as a function of alternation δ for spin chains of length $L=28, 48, 96, 144$, and 192 . The envelope of these curves is the bulk limit $\tilde{\Delta}(\delta)$, which is evident for $\delta \gtrsim 2^{-7}$. For smaller values of the alternation δ , finite-size effects are evident in the figure even for $L=192$. A power-law fit to $\tilde{\Delta}(\delta)$ as for $\tilde{e}_0(\delta)$ gives $c_0=1.94$ and $p=0.73$, shown as a dashed line in Fig. 3. The renormalization group prediction $p=2/3$ from Eq. (5) is also shown, displaced for presentation. Evidently the renormalization group exponent (without the logarithmic term) again gives a less accurate description of our DMRG data. Note that the two exponents obtained in our fits are related by a factor of 2, which implies that the $\tilde{e}_0(\delta)$ defect scales as $\tilde{\Delta}(\delta)^2$. This relation also follows from the leading-order

TABLE I. Extrapolated DMRG results for the lowest energy per spin in the spin- s sector, $e_s(L, \delta) \equiv \tilde{e}_s(L, \delta)/(1 + \delta)$, for various alternations δ and chain lengths L . The estimated error is a few units in the final digit.

δ	L	$e_0(L, \delta)$	$e_1(L, \delta)$
2^{-3}	28	-0.4110961	-0.3976678
2^{-3}	48	-0.4110928	-0.4032882
2^{-3}	96	-0.4110928	-0.407191
2^{-3}	144	-0.4110928	-0.4084913
2^{-3}	192	-0.41109284	-0.4091416
2^{-4}	28	-0.4239186	-0.4149855
2^{-4}	48	-0.4238627	-0.418895
2^{-4}	96	-0.4238617	-0.4213883
2^{-4}	144	-0.4238619	-0.422211
2^{-4}	192	-0.4238618	-0.422623
2^{-5}	28	-0.4325593	-0.4258695
2^{-5}	48	-0.4323071	-0.429086
2^{-5}	96	-0.4322899	-0.430754
2^{-5}	144	-0.432290	-0.431263
2^{-5}	192	-0.4322906	-0.431518
2^{-6}	28	-0.4378673	-0.4319820
2^{-6}	48	-0.437370	-0.435005
2^{-6}	96	-0.437284	-0.436321
2^{-6}	144	-0.437283	-0.436652
2^{-6}	192	-0.437285	-0.43681
2^{-7}	28	-0.4408870	-0.435219
2^{-7}	48	-0.440254	-0.438202
2^{-7}	96	-0.440074	-0.439410
2^{-7}	144	-0.440058	-0.439664
2^{-7}	192	-0.440064	-0.439768
2^{-8}	28	-0.4425056	-0.4368847
2^{-8}	48	-0.441826	-0.439863
2^{-8}	96	-0.44158	-0.4410442
2^{-8}	144	-0.441550	-0.441275
2^{-8}	192	-0.441550	-0.441360
2^{-9}	28	-0.4433439	-0.4377293
2^{-9}	48	-0.442650	-0.440709
2^{-9}	96	-0.442384	-0.441885
2^{-9}	144	-0.442340	-0.442109
2^{-9}	192	-0.442336	-0.442190
2^{-10}	28	-0.4437703	-0.4381546
2^{-10}	48	-0.443073	-0.441136
2^{-10}	96	-0.44281	-0.442311
2^{-10}	144	-0.442756	-0.442532
2^{-10}	192	-0.442741	-0.442614
0	28	-0.444201	-0.4385820
0	48	-0.443504	-0.441566
0	96	-0.44323	-0.442741
0	144	-0.44318	-0.442965

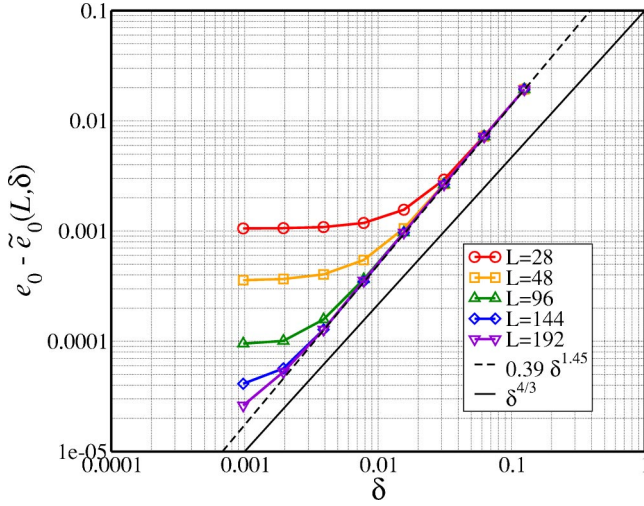


FIG. 2. Approach of $\tilde{e}_0(L, \delta)$ to the uniform-chain limit $e_0 = 1/4 - \ln(2)$ with decreasing alternation δ and increasing chain length L . The dashed line shows a fit to a power law, $c_0 \delta^p$, which gives $c_0 = 0.39$ and an exponent of 1.45. The solid line shows the renormalization group exponent $4/3$ (displaced for presentation, without logarithmic corrections).

renormalization group, Eqs. (4) and (5). Our value of $p = 0.73$ is consistent with the “effective” critical exponent quoted by Singh and Weihong.⁵ Note, however, that we estimate a different value for the \tilde{e}_0 power,¹⁷ due to their scaling of the Hamiltonian by a factor of $(1 + \delta)^{-1}$.

