

## Spin- $\frac{1}{2}$ antiferromagnetic XXZ chain: New results and insights

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We study the criticality at the isotropic limit of the  $S = \frac{1}{2}$ , antiferromagnetic, XXZ chain on approach from the Ising side. Long series are developed for the longitudinal and transverse correlation sums or structure factors  $S_{zz}$  and  $S_{+-}$  around the Ising limit. Their extrapolation indicates a divergence as the critical point is approached, with two different powers, a result quite unexpected if one employs a naive scaling argument since the critical correlations are isotropic and there is only one correlation length,  $\xi$ . An analytical calculation is presented, in which this paradox is resolved and the numerical results are confirmed.

### I. INTRODUCTION

Quantum spin chains have been of special theoretical interest owing to their exact solvability and also because they map onto various two-dimensional classical models and (1+1)-dimensional field theories.<sup>1</sup> A vast number of analytical and numerical results have been obtained which have proven useful in our general understanding of phase transitions and critical phenomena in addition to being relevant to several experimental systems.<sup>2</sup> The  $S = \frac{1}{2}$  antiferromagnetic Heisenberg chain, whose exact ground-state energy was first obtained by Bethe and Hulthén several decades ago, is one of the simplest of these models which is *exactly solvable* in many respects. It is known that in the ground state there is no sublattice magnetization and the spin-spin correlations decay algebraically. However, the complete asymptotic form of the spin-spin correlations is not known. More precisely, the correlations are known to decay in leading order like  $1/r$ , but possible logarithmic correction factors which have been anticipated<sup>3</sup> are not known exactly. One of the aims of this paper is to obtain the form of the leading logarithmic correction.

The Hamiltonian for the XXZ chain is

$$H = \sum_i [\Delta S_i^z S_{i+1}^z + (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y)], \quad (1.1)$$

where the spins may be taken as Pauli spin matrices. In this paper we shall concentrate on the behavior of the correlation sums or antiferromagnetic structure factors

$$S_{zz} = \sum_j (-1)^j (\langle S_0^z S_j^z \rangle - \langle S_0^z \rangle \langle S_j^z \rangle), \quad (1.2)$$

and

$$S_{+-} = \sum_j (-1)^j (\langle S_0^x S_j^x \rangle + \langle S_0^y S_j^y \rangle). \quad (1.3)$$

At the Heisenberg point, i.e., at  $\Delta = 1$ , the Hamiltonian is isotropic in spin space and the two structure factors are

identical apart from a factor of 2. But for  $\Delta \neq 1$ , they are clearly different. We find that as  $\Delta$  approaches unity from above, these two correlation sums diverge with different exponents. This is quite contrary to normal expectations. Its proper explanation requires a careful study of the spin-spin correlations close to criticality. Naive scaling arguments would suggest

$$S_{ab}(\Delta) \sim \int_0^\xi (-1)^r \langle S^a(0) S^b(r) \rangle_c dr, \quad (1.4)$$

where  $ab$  stands for  $zz$  or  $+-$ ,  $\xi(\Delta)$  is the correlation length, and the subscript  $c$  refers to correlations at criticality,  $\Delta_c = 1$ . Since the critical point is isotropic, the correlations are isotropic. Hence, one expects the two exponents to be the same. Let us develop the argument in further detail. Correlations at criticality are expected to decay as a power law, namely,

$$(-1)^r \langle S^a(0) S^b(r) \rangle_c \sim 1/r^\eta. \quad (1.5)$$

Also, the correlation length typically diverges on approach to criticality as

$$\xi \sim (\Delta - 1)^{-\nu} \quad (\Delta \rightarrow 1+). \quad (1.6)$$

These would imply that the structure factors should diverge with an exponent  $(1-\eta)\nu$ . In the present problem  $\eta = 1$  and  $\nu$  is infinite, since the correlation length has an essential singularity.<sup>1</sup> Hence, the exponent for the divergence of the structure factors depends on the nature of the essential singularity which characterizes the divergence of the correlation length. From the exact solutions,<sup>1</sup> one knows

$$\xi \sim \exp[\pi/(\Delta - 1)^{1/2}]. \quad (1.7)$$

Substituting this form into Eq. (1.4) we get

$$S_{ab} \sim \int^{\exp[\pi/(\Delta - 1)^{1/2}]} dr / r \sim (\Delta - 1)^{-1/2}. \quad (1.8)$$

More interestingly, however, multiplicative logarithmic corrections directly modify this exponent. Suppose we assume

$$(-1)^r \langle S^a(0)S^b(r) \rangle_c \sim (\ln r)^\lambda / r, \quad (1.9)$$

then one finds that the structure factor diverges with an exponent  $(1+\lambda)/2$  in place of  $\frac{1}{2}$ . However, as long as the correlations at criticality are isotropic and there is only one correlation length in the problem, the transverse and longitudinal correlation sums should apparently diverge with the same exponent. In the rest of the paper we shall show that the situation is more complicated. The presence of marginal variables invalidates a naive application of scaling arguments. We shall take recourse to sine-Gordon field theory to resolve the issue.

