Are Antiferromagnetic Spin Chains Representations of the Higher Wess-Zumino-Witten Models?

Timothy Ziman
Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08855

and

H. J. Schulz
Laboratoire de Physique des Solides, Université de Paris-Sud, 91405 Orsay, France
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We show that while the exactly integrable spin-$\frac{3}{2}$ Heisenberg antiferromagnet is a representation of the nonlinear σ model with nontrivial Wess-Zumino term, the generic massless antiferromagnet has long-wavelength behavior equivalent to spin $\frac{1}{2}$. This is demonstrated by comparing the predictions of conformal symmetry and rotational symmetry to the gaps calculated for finite chains. The leading corrections are eliminated, leading to stable estimates of the conformal central charge and exponents for the spin-correlation functions.

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Some years ago Haldane[1] initiated a program to calculate correlation functions of quantum spin chains by mapping the long-wavelength properties onto those of nonlinear σ models. By a semiclassical argument mapping the spin chains onto an O(3) σ model with topological term $\Theta=\pi$ or 0 for half-integer and integer spin, respectively, he argued that half-integral and integral isotropic antiferromagnets differ in that the integer chains have a singlet ground state and fluctuation-induced gap while the half-integer cases, like the exactly soluble case of spin $\frac{1}{2}$, remain massless. His predictions for spin 1 are supported by both numerical studies[2,3] and neutron-scattering experiments.[4] For higher half-integral spin the ground state is either degenerate or has massless excitations[5] which suggests but does not prove critical correlations.

The question remains: Are the higher spin $S=\frac{3}{2}, \frac{5}{2}, \ldots$ critical and if so what are the universality classes? Haldane's argument suggested asymptotically similar behavior as for spin $\frac{1}{2}$; the same conclusion was reached by Schulz[6] by a Jordan-Wigner transformation, using a procedure that strictly speaking is valid only in the easy plane region of an anisotropic XXZ Hamiltonian. On the other hand, a calculation of the conformal central charge for a special antiferromagnetic Hamiltonian integrable by the Bethe *Ansatz*[7] lead Affleck[8] to identify these models with the Lagrangean of fermions analyzed by Witten[9] possessing a topological term with integer coefficient $k=2S$. Furthermore, by a non-Abelian bosonization that, unlike the Jordan-Wigner procedure, conserves rotational isotropy, Affleck argued that the asymptotic behavior was generic for the isotropic antiferromagnet and found support for this in experimental results on the spin-$\frac{5}{2}$ antiferromagnet tetramethyl ammonium manganese trichloride.[10] This is an interesting idea in that it would allow several experimental realizations of strongly interacting many-body systems behaving quite differently from weakly interacting systems. Furthermore, recent progress in the application of conformal symmetries to quantum field theories in one spatial dimension allows us to relate the algebra of operators of the corresponding field theory to experimental observables.[11] Thus, for example, the central charge of the conformal algebra is experimentally observable as the ratio of the coefficient of linear specific heat to the spin-wave velocity as measured by inelastic neutron scattering.[8,12]

The aim of this study was to resolve the issue of the critical behavior of the antiferromagnets by calculating the exponents for general isotropic Hamiltonians. At the exactly soluble point there is no argument, nor is there for spin $\frac{1}{2}$ where the Wess-Zumino model with term $k=1$ is equivalent to free bosons. The natural choice to study is spin $\frac{3}{2}$ since for larger S convergence will be slower. In principle, this is straightforward as the different critical points have quite distinct algebras: the conformal central charge $c=3k/(2+k)$ and $\eta=3/(2+k)$. For the numerical case taken $k=2S=3$ would imply $c=\frac{9}{5}$, $\eta=\frac{3}{5}$, compared to $c=1$, $\eta=1$ for spin $\frac{1}{2}$ (η is the exponent governing the power-law decay of the spin-spin correlations).

