Logarithmic corrections in antiferromagnetic chains

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Various numerical estimates of critical exponents for antiferromagnetic chains are compared with conformal field-theory predictions. Field theory allows the explicit calculation of logarithmic corrections, and hence the value of the effective exponent that is expected to be observed numerically. Comparison is made with numerically obtained exponent values, and agreement is found to be very good, even when logarithmic corrections are as large as 70%. Logarithmic corrections can lead to misleading results, for example an incorrect phase diagram, and examples in the literature where this seems to have occurred are discussed.

The extraction of critical exponents for quantum antiferromagnetic chains by a variety of numerical techniques, including finite-size scaling, has long been plagued by the presence of marginal operators which lead to logarithmically slow finite-size convergence. For example, for the case of the $S=\frac{1}{2}$ alternating chain, there have been over twenty attempts at numerical calculation of spin-Peierls exponents. The earliest such work, real-space renormalization-group calculations by Fields, Blöte, and Bonner,[1] produced exponents significantly larger than analytic predictions of Cross and Fisher,[2] a result also typical of subsequent studies. It was later suggested that logarithmic corrections could result in such a discrepancy,[3] and numerical studies attempting to verify this suggestion include work by Spronken, Fourcade, and Lepine[4] on chains up to $L=18$ sites, and by Soos, Kuwajima, and Mihalick[5] on the longest chains with $L=26$. In addition to their power to frustrate many workers, logarithmic correction terms have frequently given rise to misleading results. It was noted by Bonner and Muller[6] that numerical scaled-gap techniques used by Botet and Jullien in their pioneering work on spin-1 XXZ chains and the Haldane conjecture[7] would also yield a Haldane-like phase diagram for the $S=\frac{1}{2}$ XXZ model, in contradiction to exact results. The culprit is the essential singularity at the Heisenberg point. In fact, recently a Haldane-like phase diagram for the $S=\frac{1}{2}$ XXZ model has actually been proposed.[8] Discrepancies resulting from logarithmic corrections can be quite large. Moreo[9] found a numerical value of $\eta=0.53$ for the spin-$\frac{3}{2}$ Heisenberg antiferromagnetic chain which differed considerably from the Haldane predicted value $\eta=1$. A resolution of this problem was provided by Ziman and Schulz, invoking logarithmic corrections.[10]

Recently, exponents have been obtained for the integrable spin-1 chain with Hamiltonian[11]

$$H=\sum_i [\mathbf{S}_i\cdot\mathbf{S}_{i+1}-(\mathbf{S}_i\cdot\mathbf{S}_{i+1})^2]\,. \tag{1}$$

Some exponents were estimated for long chains by exploiting the Bethe ansatz integrability of this model.[12,13] Generally, exponents involving nonintegrable perturbations of H cannot be obtained in this way and are calculated numerically from rather short chains. A previous comment[14] by one of the present authors on a paper by Singh and Gelfand[15] inadvertently neglected to mention prior numerical work by Oitmaa, Parkinson, and Bonner,[16] Blöte and Capel,[17] and Blöte and Bonner,[18] and others, which also agrees very well with field-theory predictions for the integrable $S=1$ antiferromagnetic chain once logarithmic corrections are taken into account. As noted in Ref. 18, an essential singularity appears explicitly in work by Babudjian,[11] in an expression for the susceptibility. The essential singularity is also apparent in a set of integrable models which are spin-s analogues of the $S=\frac{1}{2}$ XXZ model[19] and their anisotropic generalizations of the Takhtajan-Babudjian models.[11] The existence of a marginally irrelevant operator for the spin-1 isotropic model [Hamiltonian (1)] was noted in Ref. 20, but the consequent presence of logarithmic corrections was first discussed, at some length, in Ref. 18.

The assumption that a gapless, isotropic antiferromagnetic quantum spin chain should renormalize to a conformally invariant fixed point leads naturally to a discrete set of possible critical theories, the Wess-Zumino-Witten (WZW) models, labeled by the integer-valued topological coupling constant k. (Throughout this Brief Report, we have used concepts and terminology from conformal field theory. For a review see Ref. 21.) The $k=1$ model is the only stable isotropic fixed point; the higher k models are increasingly multicritical. The dimensions of all scaling fields have been calculated explicitly for these models. They each have a finite number of relevant operators and one invariant marginal operator. Such a marginal operator is a consequence of isotropy and conformal invariance in $(1+1)$ space-time dimensions. In these theories, continuous symmetries are necessarily *chiral*; i.e., there are independent symmetry groups for left and right moving excitations. Thus there are corresponding density operators J_L and J_R, which have scaling dimension one (since

their integrals along the chain give dimensionless conserved quantum numbers). The product $J_L J_R$ is the marginal operator referred to above. In the case of SU(2) symmetry, we have triplets of densities, $\mathbf{J}_{L,R}$ and the invariant operator is $\mathbf{J}_L \cdot \mathbf{L}_R$. [The operator $(\mathbf{J}_L^2 + \mathbf{J}_R^2)$ is also marginal but is redundant; it corresponds to merely shifting the spin-wave velocity. When the symmetry is only U(1), the marginal operator $J_L J_R$ does not renormalize, for a range of parameters, and labels the well-known critical line, occurring, for example, in the $s = \frac{1}{2}$ XXZ chain.]

