Ground-State Energy of Heisenberg Antiferromagnet for Spins $s=\frac{1}{2}$ and $s=1$ in $d=1$ and 2 Dimensions

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A simple real-space renormalization method yields the ground-state energy of the Heisenberg antiferromagnet. We find the ground-state energy per spin for $s=\frac{1}{2}$ (-0.4438 in 1D, -0.6723 in 2D) and $s=1$ (-1.388 in 1D and -1.907 in 2D) to three-figure accuracy, using properties of relatively small odd-numbered clusters. Our results provide reasonable proof for long-range order in the ground state of the $s=\frac{1}{2}$ Heisenberg antiferromagnet in 2D.

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Over the past decade, real-space renormalization-group (RSRG) techniques have become commonplace in the study of magnetic systems. This technique is not always successful, however, for when the size of the clusters used is smaller than the inherent correlation length the accuracy is severely impaired. In this paper, we show that it is possible to overcome this handicap and obtain results of satisfactory accuracy with relatively limited computational means.

Spin-wave theory[1-3] indicates that the ground-state energy per spin of an Heisenberg antiferromagnet, spins s, can be written in the form $\epsilon_0=e_0J$, with $e_0=-s^2[1+\gamma/2s+O(1/s^2)]$ per site, with $\gamma\approx 0.7$ in one dimension (1D) being a measure of the relatively important quantum fluctuations. But it is well known that, because of excessive long-wavelength fluctuations, spin-wave theory cannot be entirely trusted in 1D nor in 2D, and alternative calculations are a necessity. With modern computers, large-scale calculations are now commonplace and chains of varying lengths up to $n=32$ have been numerically diagonalized,[4] although this remains a relatively expensive procedure with slow convergence.

Our first attempt at an RSRG calculation[5] with *fixed* block size $n=3$ demonstrated a relatively poor accuracy, on the order of 10%, for $s=\frac{1}{2}$ and 1, and failed conspicuously at large spins (predicting $\gamma=0$ in the limit $s\rightarrow\infty$). On the positive side, it is noteworthy that this was an extremely simple calculation, performed analytically at all values of s and yielding closed-form expressions, in which rigorous upper and lower bounds to e_0 were obtained. In more recent studies,[6] we found that extending the cluster size to $n=5$ somewhat improved the accuracy, with additional improvements occurring at each step upon increasing cluster sizes to $n=7, 9, \ldots$, etc. The upper bound is always more accurate (closer to the final result) than the lower, but both converge to a common value at $n\rightarrow\infty$. Nevertheless, convergence appears slow and the relative distance between upper and lower bounds remains on the order of 1% for all attainable cluster sizes. On the face of it, RSRG does not appear to be a promising scheme.

Our new findings have changed this prognosis. They are twofold: First, we have determined that a *least-squares* extrapolation of *both* upper *and* lower bounds to $n\rightarrow\infty$ (where they must meet) allows calculation of the extrapolated ground-state energy to much better accuracy than can be achieve with either one alone. For example, this extrapolation method yields $e_0=-0.44378$ for $s=\frac{1}{2}$ in 1D [the error is in the fourth decimal place as compared with the Bethe-Hulthén exact value,[3] $e_0=(\frac{1}{4}-\ln 2)=-0.44315\ldots$]. The relative error $|\Delta\epsilon_0/\epsilon_0|=0.14\%$ is satisfactory for most applications.

In order to obtain e_0, we fitted some RSRG upper and lower bounds $e_\pm(n)$ that we had calculated previously[6] on relatively short chains of lengths $n=3,5,7,9,11$, and 13, by the following polynomial:

$$e_\pm(n)=e_0(\infty)+A_\pm/n+B_\pm/n^2, \tag{1}$$

where $+/-$ refer to upper/lower bounds. There are twelve data points with which to determine five parameters: $A_\pm$, $B_\pm$, and a common limit point $e_0=e_0(\infty)$. The least-squares fit yields the energy estimate above, with

$$A_+=0.22522,\quad A_-=-0.16581,$$

$$B_+=-0.19598,\quad B_-=0.79132\quad (s=\tfrac{1}{2}).$$

Aside from the exact Bethe-Hulthén result[3] for $e_0(\infty)$, there exist numerical estimates based on finite-length (n) chains with periodic boundary conditions. These always approach the asymptotic value ($n\rightarrow\infty$) from below.

For $s=\frac{1}{2}$, using even-length chains ranging from $n=4$ to 24, Gagliano *et al.* find[7] an extrapolated value $e_0(\infty)=-0.4431\pm0.0001$, which is distinctly closer to the exact answer than is our result.