We used the same method for calculating the critical exponents as we did[2] in the study of spin $\frac{1}{2}$ and spin 1: The conformal mapping of the infinite space-time plane to the cylinder relates the power-law decay of correlations in the plane to the amplitude of the scaled gap on the finite cylinder.[11] For quantum systems the infinite axis of the cylinder is taken to be the time coordinate; the finite periodic coordinate, the spatial direction. The novelty compared to the analysis of statistical mechanical models defined on a two-dimensional lattice is that we must scale the time and space dimensions by calculating a spin-wave velocity by diagonalizing the Hamiltonian for finite wave number.

The different correlation functions are distinguished by the different quantum numbers of the excited states that contribute. Thus by solving the Hamiltonian in different orthogonal subspaces we can, in principle, determine the whole operator algebra. We did this previously to distinguish different massless phases in the spin-1 chain with easy-axis anisotropy.[2] The conformal central charge can be calculated from the $1/L^2$ correction to the ground-state energy density,[8,12] again normalized by the spin-wave velocity. In practice the difficulty is that the matrix dimensions increase exponentially with chain length L; for spin $\frac{3}{2}$ one is restricted to chains of $L=12$ long and corrections to scaling decay logarithmically slowly with L.[11,13] Monte Carlo methods could roughly double the accessible chain lengths but with the cost of introducing numerical uncertainties.

Early results for a nearest-neighbor antiferromagnet gave exponents that were interpreted to be in favor of Affleck's conjecture,[14] but as we shall see, are correctly understood as crossover effects. The remedy for the slow convergence is to study a more complete spectrum of levels for finite chains. By measuring scaling dimensions that are predicted to be degenerate in the thermodynamic limit we can estimate corrections due to finite size from a fixed length rather than by a hazardous extrapolation. The crucial point is that for all coefficients k at the fixed point as well as conformal symmetry there is an SU(2)⊗SU(2) symmetry, higher than the original SU(2) lattice symmetry. Then, in addition to the conformal towers of operators predicted by the Virasoro algebra of the conformal group, the Kac-Moody algebra of the SU(2)⊗SU(2) group[15] determines a set of operator dimensions distinct for each coupling k. However, there are degeneracies which are independent of k. In particular the triplet level that is the lowest excitation of the finite chain is predicted, for all k, to be degenerate with a singlet level in the limit $L\rightarrow\infty$. The two levels are associated with the representations $s_l=\frac{1}{2}$, $s_r=\frac{1}{2}$ of the left and right SU(2) symmetry groups. The leading correction comes from a single marginally irrelevant variable whose contribution to the two levels is the scaled variable g times a Clebsch-Gordan coefficient[16]:

$$\eta_t=\eta+(s_l s_r)_t g(L)+O([g(L)]^2),$$

$$\eta_s=\eta+(s_l s_r)_s g(L)+\ldots.$$

To leading order g decays logarithmically:

$$g(L)=\frac{g_0}{1+\pi b g_0 \ln L}+O\left[\frac{\ln\ln L}{(\ln L)^2}\right].$$

As the singlet and triplet excitations have different quantum numbers it is simple to determine their splitting. By taking as our estimate of the scaling exponent an average $\bar{\eta}=(\eta_s+3\eta_t)/4$ we eliminate the contribution of the leading logarithmic correction. This may be futher refined by the fitting of length corrections for next-to-leading terms.

To demonstrate the reliability of the results for the general spin-$\frac{3}{2}$ Hamiltonian, for which we have results for L up to 12, we examined the exactly integrable model[7] whose eigenvalues may be found from the Bethe *Ansatz* for very large lengths—for length L we have $3L/2$ coupled nonlinear equations. In Fig. 1 we show the results for lengths up to 100. While the individual levels of the singlet and triplet converge extremely slowly, the average $\bar{\eta}$ is accurately given by the asymptotic value plus a correction linear in $1/\ln^2 L$ over the whole range $L\geq 10$. We note that the $(\ln\ln L/\ln^2 L)$ term found in Ref. 13 comes from a cubic term in the β function for $g(L)$ and should therefore also be correctly subtracted. Similarly the conformal central charge converges with a term in $1/\ln^3 L$. This shows that, for this Hamiltonian at least, it is possible to extract reliable scaling dimensions for the most relevant operators from the results for