Exponents which have been "measured" numerically for the spin-1 chain include the spin-spin correlation exponent η, the exponent determining the scaling of the gap with the addition of an alternating interaction v_a, the exponent determining the scaling of the gap with respect to a change in biquadratic strength v_b, and the exponent determining the scaling of the gap with XXZ anisotropy v_z. The field-theoretic treatment[13] gives the following expressions for these exponents: $\eta = 2x_t$, $v_a = (2 - x_s)^{-1}$, $v_b = (2 - x_{s1})^{-1}$, and $v_z = (2 - x_{t1})^{-1}$. The quantities x_t, x_s, x_{s1}, and x_{t1} are the dimensions of $\mathrm{tr} g\sigma$, $\mathrm{tr} g$, $(\mathrm{tr} g)^2$, and $\mathrm{tr} g^2\sigma$, respectively, where g is the fundamental field of the WZW model with topological coupling constant k. (Note that $k = 1$ corresponds to $S = \frac{1}{2}$, $k = 2$ to $S = 1$, etc.; and x_{s1}, x_{t1} do not exist for $k = 1$.) For the $k = 2$ model [Eq. (1)], the dimensions are $x_t = x_s = \frac{3}{8}$, and $x_{s1} = 1$. The effect of the marginal operator is to shift the effective dimensions for chains with large but finite length L according to the following expression:[13]

$$\delta x = -\lambda(L)(4\pi/\sqrt{3}k)\mathbf{S}_L \cdot \mathbf{S}_R + O(\lambda^2) , \tag{2}$$

where $\mathbf{S}_{L,R}$ are the left and the right spin quantum numbers of the operators of the SU(2)×SU(2) algebra, and $\lambda(L)$ is the marginal coupling constant which flows logarithmically slowly to zero with L. Equation (2) is the result of first-order perturbation theory in λ, and corrections exist which are $O(\lambda^2)$ and higher. It is possible to calculate them explicitly, but we have not done so. Thus efforts to estimate λ from an exponent shift can only be accurate up to corrections of $O(\lambda^2)$ [or more precisely $O((4\pi/\sqrt{3})\lambda^2)$]. For example, three estimates of $\lambda(20)$ were made in Ref. 13 for the $k = 2$ WZW model of Eq. (1); namely, 0.064, 0.073, and 0.041, showing the expected differences of $O(\lambda^2)$. The quantum number $\mathbf{S}_L \cdot \mathbf{S}_R$ can be expressed in terms of S_L, S_R and the total spin quantum number, $\mathbf{S}_T \equiv \mathbf{S}_L + \mathbf{S}_R$:

$$\mathbf{S}_L \cdot \mathbf{S}_R = \tfrac{1}{2}(\mathbf{S}_T^2 - \mathbf{S}_L^2 - \mathbf{S}_R^2) . \tag{3}$$

In Table I, values of x are calculated for $S = 1$, and also $S = \frac{1}{2}$ for completeness. The quantities $\delta x_t(x_t)$ and $\delta x_s(x_s)$ were obtained previously.[13] The effective exponents x_{sl} and x_{tl} were not calculated in Ref. 13, but have been estimated using formula (2) and taking for $\lambda(20)$ the average of that estimated from δx_t and δx_s. (This is simply a guess and given the spread in the estimates of λ we might estimate an uncertainty in x_{s1} and x_{t1} of about $\pm 10\%$.) We make the following observations from Table I. Note that δx_{sl} (for the $k = 2$ model) is considerably larger than the values $\delta x_t = -0.037$ and $\delta x_s = 0.199$ obtained for lower values of S_L, S_R. In general the dimension shifts increase with S_L, S_R, with correspondingly larger deviations of effective exponents from their limiting values.

Field theory predicts that numerical values for the conformal anomaly c should show relatively smaller deviations from the limiting values than the critical exponents, i.e., should differ by $O(\lambda^3)$ rather than $O(\lambda)$. Specifically the formula is[13]

$$c_{\mathrm{eff}} = c(k) + [2\pi\lambda(L)^3]/\sqrt{3}k , \tag{4}$$

where $c(k) = 3k/(2+k)$. If this prediction is verified, the implication is that numerical values for c are easier to use for determining the critical behavior of a particular model than values for exponents, since c values are much less sensitive to the effects of marginal operators.

