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Quantum spin chains and the conformal anomaly

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The conformal anomaly c determines the universality class of a model system in statistical mechanics. The value of c characterizes both 2D classical models and their 1D quantum counterparts. The conformal anomaly may therefore be determined numerically for quantum spin chains using the relation: $E_0(N) \approx E_0(\infty) - (N\Delta E/12)c(1/N^2)$, where $E_0(N)$ is the ground-state energy of an N -spin finite system, $E_0(\infty)$ is the ground-state energy in the thermodynamic limit, and ΔE is the energy gap between the ground state at $k=0$ and the first excited state of the dispersion curve at $k=2\pi/N$. The numerical approach is highly successful when tested on the integrable $s = \frac{1}{2}$ Heisenberg antiferromagnetic XXZ chain and the integrable $s = 1$ $SU(2)$ model. The method gives $c = 1$ to within 2% accuracy for the $s = 1$ and $\frac{3}{2}$ XY chains, placing them in the universality class of the 2D XY model. The result $c = 1$ (2% accuracy) is obtained for the $s = \frac{3}{2}$ Heisenberg antiferromagnetic chain, in agreement with the Haldane prediction. The $s = 1$ pure antiferromagnetic biquadratic chain and the $s = 1$ XXZ model with uniaxial anisotropy in the vicinity of the critical point $\Delta = \Delta_2 \sim 1.15 - 1.18$ have also been studied.

INTRODUCTION

Conformal invariance^{1,2} has provided a powerful tool for classifying statistical mechanical systems according to their critical behavior. A system at criticality is invariant with respect to a conformal algebra,³ and is characterized by a number, the conformal anomaly, or central charge c that determines the universality class of the system. The same value of c characterizes both 2D classical models and their 1D quantum counterparts. Blöte, Cardy, and Nightingale,⁴ and Affleck⁵ have shown that the conformal anomaly can be found by studying the large- N behavior of finite N chains, according to the expression

$$E_0(N) = E_0(\infty) - (\pi v/6)c(1/N^2) + (\text{higher terms}), \quad (1)$$

where $E_0(\infty)$ is the ground state energy per spin in the thermodynamic limit, $N \rightarrow \infty$; $E_0(N)$ is the ground state energy per spin of a finite, N -spin chain; v is the velocity of sound for the model (i.e., the initial slope of the ΔE vs k dispersion curve). Expression (1) holds only for chains with periodic boundary conditions.

It is known that $c = \frac{1}{2}$ for the spin- $\frac{1}{2}$ transverse Ising chain (universality class of the 2D Ising model) and $c = 1$ for the spin- $\frac{1}{2}$ XXZ chain with continuous symmetry (universality class of the 2D Baxter model) from planar anisotropy analytic results.⁴ Quantum spin chains with higher-spin provide examples of models with $c > 1$. For a class of Bethe Ansatz integrable models with $SU(2)$ symmetry,^{6,7} Affleck⁵ has predicted the following expression for c :

$$c = 3s/(1+s). \quad (2)$$

Obviously, each member of the class is in a different universality class, where $c = 1$ for $s = \frac{1}{2}$, $c = 1.5$ for $s = 1$, $c = 1.8$ for $s = \frac{3}{2}$, etc.

It has been realized by several authors⁸⁻¹⁰ in addition to ourselves (see brief summary in Ref. 11) that Eq. (1) may be

formulated in a way that allows calculation of a series of estimates, $c(N)$, for a sequence of chains of increasing N , and extrapolation to $N = \infty$ to obtain the value of c . This numerical approach will be discussed in detail in the next section.

Voynarovich and Eckle⁹ studied the leading and next-to-leading finite-size corrections to the ground and first excited states for the spin- $\frac{1}{2}$ anisotropic Heisenberg model in the critical region. Since this model is Bethe Ansatz integrable they could obtain the analytic form of the corrections. The Hamiltonian has the form

$$H = J \sum_{i=1}^N (s_i^x s_{i+1}^x + s_i^y s_{i+1}^y + \Delta s_i^z s_{i+1}^z), \quad (3)$$

where Δ is an anisotropy parameter. They showed explicitly the presence of $\ln N$ factors in the correction terms and also why a naive finite-size scaling analysis on this system yields a critical point substantially in error.^{12,13}

Moreo¹⁰ and the present authors are particularly interested in the critical behavior of spin- $\frac{3}{2}$ Heisenberg antiferromagnetic chains (HB AFM's) in comparison with the spin- $\frac{1}{2}$ HB AFM. The Haldane prediction¹⁴ is that both systems should be in the same universality class and thereby possess the same set of critical exponents, for example, $c = 1$ and $\eta = 1$. Affleck, on the other hand, initially conjectured that the spin- $\frac{3}{2}$ HB AFM should be in the universality class of the $s = \frac{3}{2}$ integrable $SU(2)$ model, with $c = 1.8$ and $\eta = 0.6$.¹⁵

Essentially all workers in this area have tested the numerical approach on the spin- $\frac{1}{2}$ XXZ AFM with continuous symmetry, given by Eq. (1). The expected value $c = 1$ has been found to high numerical accuracy in the appropriate parameter range $0 \leq \Delta < 1$. In addition, we have studied the $s = 1$ integrable $SU(2)$ chains,^{6,7} again finding numerical

results in excellent agreement with Affleck's predicted value.