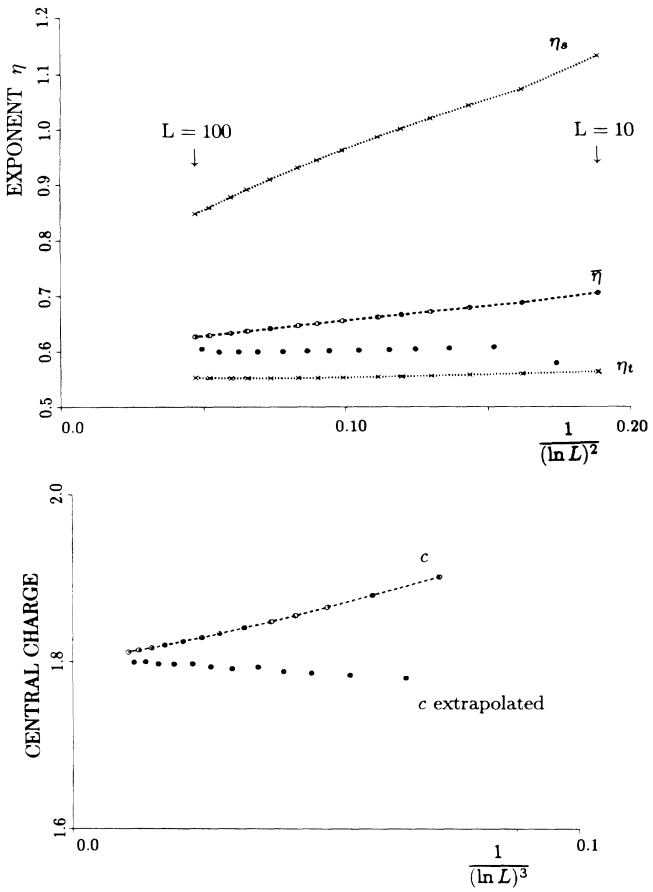

FIG. 1. The exponents calculated as a function of length L ($10\leq L\leq 100$) from the exact solution of $\mathcal{H}_b$. η_s and η_t contain a logarithmic correction eliminated in $\bar{\eta}$ which is accurately given by 0.6 plus a correction linear in $1/\ln^2 L$. For central charge c the correction is asymptotic linear in $1/\ln^3 L$. The filled circles are values of $\bar{\eta}$ and c linearly extrapolated from successive points.

$L=10$ and 12 extrapolated with the corrections discussed.

We now proceed to apply the same method to generic Hamiltonians, in particular the simple nearest-neighbor exchange. In addition to the gaps we must also estimate the velocity, which we do by diagonalizing the Hamiltonian in subspaces of nonzero wave number and fitting corrections analytic in $1/L$ up to second order. While we expect corrections of the same functional form in $\bar{\eta}$ and c it is not obvious that the results will be as good as at the integrable point. We can further test reliability in two ways: One is to vary the original Hamiltonian by addition of a second term of the same symmetry, in practice an antiferromagnetic exchange between second nearest neighbors:

$$\mathcal{H}_1(J_2)=\sum_i (\mathbf{S}_i\cdot\mathbf{S}_{i+1}+J_2\mathbf{S}_i\cdot\mathbf{S}_{i+2}). \quad (1)$$

The amplitude of the marginal operator producing logarithmically decaying corrections to exponents decreases with increasing positive J_2 and eventually vanishes at a transition to a spontaneously dimerized singlet state.[17] We see in the right-hand part of Fig. 2 that as a function of J_2 the individual values for η_s and η_t vary sharply while the weighted average and estimated central charge are essentially constant up to the transition at $J_2\approx 0.33$. Very close to the transition the extrapolation is inaccurate, since there should be power-law rather than logarithmic convergence. For larger values of J_2 the singlet level drops sharply, converging exponentially to the ground state which has a broken Ising symmetry, corresponding to the choice of a given spin to form a singlet to the left or the right. The triplet develops into a massive excitation.