The plan of the paper is as follows: In Sec. II we shall discuss series expansions and their analyses for the structure factors and estimate the exponents for their divergences. This is how the paradox was discovered. In Sec. III we introduce the appropriate bosonic field theory that describes criticality in these systems and obtain the logarithmic corrections to the  $1/r$  decay of correlations at criticality. By a careful consideration of the correlations close to, but not at, criticality, we shall explain the origin of two different exponents. Our conclusions are summarized in Sec. IV.

## II. SERIES EXPANSION FOR THE $S = \frac{1}{2}$ $XXZ$ CHAIN

We wish to obtain power series expansions for the longitudinal and transverse correlation sums around the Ising limit. Such expansions, in powers of  $y = 1/\Delta$ , have been obtained before<sup>4</sup> for the ground-state energy,  $e_0$ , and the sublattice magnetization,  $m^\dagger$ , but only to sixth order. We have obtained expansions for  $e_0$ ,  $m^\dagger$ , and  $S_{zz}$  to order  $\Delta^{-22}$ , and for  $S_{+-}$  to order  $\Delta^{-12}$  by the method developed by Singh, Gelfand, and Huse.<sup>5</sup> The expansion for  $S_{zz}$  in powers of  $x = (1/\Delta)^2$  is

$$\begin{aligned} S_{zz} = & 4x + 4x^2 + 4.75x^3 + 5.125x^4 + 5.2813x^5 \\ & + 5.3516x^6 + 5.4287x^7 + 5.4761x^8 \\ & + 5.5881x^9 + 5.5612x^{10} + 5.8508x^{11} + \dots, \end{aligned} \quad (2.1)$$

where the coefficients are correct to five significant digits. The expansion for  $S_{+-}$  in powers of  $y = 1/\Delta$  is, likewise,

$$\begin{aligned} S_{+-} = & 1 + 2y + y^2 + 0.5y^3 + y^4 + 0.875y^5 \\ & + 0.8125y^6 + 0.78125y^7 + 0.73438y^8 \\ & + 0.69531y^9 + 0.65625y^{10} \\ & + 0.66602y^{11} + 0.64941y^{12} + \dots \end{aligned} \quad (2.2)$$

As discussed, the critical point is at  $\Delta_c = 1$ . Let us denote the deviation from criticality by  $t = \Delta - 1$ . We expect the correlation sums diverge as

$$S_{zz} \sim t^{-\sigma^{zz}}, \quad S_{+-} \sim t^{\sigma^{+-}}. \quad (2.3)$$

Given this assumption of power-law divergence as  $t \rightarrow 0$ , the series may be analyzed by biased  $D$ log Padé and inhomogeneous differential approximants.<sup>6</sup> The critical point is set at  $x = 1$ . A list of exponent estimates for the two cases is given in Tables I–IV. Based on these we estimate the exponents to be

$$\sigma^{zz} = 1.1 \pm 0.1, \quad \sigma^{+-} = 0.75 \pm 0.15, \quad (2.4)$$

which values seem quite distinct.

## III. RENORMALIZATION-GROUP ANALYSIS

In this section we introduce the appropriate field theory that describes criticality in these systems and carry out a renormalization-group analysis of the problem. Following the standard steps of Jordan-Wigner transformation and bosonization, one can map the  $XXZ$  model on to the following sine-Gordon Hamiltonian (for a recent treatment of the steps involved see Sachdev and Shankar<sup>7</sup>)

$$\begin{aligned} H = & \frac{1}{2} \int dx \{ \Pi^2 + (d\phi/dx)^2 \\ & - \alpha_0 \Lambda_0 \cos[(16\pi/K_0)^{1/2} \phi] \}. \end{aligned} \quad (3.1)$$

Here  $\phi$  is the boson field and  $\Pi$  its conjugate momentum while  $K_0$  and  $\alpha_0$  are smooth and monotonic functions of  $\Delta$  in the region of interest<sup>7</sup> and  $\Lambda_0$  is the momentum cutoff. The correlation functions we need for the structure factors are

$$G_{+-}(R) = \langle e^{-i(\pi K_0)^{1/2} \theta(R)} e^{i(\pi K_0)^{1/2} \theta(0)} \rangle, \quad (3.2)$$

where

$$\theta(x) = \int_{-\infty}^x \Pi(x') dx' \quad (3.3)$$

and

$$G_{zz}(R) = 4 \langle \cos[(4\pi/K_0)^{1/2} \phi(R)] \cos[(4\pi/K_0)^{1/2} \phi(0)] \rangle. \quad (3.4)$$