Our interest in numerical estimation of c has been broader than that of other authors. We have employed the technique in the following connections.

(a) We have analyzed quantum spin chains which are not integrable to determine from the c value the universality classes of these models. The spin- $\frac{3}{2}$ HB AFM noted above is one example. Others of interest are the $s = 1$ and $s = \frac{3}{2}$ XY models, believed to be in the universality class of the Gaussian, 2D XY, or Baxter models. In the case of the spin-1 XXZ chain, the uniaxial critical point at $\Delta = \Delta_2$ is predicted to be in the universality class of the 2D Ising model.¹⁴

(b) A c value can only be defined if the statistical mechanical model is critical, i.e., gapless. If the numerical analysis is performed on a system which has an excitation gap, the result is a $c(N)$ sequence which plunges to zero. Hence, in principle, this method can be used to determine whether or not a given system is gapless, a question of considerable interest since the controversial advent of the Haldane conjecture.^{12,14} Tested on the integrable $s = \frac{1}{2}$ XXZ AFM with uniaxial anisotropy (discrete symmetry) and a gap, the approach appears to work. Consequently, we have examined the $s = 1$ XXZ model at $\Delta = 1$ (HB AFM) and also for Δ values in the range 1.1–1.2, encompassing the critical point $\Delta_2 \sim 1.18$. The $s = 1$ chain with pure AFM biquadratic exchange is also interesting. Oitmaa, Parkinson, and Bonner,¹⁶ and Blöte and Capel¹⁷ obtained numerical evidence for a gap, in agreement with theoretical arguments of Affleck, Kennedy, Lieb, and Tasaki.¹⁸ Sólyom, however, has numerical evidence against the presence of an excitation gap in the biquadratic model.¹⁹

(c) The common assumption is that nonintegrable systems will display critical behavior analogous to their integrable counterparts, with unique T_c , associated scaling behavior, and a clearly defined universality class. However, the dramatically different dynamical behavior of both types of system suggest the possibility of differences in the static (spectral) properties also. Some unusual spectral phenomena in nonintegrable systems have already been observed.²⁰ Hence c -number calculations on nonintegrable systems are of particular interest.

NUMERICAL APPROACH

Neglecting higher terms, we may write (1) as

$$N^2[(E_0(\infty) - E_0(N))] = (\pi v/6)c. \quad (4)$$

The left-hand side (LHS) is essentially the asymptotic slope of a graph of $E_0(N)$ plotted versus $(1/N^2)$, the intercept giving $E_0(\infty)$, which is generally not known for a nonintegrable system. Assuming a gapless $\sin k$ -like, dispersion curve, the slope as $k \rightarrow 0$ is v , and is obtained numerically as

$$v = \lim_{N \rightarrow \infty} (N\Delta E/2\pi), \quad (5a)$$

where ΔE is the energy gap to the first excitation at $k = 2\pi/N$, since the finite- N excitations are distributed

across the Brillouin zone as multiples of $2\pi/N$. Hence,

$$(\pi v/6) = \lim_{N \rightarrow \infty} (N\Delta E/12). \quad (5b)$$

The value of c can therefore be obtained in two ways.

(a) Extrapolate the slopes $s(N+2, N)$ of neighboring points on an $E_0(N)$ vs N^{-2} plot, i.e., find

$$\begin{aligned} S &= \lim_{N \rightarrow \infty} s(N+2, N) \\ &= \lim_{N \rightarrow \infty} \frac{[E_0(N) - E_0(N+2)]}{[1/(N+2)^2 - 1/N^2]}. \end{aligned} \quad (6)$$

Then

$$c = \lim_{N \rightarrow \infty} \frac{s(N+2, N)}{N\Delta E/12}. \quad (7)$$

(b) Calculate finite- N approximations to c :

$$c(N) = \frac{s(N+2, N)}{N\Delta E/12}$$

$$\text{and then take limit } c = \lim_{N \rightarrow \infty} c(N). \quad (8)$$

Both approaches differ somewhat from the numerical approach of Moreo¹⁰ and seem to give more consistent results. Our calculations extend to rings of $N = 14$ spins for $s = 1$ and to $N = 10$ spins for $s = \frac{3}{2}$.

RESULTS

$s = \frac{1}{2}$ AFM XXZ chain: As noted, for $0 < \Delta < 1$, the value $c = 1$ is obtained to within 1% accuracy.