Exact, effective, and numerical critical parameters, exponents and c values from Refs. 16–18, and also Ref. 22, are given in Table II. We observe, in the case of c, that both effective and numerical exponents differ from the exact values only by 1–2%, in agreement with predictions.[23] In the case of the exponents, the agreement is very good in all cases once logarithmic corrections are included; however, the correction varies from about 12% to as much as 70%, in contrast to the much smaller correction in the case of c. [Since x_{s1}^{eff} is quite close to two and $v_b = (2 - x_{s1})^{-1}$, our estimate of v_b would change by a large amount if we took a different estimate of x_{s1}^{eff} based on a different guess at the value of $\lambda(20)$.]

Let us note some specific features of interest in connection with particular exponents. First of all, our numerical value of η for $S = 1$ was obtained using spectral gap ratios. However, the theory discussed here uses the values of x_t and x_s obtained from the finite chain triplet and singlet gaps as input. Hence the numerical value of η in Table II agrees with the effective value by definition, since it was calculated as $2x_t$, i.e., the $S = 1$ exponent of Table II is not

TABLE I. Parameters required for calculating the anomalous dimension shifts δx_a governing the effective exponents for $s = \frac{1}{2}$ and 1.

$k(2s)$	Operator	$S_L = S_R$	S_T	$\lambda(20)$	a	x	δx	x^{eff}	Exponent
1	$\mathrm{tr} g\sigma$	$\frac{1}{2}$	1	0.032	t	0.5	−0.058	0.42	η
1	$\mathrm{tr} g$	$\frac{1}{2}$	0	0.038	s	0.5	0.21	0.71	v_a
2	$\mathrm{tr} g\sigma$	$\frac{1}{2}$	1	0.041	t	0.375	−0.037	0.34	η
2	$\mathrm{tr} g$	$\frac{1}{2}$	0	0.073	s	0.375	0.199	0.57	v_a
2	$(\mathrm{tr} g)^2$	1	0	0.057	s_1	1	0.41	1.41	v_b
2	$\mathrm{tr} g^2\sigma$	1	1	0.057	t_1	1	0.21	1.21	v_z

TABLE II. Exact and effective exponents compared with numerical exponents from Refs. 1 and 16–18.

S	Parameter	Exact	Effective ($L=20$)	Numerical
$\frac{1}{2}$	c	1	1.01	0.98
	η	1	0.84	0.85
	ν_a	$\frac{2}{3}=0.67$	0.78	0.75–0.76
1	c	1.5	1.52	1.47
	η	0.75	0.68	0.65
	ν_a	$\frac{8}{13}\approx 0.614$	0.70	0.67
	ν_b	1	1.7	1.8
1	ν_z	1	1.26	1.11

a real test of the theory. However, other numerical calculations have been performed which allow an independent test. Recently, Uchinami, using a Monte Carlo approach, found a value $\eta=0.64$.[24] In fact, two early approaches have examined values of η at a special multicritical point in the phase diagram of the $S=1$ XXZ chain with single-ion anisotropy. Glaus and Schneider, using a finite-size scaling method, obtained a value $\eta=0.64$,[25] and Schulz and Ziman, the first to use the spectral gap approach for calculating η, found a value $\eta=0.67$ (Ref. 26) for this special point. If we make the assumption that this special multicritical point lies in the same universality class as the $S=1$ WZW point, we find very good agreement with our value $\eta=0.65$ using the spectral gap method and, of course, very good agreement with theory.[13]

In the case of $S=\frac{1}{2}$, our numerical exponent, $\eta=0.85$ was also obtained by the spectral gap method, as was the value $\eta=0.87$ obtained by Schulz and Ziman.[26,27] An independent approach was taken by Moreo[9] who evaluated $\eta(S=\frac{1}{2})$, as a function of anisotropy, directly from the spin-spin correlation functions. Moreo observes that the direct evaluation of η seems to avoid logarithmic correction difficulties. Certainly, her value for η at the isotropic point is very close to unity. However, this agreement with the exact value may be fortuitous, since η values over the range of anisotropy are in only fair agreement with exact analytic results.