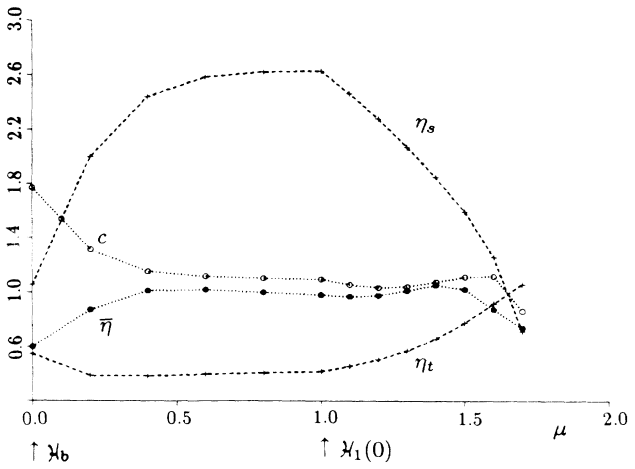

FIG. 2. Exponents for Hamiltonians starting from the exactly soluble $\mathcal{H}_b$ to the left and varying linearly: $\mathcal{H}=(1-\mu)\mathcal{H}_b+\mu\mathcal{H}_1(0)$ for $0\le\mu\le 1$ on the left-hand side to the nearest-neighbor exchange at the center $\mu=1$. On the right-hand side of the graph there is an increasing second-nearest-neighbor term $\mathcal{H}=\mathcal{H}_1(J_2)$ with $J_2=(\mu-1)/2$ for $1\le\mu\le 1.7$, i.e., $0\le J_2\le 0.35$. η_s and η_t are from gaps for $L=12$ and velocities extrapolated for $L=8$, 10, and 12; $\bar{\eta}$ and c are extrapolated as in Fig. 1 from the gaps for $L=8$, 10, and 12.

In the left-hand part of Fig. 2 we display results on a line in parameter space linearly interpolating between the Hamiltonian $\mathcal{H}_1(J_2=0)$ and the soluble[7]

$$\mathcal{H}_b=\sum_i [-\mathbf{S}_i\cdot\mathbf{S}_{i+1}+\tfrac{8}{27}(\mathbf{S}_i\cdot\mathbf{S}_{i+1})^2 + \tfrac{16}{27}(\mathbf{S}_i\cdot\mathbf{S}_{i+1})^3]. \quad (2)$$

It is evident that in both c and $\bar{\eta}$ there is a smooth crossover from the multicritical $k=3$ to the generic $k=1$ values. Except for a range close to the soluble point, where crossover effects predominate, the estimated values of c and η are stable, justifying our procedure. Other conflicting results[14] are seen to be a consequence of the leading logarithmic correction: For example, the apparent value of η_t *decreases* as we move from the multicritical point towards the simple antiferromagnet.

In conclusion, we have demonstrated that the numerical results for finite chains, in conjunction with the level structure predicted from the conformal and SU(2) $\otimes$SU(2) symmetries, enable us to show unambiguously that the antiferromagnetic models exactly soluble by the Bethe *Ansatz* are not typical. The lattice representation (2) of the higher Wess-Zumino model constitutes a multicritical point in parameter space, a point of transition between the generic massless phase of the isotropic antiferromagnet and a singlet phase. We expect this to be generally true of the half-integer cases; for each $k>1$, there is a relevant operator[10,18] $(\mathrm{tr}g)^2$ of dimension $4/(2+k)$. This induces a crossover from the $k=2S$ representation. However, the present numerical results show that the antiferromagnet stays massless, and crosses over to a new fixed point with the critical properties of $k=1$, in accord with Haldane's original hypothesis. The apparent agreement of earlier studies and the experimental results must be understood to be the slow crossover from large-S behavior at relatively short distances to the true asymptotic behavior of free bosons at long distances. While the primary aim in the study of the scaling corrections was numerical, to provide accurate exponents, such corrections are also relevant for experiment: The corresponding length scale is the thermal correlation length. In any real quasi one-dimensional antiferromagnet the strength of interchain coupling bounds the correlation lengths for which one-dimensional effects can be observed. The present study suggests that for $S>\frac{1}{2}$ a large correlation length and therefore very weak interchain coupling are necessary to observe the true asymptotic behavior, and that in many cases crossover effects dominate.