Applying the RSRG least-squares method to $s=1$ with somewhat sparser data ($n=3$, 5, 7, 9, and 11), we have obtained a ground-state energy per spin $e_0=-1.38814$, and

$$A_+=0.66155,\quad A_-=-0.56895,$$

$$B_+=-0.53447,\quad B_-=2.36447\quad (s=1).$$

There is no exact result with which to compare the $s=1$ ground state, as the Heisenberg antiferromagnet is known[8] to be nonintegrable for $s\geq 1$. Nevertheless, there exist a number of numerical estimates based on finite chains. One of the most recent, that of Nightingale and Blöte,[4] obtains Monte Carlo estimates of the ground-state energy at several values of $n\leq 32$. At $n=16$, they find $e_0(16)=-1.4029\pm0.0001$ and at $n=32$, $e_0(32)=-1.4016\pm0.0002$, which suggests a limiting value $e_0(\infty)\approx-1.400\pm0.002$. This agrees substantially with the work of Moreo ($n\leq 16$), both differing from our RSRG estimate ($n\leq 11$) by 0.86% only. Thus, in 1D the present method is competitive with, but not quite as good as, the standard approaches. The attainable accuracy is, however, always better than 1%.

In 2D there is an extraordinary amount of interest in properties of magnetic systems, because of a number of plausible applications[9] to the new high-T_c superconductors. Here, the present procedure involves (in principle) our taking $n\times n$ blocks, again extrapolating upper and lower bounds to the energy per site, e_0, to a common intersection at $n=\infty$.

In practice, we have found that the accuracy of the RSRG upper bound at 3×3 (nine spins) is now *quite superior* to results on 4×4 clusters (sixteen spins) with periodic boundary conditions,[10] being rather comparable to studies of finite-sixed 8×8 clusters subject to periodic boundary conditions (perforce carried on by Monte Carlo[11] techniques). If we were to adapt Monte Carlo techniques to the present procedure, we could proceed to 5×5 and perhaps 7×7 for both spins $s=\frac{1}{2}$ and $s=1$. Pending these developments, in view of the considerable computational economy that our preliminary finding represents, we have thought it useful to bring it to the attention of our colleagues without further delay.

The finite-sized cluster has to mimic the original unit. Thus, in the Heisenberg antiferromagnet, one is led to compact, odd-numbered clusters, which have a ground-state degeneracy $g=2s+1$ identical to that of a single spin. (By contrast, the "standard approach" studies even-sized clusters with singlet ground states, subject to periodic boundary conditions.) The infinite array is decomposed into such clusters; for the square lattice, we take odd-sized *square* clusters, $n\times n=3\times3$, 5×5,... (rectangular clusters 3×5, etc., even though odd, violate the point-group symmetry). Bonds connecting neighboring clusters are then reevaluated in the subspace of the $2s+1$ ground states of each cluster, by adaptation of a procedure previously described[5,6] for 1D.

In 2D there are n bonds connecting a square cluster to each of its neighbors, for a total of $4n$. This large perimeter might be thought to cause slow convergence (as compared to 1D where there are only two "surface" bonds regardless of the size of the cluster) but quite the opposite turns out to be true [i.e., A_+ in Eq. (1) is unexpectedly small].

Consider a typical cluster and one of its neighbors. The two corner bonds which connect them have identical renormalization parameters ($J\rightarrow\lambda_1^2J$); the two bonds which neighbor them are characterized by a different renormalization-group parameter ($J\rightarrow\lambda_2^2J$), etc., with the middle bond [$(n+1)/2$ from the corner] being unique [$J\rightarrow(\lambda_{(n+1)/2})^2J$]. With use of the Wigner-Eckart theorem, the λ's are calculated in the $(2s+1)$-fold degenerate ground state, by the standard projection technique.[5] Together with the calculated ground-state energy of a cluster, $E_0(n)$, these $(n+1)/2$ parameters are all that are required for a final answer. That is because each cluster, with its $2s+1$ ground-state degeneracy, now resembles a single-spin interacting with its neighbors by means of a renormalized coupling constant $J'=\Lambda^2J$, with $\Lambda^2\equiv[2(\lambda_1^2+\lambda_2^2+\cdots)+(\lambda_{(n+1)/2})^2]$. The scheme is iterated *ad infinitum*.

If J_z differed from J_x or J_y, or if an external field distinguished one spin orientation from the others, then aside from E_0 and Λ the renormalization scheme would involve the flow of one or more additional parameters (e.g., the ratio J_z/J_x) and the series would have to be constructed term by term. This presents no difficulty in principle, and in particular, extension to the ubiquitous quantum XY model is feasible.[12]

In the *isotropic* case considered here, the simple geometric series which ensues for the ground-state energy per spin $\epsilon_0(n)\equiv e_0(n)J$ is summed analytically,

$$e_+(n)=[E_0(n)/(n^2-\Lambda^2)], \tag{2}$$

and represents a (rather tight) variational upper bound to $e_0(\infty)$, while

$$e_-(n)=E_0(n)/n(n-1), \tag{3}$$

obtained by our setting $\Lambda^2=n$, is a (loose) lower bound to $e_0(\infty)$.