The behavior of this theory under renormalization is well known.<sup>8</sup> Let us define scaled variables

$$x_0 = 4/K_0 - 2, \quad \text{and} \quad y_0 = 2\alpha_0\pi. \quad (3.5)$$

Then the renormalization-group flow equations are

$$\frac{dy}{dZ} = -xy, \quad \text{and} \quad \frac{dx}{dZ} = -y^2, \quad (3.6)$$

where  $Z = \ln(\Lambda/\Lambda_0)$  is the length rescaling factor. The fixed point is at  $x^* = y^* = 0$ , or  $K^* = 2$  and  $\alpha^* = 0$ . The flows are shown schematically in Fig. 1. The physical manifold is depicted by the dashed line. The Heisenberg point,  $A$ , must lie on the separatrix  $C$  given by  $x = y$ .<sup>9</sup> Any point on this separatrix flows into the fixed point  $O$ . To the right of  $C$  is the  $XY$  ordered region, which flows into the fixed line. To the left is the Ising-like region which ultimately flows to strong coupling under renormalization.

Let us begin by computing the asymptotic decay of spin-spin correlations at the Heisenberg point  $A$ . On the separatrix we can parametrize the flows by

$$x = y = g/\pi, \quad (3.7)$$

so that  $dg/dz = -g^2/\pi$ . The Callan-Symanzik equation expresses the critical correlation function as<sup>10</sup>

TABLE I. Estimates of  $\sigma_s^{zz}$  from biased Dlog Padé approximants:  $M$  and  $N$  are the orders of the polynomials in the numerator and denominator, respectively.

$M \backslash N$	1	2	3	4	5	6	7	8	9
1	1.38	1.30	1.04	1.06	1.07	1.08	1.09	1.09	1.11
2	1.28	1.46	1.07	1.02	1.08	1.11	1.09	1.09	
3	1.09	0.93	1.13	1.09	1.09	1.09	1.10		
4	1.00	1.03	1.05	1.09	1.09	1.09			
5	1.06	1.06	1.04	1.09	1.09				
6	1.06	1.06	1.26	1.12					
7	1.20	1.10	1.14						
8	0.91	1.12							
9	1.12								

TABLE II. Estimates of  $\sigma_s^{zz}$  from biased inhomogeneous differential approximants  $[0/M;N]$ , with a constant-background term:  $N$  and  $M$  are the orders of the polynomials multiplying the derivative of the series and the series, respectively (Ref. 6).

$M \backslash N$	1	2	3	4	5	6	7	8
1	1.38	1.10	1.06	1.02	1.04	1.10	1.09	1.05
2	0.89	1.04	1.02	1.02	1.10	1.10	1.10	
3	1.00	1.05	1.05	1.09	1.09	1.10		
4	1.01	1.05	1.05	1.10	1.09			
5	1.06	1.05	1.06	1.04				
6	1.00	1.05	1.08					
7	1.34	0.89						
8	1.41							

TABLE III. Estimates of  $\sigma_s^{+-}$  from biased Dlog Padé approximants as in Table I. An asterisk indicates an approximant with  $\gamma_s^{+-} < 0.5$  or  $\gamma_s^{+-} > 1.0$ .

$M \backslash N$	2	3	4	5	6	7	8	9	10
2	0.75	0.87	0.84	0.76	0.76	0.67	0.70	0.72	0.73
3	0.84	0.85	0.88	0.76	0.76	0.69	0.88	0.73	
4	0.85	0.84	0.79	*	*	0.71	0.73		
5	0.77	0.69	0.97	*	*	0.72			
6	0.74	0.80	*	0.84	0.74				
7	0.64	0.63	0.67	0.71					
8	0.63	0.64	*						
9	0.67	0.60							
10	0.74								

TABLE IV. Estimates of  $\sigma_s^{+-}$  from biased inhomogeneous differential approximants  $[0/M;N]$ . An asterisk indicates an approximant with  $\gamma_s^{+-} < 0.5$  or  $\gamma_s^{+-} > 1.0$ .