It is especially interesting to determine whether there is numerical evidence for logarithmic corrections to pure power-law behavior, as predicted by the renormalization group in Eqs. (4) and (5). We first consider the bulk-limit ground-state energy per spin, predicted to asymptotically approach the uniform chain limit as

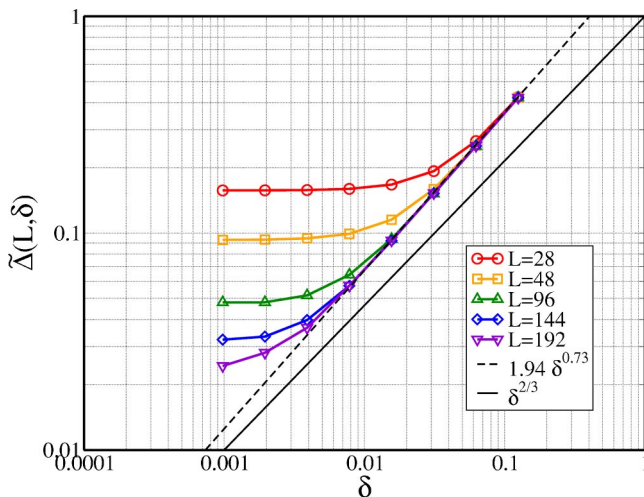


FIG. 3. Critical behavior of the singlet-triplet gap $\tilde{\Delta}(L, \delta)$ as a function of alternation δ for spin chains of length L . The dashed line shows a power-law fit, $c_0 \delta^p$, which gives $c_0 = 1.94$ and exponent $p = 0.73$. The solid line shows the renormalization group exponent $p = 2/3$ (displayed as in Fig. 2).

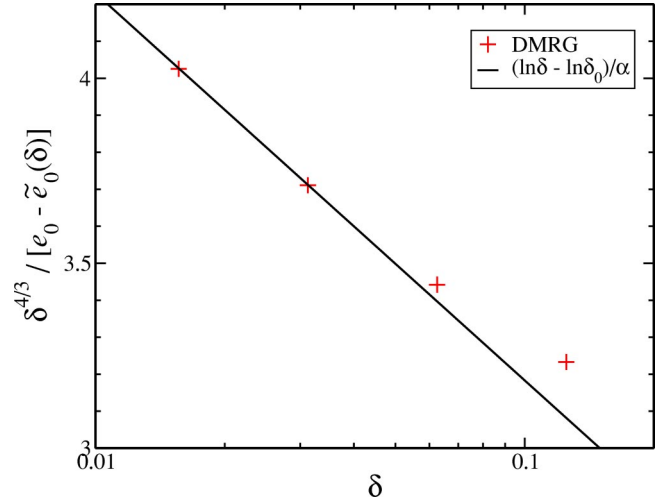


FIG. 4. Estimation of the constants α and δ_0 in Eq. (6) from our DMRG data.

$$e_0 - \tilde{e}_0(\delta) = \alpha \frac{\delta^{4/3}}{\ln(\delta/\delta_0)}. \quad (6)$$

Here we have introduced an overall constant α and scale parameter δ_0 , which we will estimate from our DMRG data. On rearranging Eq. (6) we obtain the easily visualized form

$$\frac{\delta^{4/3}}{e_0 - \tilde{e}_0(\delta)} = \alpha^{-1} (\ln \delta - \ln \delta_0). \quad (7)$$

Figure 4 shows our DMRG results for $\delta^{4/3}/[e_0 - \tilde{e}_0(\delta)]$ [the left-hand side of Eq. (7)] versus $\ln \delta$. The data clearly disagree with the leading-order renormalization group prediction, Eq. (6), over this range of δ , since the points do not lie on a straight line. Assuming that the two smallest- δ points are close to asymptotic, we estimate $\alpha \approx -2.2$ and $\delta_0 \approx 110$. A similar fit to the singlet-triplet gap gives

$$\left(\frac{\delta^{2/3}}{\tilde{\Delta}(\delta)} \right)^2 = \alpha_{gap}^{-1} (\ln \delta - \ln \delta_0), \quad (8)$$

with $\alpha_{gap} \approx -19.4$ and $\delta_0 \approx 115$. With these constants the theoretical renormalization group results, Eqs. (4) and (5), are barely distinguishable from our power-law fits in Figs. 2 and 3. There are no predictions of these constants in the literature to our knowledge.

Equation (6) can be reexpressed as an effective power $p_{eff}(\delta) = 4/3 + 1/\ln(\delta_0/\delta)$. With $\delta_0 = 110$, the range $\delta = 10^{-3} \rightarrow 10^{-1}$ corresponds to $p_{eff} = 1.42 \rightarrow 1.47$, which may explain our good numerical agreement with a pure power of exponent $p = 1.45$.