$s = 1$ SU(2) chain: Method (a) gives a value $c \sim 1.48$ and method (b) gives $c \sim 1.46$, in excellent agreement with the Affleck prediction $c = 1.50$. The ground-state energy per spin $-E_0(\infty) \approx 4.000$.

$s = \frac{3}{2}$ HB AFM: Method (a) gives $c \sim 0.99$ and method (b) gives $c \sim 0.97$, in excellent agreement with the Haldane prediction $c = 1$, and complete disagreement with the integrable SU(2) predicted value of 1.8. The ground-state energy per spin $-E_0(\infty) \approx 5.080$.

$s = 1$ XY: Method (a) gives $c \sim 0.98$ and method (b) gives $c \sim 0.97$, strongly indicating the expected value $c = 1.0$. The ground state energy per spin is $-E_0(\infty) \approx 1.116$.

$s = \frac{3}{2}$ XY: Method (a) gives $c \sim 1.01$ and method (b) gives $c \sim 0.99$, strongly indicating the expected value $c = 1.0$, as found also by Moreo.¹⁰ The ground-state energy per spin is $-E_0(\infty) \approx 2.4149$.

$s = 1$ biquadratic AFM: This model is interesting since Refs. 16–18 predict a gap, albeit a small one, whereas Ref. 19 predicts no gap. Our extrapolations behave quite smoothly, with no indications up to $N = 14$ spins of a sharp downward turn to zero, consistent with the presence of an excitation gap. Method (a) gives $c \sim 1.19$ and method (b) gives $c \sim 1.16$, consistent with a "round number" value $c = 1.2$. This apparent c value does not correspond to any known prediction for an $s = 1$ spin chain. It is possible that the method is not sensitive to the presence of a very small gap until $N > 14$, i.e., the asymptotic behavior of the $c(N)$ extrapolations changes for $N > 14$. By comparison, in the case

of the nonintegrable spin- $\frac{3}{2}$ HB AFM, however, all previous numerical studies have tended to indicate the presence of a gap, more like the case of spin-1 than spin- $\frac{3}{2}$.^{21,22} Affleck and Lieb²³ have given a proof that all half-integer Heisenberg antiferromagnetic spin chains are gapless, but our c calculation is essentially the first piece of numerical evidence of gapless behavior, predicted by Haldane.¹⁴

$s=1$ XXZ chain, $\Delta > 1$: We have studied anisotropy values $\Delta = 1.1$ and 1.2 , encompassing the expected critical point $\Delta = \Delta_2 \sim 1.15-1.18$. In both cases, the $c(N)$ start from high values of ~ 1.5 and plunge downwards to zero, consistent with the presence of a gap. According to Haldane, at the critical point Δ_2 the quantity $c \sim \lim_{N \rightarrow \infty} c(N) = 0.5$. We are "fine-scanning" the interval $1.1 < \Delta < 1.2$ to observe this phenomenon.

CONCLUSION

We have used a numerical approach involving finite chain calculations to determine the value of the conformal anomaly c for a variety of spin chain models. Tested on the exactly integrable $s = \frac{1}{2}$ XXZ chain with planar anisotropy and the $s = 1$ integrable SU(2) model, our method gives excellent agreement with predicted values, which can also be obtained analytically. When applied to the $s = 1$ and $s = \frac{3}{2}$ XY models, our method yields the value $c = 1$ to within 2% accuracy, indicating that XY models of general spin s all belong to the same universality class, that of the 2D XY, 2D Gaussian, or Baxter model. When applied to the spin- $\frac{3}{2}$ HB AFM, the method again yields the value $c = 1$ to within about 2% accuracy, supporting the Haldane prediction that all half-integer spin HB AFM's are in the same universality class. The fact that the $s = 1$ and $\frac{3}{2}$ XY chains, and the $s = \frac{3}{2}$ HB AFM chain, comprising three models thought to be non-integrable, all yield c values as well-defined as those associated with integrable models, supports the belief that critical behavior is unaffected by nonintegrability.

The situation is at present less conclusive in the case of two additional models of interest. In the case of the $s = 1$ chain with pure AFM biquadratic exchange, the existence of a gap is somewhat controversial, although strongly supported by theoretical arguments. We obtain an apparently well-

defined c value in the vicinity of 1.20, instead of a trend to $c = 0$ expected in the presence of a gap. In the case of the $s = 1$ XXZ model with uniaxial anisotropy, in the vicinity of the critical point $\Delta_2 \approx 1.15-1.18$, we hope to observe the value $c = \frac{1}{2}$ predicted by Haldane. Calculations at $\Delta = 1.1$ and 1.2 indicate the presence of a gap, which is expected to vanish at, and only at, $\Delta = \Delta_2$. Further study of both models is indicated.

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