$M \backslash N$	2	3	4	5	6	7	8	9
2	0.78	0.86	0.81	0.76	0.72	0.69	0.71	0.72
3	0.84	0.83	0.53	*	0.55	0.70	0.75	
4	0.82	0.87	*	*	*	0.71		
5	0.75	*	0.59	*	0.54			
6	0.70	*	*	0.79				
7	0.64	0.65	0.69					
8	0.65	0.64						
9	0.70							

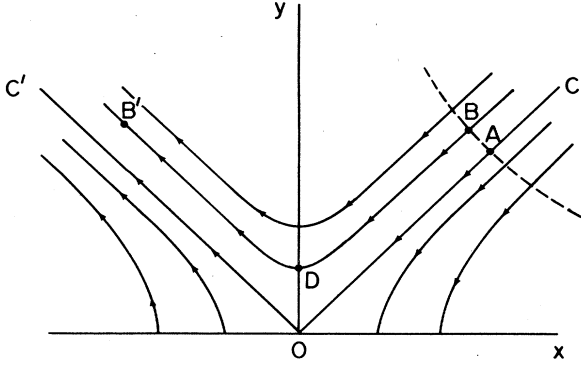


FIG. 1. Renormalization-group flow diagram for the sine-Gordon field theory.

$$G_{ab}(R, g_0) = \exp \left[ - \int_0^{\ln R} \gamma_{ab}[g(z)] dz \right] G_{ab}(1, g(R)), \quad (3.8)$$

where

$$\gamma_{ab}(g) = d \ln(Z_{G_{ab}}) / d \ln(\Lambda), \quad (3.9)$$

$Z_{G_{ab}}$  being the prefactor which renormalizes  $G_{ab}$  multiplicatively.

To obtain the leading logarithmic correction we need  $\gamma_{ab}(g)$  only<sup>8</sup> to order  $g$ . To compute this, it suffices to know that in the free-field measure, one has

$$\langle \Pi e^{i\alpha_i \phi_i(x)} \rangle = \delta \left[ \sum_i \alpha_i \right] \exp \left[ \sum_{\substack{i,j \\ i < j}} \frac{\alpha_i \alpha_j}{2\pi} \ln \Lambda |x_i - x_j| \right], \quad (3.10)$$

and similarly for a string of factors  $e^{i\beta\theta}$ . (A mixed string vanishes unless the  $\alpha_i$  and  $\beta_i$  separately add up to zero.)

Consider first  $G_{+-}(\Lambda)$ , to order  $g$  in the interaction. We can ignore the interaction by virtue of the  $\delta$  function in Eq. (3.10). The free-field integration gives, to order  $g$ ,

$$G_{+-}(R, g, \Lambda) = \frac{1}{(R\Lambda)^{1-g/2\pi}} = \left[ \frac{\Lambda_0}{\Lambda} \right]^{1-g/2\pi} G_{+-}(R, g, \Lambda_0), \quad (3.11)$$

so that using (3.9) we have

$$\gamma_{+-} = 1 - g/2\pi + O(g^2). \quad (3.12)$$

Notice that the entire  $g$  dependence of  $G_{+-}$ , and hence of  $\gamma_{+-}$ , comes from the  $(\pi K)^{1/2}$  term which multiplies the  $\theta$ 's in (3.2). Substituting this into Eq. (3.8) we get

$$G_{+-}(R, g_0) = \frac{(\ln R)^{1/2}}{R} [1 + O(g(R))]. \quad (3.13)$$

This calculation thus yields the leading logarithmic correction to the  $1/r$  decay of the correlation function up to  $O(g(R))$ , which goes as  $1/\ln R$ .

We know that  $G_{zz}$  should have similar behavior. Let

us, however, verify that this is so, both as a check on the calculation and to pave the way for later discussions.

In the  $O(g)$  computation of  $G_{zz}$  the interaction term comes in. Indeed, if it did not, the fact that the  $\phi$ 's in (3.4) are multiplied by  $(4\pi/K)^{1/2}$ , where  $K$  comes in the denominator, rather than in the numerator as for  $G_{+-}$ , implies that as  $K$  moves away from  $K^*=2$  (i.e.,  $g$  moves away from  $g^*=0$ ) the  $O(g)$  contribution of  $\gamma_{zz}$  would be the negative of that of  $\gamma_{+-}$ . Hence implying that  $G_{zz}$  would have the  $(\ln R)^{1/2}$  in the denominator if we used free-field theory. But we will see that interactions turn this around. Using Eq. (3.10), a short calculation, correct to  $O(g)$ , yields

$$G_{zz}(R, g, \Lambda) = \frac{1}{(R\Lambda)} \left[ 1 - \frac{g}{2\pi} \ln(\Lambda R) + \frac{g}{4\pi^2} \int \frac{R^2}{x^2 |R-x|^2} d^2x \right], \quad (3.14)$$

where the second term comes from the  $g$  dependence of  $K$  implied by (3.5)–(3.9), as in the case of  $G_{+-}$ , but the third term comes from the  $g$  dependence of the interaction  $\alpha$ . The  $\ln(\Lambda R)$  piece of the integral in the third term is found to have a coefficient  $g/\pi$ , which reverses the sign of the second term so restoring the rotational invariance along  $C$ , i.e.,  $\gamma_{zz} = \gamma_{+-} = 1 - g/2\pi$ .