With only the $n=3$ cluster available so far, there is, of course, no need for least-squares analysis nor is there a possibility of extrapolation to $n\rightarrow\infty$. However, the upper bound, Eq. (2), is remarkably close to known results already at $n=3$. Table I lists $E_0(3)$; its degeneracy, g; the energy and degeneracy of several low-lying excited states E_1, E_2,... (within the cluster); the ground-state values of λ_1^2, λ_2^2 ($\Lambda^2=2\lambda_1^2+\lambda_2^2$); the resulting upper

TABLE I. Calculated parameters for 3×3 cluster.

$E_i(3)$	g	λ_1^2	λ_2^2	e_0
	$s=\frac{1}{2}$			
−5.2935667	2	0.4090165	0.3079162	−0.67228
−4.1932990	2			
−3.5461862	2			
−3.3113915	2			
Kubo,[1] Nishimori and Miyake[a] (spin waves)				−0.670
Oitmaa and Betts[b] (exact, 4×4)				−0.702
Oitmaa and Betts[b] (estimate for $n\to\infty$)				−0.655
Barnes and Swanson[c] (8×8)				−0.6766
Barnes and Swanson[c] (estimate for $n\to\infty$)				-0.6727 ± 0.0009
Lin[d] (exact, 26 sites)				−0.67201
	$s=1$			
−15.4223967	3	0.3466383	0.2203354	-1.907 ± 0.002
−14.1828763	3			
−13.2539046	0			
−12.7220590	3			

[a]Reference 13.
[b]Reference 10.
[c]Reference 11.
[d]Reference 14.

bound $e_+(3)$ to the ground-state energy for $s=\frac{1}{2}$ and 1 (denoted e_0 in the table); and estimates of e_0 based on a number of other techniques. The lower bounds [$e_-=E_0(3)/6\approx-0.88$ for $s=\frac{1}{2}$, ≈-2.57 for $s=1$] remain quite wide of the mark and so are not useful at this stage.

The small even-numbered clusters underestimate the ground-state energy. It is noteworthy that our 3×3 results (calculated in Hilbert spaces of some 10^3-10^4 states) are much better than the conventional 4×4, and indeed are comparable to the conventional 8×8 (which can only sample, perforce, some 10^{19}-10^{30} states). This implies that $A+,B+$ are much smaller in 2D than in 1D. This unexpected, serendipitous, result should prove beneficial in future investigations.

For $s=1$ in 2D, our numbers are essentially new and there is no reliable basis for comparison.

Finally, it is interesting to note that Table I, combined with the variational principle, yields a practical proof of the existence of long-range order (LRO) in two-dimensional $s=\frac{1}{2}$ antiferromagnets. This topic has been controversial. On the one hand there exist good arguments by Anderson[9] and Wiegmann,[15] as well as numerical results,[16] militating *against* the existence of LRO for $s=\frac{1}{2}$. On the other hand, there exists a rigorous proof for the existence of LRO for $s\geq\frac{3}{2}$ due to Neves and Perez,[17] recently extended to $s=1$ by Kubo[18] and by Affleck *et al.*[19] Although these proofs fail for $s=\frac{1}{2}$, numerical evidence *for* LRO and for a ground-state staggered magnetization $\omega\approx0.6$ comes from several sources.[20] Although it might have been both interesting[9] and surprising for $s=\frac{1}{2}$ to be on a special footing, we shall now supplement the actual calculations in Ref. 10 and prove this not to be the case.

The argument can be stated simply. The calculated $\Lambda^2=2\lambda_1^2+\lambda_2^2$ in a 3×3 cluster ground state is a lower bound for this renormalization-group parameter in this size cluster. Excited states, having energies higher than $E_0(3)$, would be included in a better variational ground state *only insofar as they boosted* Λ^2 and thereby lowered the total energy Ne_0. Any value of $\Lambda^2>1$ implies that the natural antiferromagnetic short-range order of each cluster translates into finite antiferromagnetic LRO (i.e., into a finite ω), because spins which are an infinite distance apart will become *rigidly* connected by bonds involving arbitrarily high powers of $\Lambda^2\to\infty$. The value calculated for $s=\frac{1}{2}$ from Table I is $\Lambda^2=1.1259492$, which substantially exceeds the minimum for LRO, yet variationally underestimates the "true" value. This basically proves the result.

Unfortunately we cannot extend the argument to $s=1$. Our calculated $\Lambda^2=0.913612$ in this case; if this number were definitive, it would indeed *disprove* LRO for $s=1$, as high powers of $\Lambda^2\to0$. However, because the calculated Λ^2 is merely a lower bound to the true value, there is no contradiction with rigorous proofs for $s\geq1$, but merely an intimation that our estimated e_+ for the ground state of $s=1$ could be further improved by some additional ~1%, through the inclusion of such excited states as would boost Λ^2 by the additional 10%.

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