While we have discussed the relevance to spin chains the results elucidate the mechanism by which the presence of topological terms in the action of nonlinear σ models can restore criticality, a matter of more general

import, for example, in the theory of the quantum Hall effect.[19] For the case studied of spin chains, to find a realization of higher Wess-Zumino models for odd k we must find a multicritical point at the edge of a massless phase. The semiclassical limit[3] $S \to \infty$ is reached, for a generic Hamiltonian, by a diverging crossover length[1] rather than by critical exponents that tend to classical values, such as those associated with the higher models for $k \to \infty$. This provides further evidence that the O(3) σ model with topological angle $\Theta = \pi$ is equivalent to free bosons.[1,8] Similarly for even k the higher models appear as multicritical points[2,10,20] in the space of integer-spin Hamiltonians but the crossover in this case is to a massive model, as for $\Theta = 0$.

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[1]F. D. M. Haldane, Phys. Lett. **93A**, 464 (1983), and Phys. Rev. Lett. **50**, 1153 (1983).

[2]R. Botet and R. Jullien, Phys. Rev. B **27**, 613 (1983); R. Botet, R. Jullien, and M. Kolb, Phys. Rev. B **28**, 3914 (1983); M. P. Nightingale and H. W. J. Blöte, Phys. Rev. B **33**, 659 (1986); H. J. Schulz and T. A. L. Ziman, Phys. Rev. B **33**, 6546 (1986); S. Takada, to be published. For a dissenting opinion see, however, J. Sólyom, Phys. Rev. B **32**, 7524 (1985).

[3]H. Nishimori, Prog. Theor. Phys. **73**, 1577 (1985). This extends the spin-wave theory of J. Villain, J. Phys. (Paris) **35**, 27 (1982).

[4]W. J. L. Buyers, R. M. Morra, R. L. Armstrong, M. J. Hogan, P. Gerlach, and K. Hirakawa, Phys. Rev. Lett. **56**, 371 (1986); J. P. Renard, M. Verdaguer, L. P. Regnault, W. A. C. Erkelens, J. Rossat-Mignod, and W. G. Stirling, Europhys. Lett. **3**, 945 (1987).

[5]I. Affleck and E. Lieb, Lett. Math. Phys. **12**, 57 (1986).

[6]H. J. Schulz, Phys. Rev. B **34**, 6372 (1986).

[7]L. Takhtajan, Phys. Lett. **87A**, 479 (1982); H. M. Babudjian, Nucl. Phys. **B215 [FS7]**, 317 (1983).

[8]I. Affleck, Phys. Rev. Lett. **56**, 746 (1986).

[9]E. Witten, Commun. Math. Phys. **92**, 455 (1984).

[10]I. Affleck, Phys. Rev. Lett. **56**, 2763 (1986), and Nucl. Phys. **B265**, 409 (1986).

[11]A. A. Belavin, A. M. Polyakov, and A. B. Zamolodchikov, Nucl. Phys. **B241**, 333 (1984); J. L. Cardy, J. Phys. A **17**, L385 (1983), and A **19**, L1093 (1986), and Nucl. Phys. **B270**, 186 (1984).

[12]H. Blöte, M. P. Nightingale, and J. L. Cardy, Phys. Rev. Lett. **56**, 742 (1986).

[13]F. Woynarovich and H.-P. Eckle, J. Phys. A **20**, L97 (1987).

[14]D. Kung, to be published; A. Moreo, to be published.

[15]V. G. Knizhnik and A. B. Zamolodchikov, Nucl. Phys. **B247**, 83 (1984).

[16]I. Affleck, unpublished.

[17]F. D. M. Haldane, Phys. Rev. B **25**, 4925 (1982).

[18]For a more complete stability analysis, see I. Affleck and F. D. M. Haldane, unpublished.

[19]H. Levine, S. Libby, and A. Pruisken, Phys. Rev. Lett. **51**, 1915 (1983); I. Affleck, Nucl. Phys. **B257**, 397 (1985).

[20]Schulz, Ref. 6 and unpublished results.