Regarding the dimerization exponent ν_a, the case of $S=\frac{1}{2}$ has already received an introductory discussion. Many different numerical calculations have yielded values of ν_a ranging from 0.75 to 0.9, with values clustered towards the lower end of the range, in agreement with the effective exponent value of 0.78.[28] For the case of $S=1$, in addition to the finite-size scaling value $\nu_a=0.67$ by Blöte and Bonner, there have recently appeared estimates by Singh and Gelfand using series-expansion techniques.[15] The Singh-Gelfand estimates are consistent with the Blöte-Bonner estimates, and consequently also give very good agreement with the effective exponent value.[14]

In the case of ν_b, we observe that agreement is good despite the fact that the logarithmic correction amounts to as much as 70% in this case. This large logarithmic correction has already caused confusion. Many groups have investigated the properties of the Hamiltonian (1) generalized by a parameter β which varies the strength of the biquadratic term. As noted by Bonner, Parkinson, Oitmaa, and Blöte,[29] the fact that the effective exponent is much larger than the ideal exponent means that the gap, implying a noncritical phase, which should ideally open up immediately for $\beta>1$, appears numerically to open up much more slowly, making it difficult to detect near the integrable point. Furthermore, the gap and inverse correlation length ξ^{-1} for the pure biquadratic model ($\beta\rightarrow\infty$) were recently calculated exactly using the Bethe ansatz[30] and shown to be very small ($\xi>20$). The $\beta=\infty$ gap may well be an upper bound for all $\beta>1$. Workers using various methods, including finite-size scaling, composite spin model, quantum transfer matrix, and Monte Carlo, have concluded that a critical region of finite extent occurs around the integrable $S=1$ point[20,24,31,32] while in Ref. 33, it was conceded that if this region is not critical, ξ must in any event be rather large. These results can now be specifically attributed to the strong logarithmic corrections associated with the exponent of the biquadratic mass gap,[13] together with the smallness of the gap for all $\beta>1$. This is an example of the situation discussed earlier, where operators occur with $S_L,S_R>1$, corresponding to large dimension shifts, of the order of 100%. If this situation is common, there is obvious significant impact on the study of critical behavior by numerical means. While such operators do indeed exist for $S\geq 1$, most exponents are governed by low-dimension (low S) operators. The operators considered here which have $S_L,S_R=\frac{1}{2},1$ (see Table I), namely the field g and g^2 determine most of the exponents respecting symmetry of translation by one site (which corresponds to $g\rightarrow -g$ in the WZW model). These estimates of the effective values of ν_b and ν_z contain an additional uncertainty compared to the others because the appropriate effective values of λ are not known. These could be obtained by measuring the gaps to the lowest excited states of wave vector 0 and spin 0 and 1, respectively. We arbitrarily chose to use the average of the two estimates of λ from x_t and x_s. If, instead, we had used the values of λ from x_t for estimating x_{t1} and from x_s for x_{s1} we would have obtained the effective exponents, $\nu_b=2.11$, $\nu_z=1.18$. Without calculating to second order in perturbation theory in λ it is unclear which is a better estimate.

Note that the first-order exponent shift of Eq. (2) can be larger either because $\mathbf{S}_L\cdot\mathbf{S}_R$ is large or because $\lambda(L)$ is large. We should emphasize that this approach to calculating effective components is based on first-order perturbation theory in the marginal coupling constant. Its success depends on the fact that the marginal coupling is fairly small at the largest length scale probed. How small it must be depends in detail on the coefficients of the higher-order terms in perturbation theory (which is expected to give only an asymptotic, not a convergent, expansion). Although none of these higher-order coefficients has been calculated, it was found empirically in Ref. 13 that, for a given chain length, the higher-order effects were larger for integrable chains of larger S. This effect is encountered in the case of the $S=\frac{3}{2}$ Heisenberg antiferromagnetic chain, where the "measured" exponent η differs from its exact value by 50% or more, in contrast

to the $S=\frac{1}{2}$ case, where the difference is only about 12%. It has been noted by Ziman and Schulz[10] that the effects of the logarithmic corrections in this situation can be minimized by taking a suitable weighted combination of η values obtained by considering both singlet and triplet gaps.

The fact that effective $\lambda(L)$ estimates depend on the particular energy level involved should not be too great a concern, at least for models with $S=\frac{1}{2}$ and 1. The effective exponent estimates for η and ν_a of Table II would change only about 5% ($S=\frac{1}{2}$ case) or 10% ($S=1$ case) if just a single input (either x_t or x_s) from finite-size measurement were allowed in determining $\lambda(L)$. More care must be exercised in connection with higher-dimensional exponents such as ν_b in Table II, and some $S=\frac{3}{2}$ exponents, since the effective exponent may vary by considerably more. However, our main purpose in presenting this report is to call attention to the fact that the appropriate technology is now available. We conclude that finite-size scaling can be a useful and quantitative way of calculating critical exponents even in the presence of a single marginal operator, provided that the leading-order shifts in effective exponents are taken in account using Cardy's technique[34] as implemented in Ref. 13 for quantum spin chains. The success of this approach depends on the property that the effective coupling is reasonably small at the largest accessible length scale. It is not too surprising that this often appears to be the case, since the decrease of $\lambda(L)$ with increasing length can be quite rapid until λ gets small enough that the slow decrease predicted by the lowest-order β function takes over.

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