We have also investigated finite-size effects in the uniform Heisenberg chain ($\delta = 0$). This serves as a consistency check for our numerical computations since comparison with analytical result is possible. Woynarovich and Eckle¹⁸ and Affleck *et al.*⁴ quote Bethe-ansatz predictions and results from conformal field theory, respectively, for the leading finite-size contributions to the ground-state energy per spin and singlet-triplet gap,

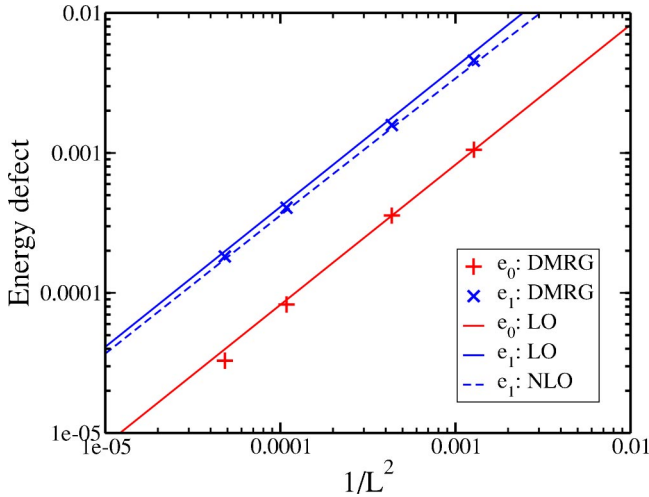


FIG. 5. Finite-size energy defects $|e_s(L) - e_0|$ of the lowest spin- s levels on the uniform chain vs chain length L . The data points are DMRG (+: spin-0, \times : spin-1) and the lines are analytical results [leading order (LO), solid line; next-to-leading order (NLO), dashed line], from Eqs. (9) and (10).

$$e_0 - e_0(L) = \frac{\pi^2}{12L^2} [1 + O((\ln L)^{-3})] \quad (9)$$

and

$$e_1(L) - e_0 = \frac{5\pi^2}{12L^2} \left(1 - \frac{3}{5} (\ln L)^{-1} + O((\ln L)^{-2}) \right). \quad (10)$$

Figure 5 shows our DMRG data for these energy defects on uniform chains of length $L=28, 48, 96,$ and 144 , together with the analytical results.

The agreement between the leading-order analytical predictions for finite-size corrections to the ground-state energy per spin [Eq. (9)] and our DMRG results is evidently very good on the shorter chains. The discrepancy evident at $L=144$ may be due to convergence problems encountered by the DMRG algorithm when applied to this asymptotically gapless system on large lattices. The DMRG results for the spin-1 energy defect depart significantly from the leading-order term in Eq. (10), but are consistent with this prediction when we include the $O(L^{-2}(\ln L)^{-1})$ correction.

Finally we consider the dependence of the ground-state energy per spin $\tilde{e}_0(L, \delta)$ on the chain length L for fixed, nonzero alternation δ . This is especially relevant to exact diagonalization studies, which extrapolate to the bulk limit from rather small systems of at most about 30 spins. To test

the accuracy of finite size extrapolations we used DMRG to compute the ground-state energy per spin and singlet-triplet gap on chains of length $L=28, 32, 36, 40, 44,$ and 48 , and fitted the results to $f(L) = a + b \exp(-L/c)/L$ and $g(L) = a + b \exp(-L/c)$, respectively. (These forms were used to extrapolate exact diagonalization results to the bulk limit by Barnes *et al.*⁶ and Yu and Haas.⁷) Both functions yield reasonably good fits to our six data points in the range $L=28, \dots, 48$. However, on comparing this extrapolation with our DMRG results on $L=96, 144,$ and 192 lattices, we noted clear discrepancies as the alternation δ decreases. This is likely due to a rapid increase in the characteristic length [modeled by c in the exponents of $f(L)$ and $g(L)$], which makes subleading terms in the asymptotic behavior more important. Our results thus suggest caution in attempting to establish critical behavior from studies of relatively small systems. For this reason, we prefer not to extrapolate our DMRG data to larger system sizes. It would be of great interest to study the asymptotic forms of the large- L finite-size dependence both numerically and analytically, since these are required for accurate estimates of bulk-limit properties.

IV. SUMMARY

We have employed the DMRG algorithm to determine the ground-state energy per spin and singlet-triplet gap of the alternating Heisenberg chain and studied the critical behavior of this model in the limit of small alternation. We find that the approaches of the bulk-limit ground-state energy per spin and singlet-triplet gap to the uniform chain limits are well described by power laws in the alternation parameter δ over the range $0.008 \leq \delta \leq 0.1$ and scale approximately as $\delta^{1.45}$ and $\delta^{0.73}$, respectively. The renormalization group predictions of power laws times logarithmic corrections also appear consistent with our results, provided that a surprisingly large scale factor δ_0 is present in the logarithms.

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¹A frequently used equivalent definition has alternating couplings of $(J, J\alpha) = ((1 + \delta)\tilde{J}, (1 - \delta)\tilde{J})$.

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