If we now integrate  $G_{ab}(R, t=0)$  up to the correlation length  $\xi(t) = e^{\pi/\sqrt{t}}$ , we find that

$$S_{+-} \sim S_{zz} \sim t^{-3/4}.$$

This is in agreement with our earlier conclusion for  $\sigma^{+-}$  but not with  $\sigma^{zz}$  in (2.4). Since the critical theory is rotationally invariant and there is only one correlation length how can different powers possibly emerge? This is the paradox we now wish to resolve.

The answer lies in the behavior of the correlation functions close to but not at criticality. Here the two correlation functions have different behavior. Consider a point  $B$  in Fig. 1 on the physical manifold, away from  $A$  by an amount  $t = \Delta - 1$ . Let us integrate the flow out to  $B'$  which has  $t \sim 1$ . During the flow along  $BD$  one follows close to the separatrix  $C$ , where the correlations are isotropic. However for the second half of the journey, along  $DB'$  the correlations, even along  $C'$ , are not necessarily isotropic. The precise balance between the interactions  $\alpha$  and  $K$  that exists on  $C$  does not exist on  $C'$ . More precisely, we have,  $\gamma_{zz} = \gamma_{+-}$  on  $C$  because the  $\alpha$  term reversed the sign of the second term in Eq. (3.14). When  $\alpha$  is positive and  $g$  is negative, however, the two terms have the same sign and thus  $\gamma_{zz} \neq \gamma_{+-}$ . Before we make this precise and also compute the power-law divergences for the correlation sums, let us go back to the arguments in the introductory sections and see what modifications are needed to accommodate the correct answer within the scaling ansatz.

Schematically, the structure factors can be expressed as

$$S_{ab}(\Delta) \sim \int_1^\infty G_{ab}(\Delta, r) dr. \quad (3.15)$$

The correlation functions are expected to have the scaling form

$$G_{ab}(\Delta, r) \sim (\ln r)^{1/2} X_{ab}(r/\xi)/r, \quad (3.16)$$

where the scaling function  $X_{ab}(x)$  depends on a single combination of the variables  $r$  and  $\Delta$ . The integral in Eq. (3.15) can be split up as

$$\int_{a_0}^{\infty} = \int_{a_0}^{\epsilon\xi} + \int_{\epsilon\xi}^{\xi} + \int_{\xi}^{\infty}. \quad (3.17)$$

For large values of its arguments, the scaling function decays exponentially, corresponding to the exponential decay of correlations away from criticality, namely,

$$X(x) \sim e^{-x}. \quad (3.18)$$

Hence, as long as the scaling function is bounded for small and finite values of its arguments, this does not affect the integrals and one is led to the result

$$\int_a^{\epsilon\xi} (\ln r)^{1/2} \frac{1}{r} dr \sim (\ln \xi)^{3/2} \sim t^{-3/4}, \quad (3.19)$$

where we have used Eq. (1.7). If, on the other hand, the scaling function does affect the first integration in Eq. (3.17), we can get additional divergences. We shall find that for  $r$  large but  $r/\xi$  small, the scaling function for  $S_{zz}$  is anomalous and so the integral does pick up additional divergences. To show this explicitly, we shall compute

the form of the correlation functions away from criticality for  $r/\xi$  small, and carry out the integration in Eq. (3.17).

Let the point  $B$  have coordinates  $x_0$  and  $y_0$  with

$$y_0^2 = x_0^2 + t. \quad (3.20)$$

Under renormalization via Eq. (3.6), this point flows accordingly to

$$\tan^{-1}(x/\sqrt{t}) = \tan^{-1}(x_0/\sqrt{t}) - Z\sqrt{t}, \quad (3.21)$$

or,

$$\tan^{-1}(x/\sqrt{t}) \approx \frac{\pi}{2} - \frac{\sqrt{t}}{x_0} - Z\sqrt{t}, \quad (3.22)$$

where we have used the fact that  $\sqrt{t}/x_0$  is small. This gives

$$x \approx \sqrt{t} \cot[\sqrt{t}(Z + 1/x_0)]. \quad (3.23)$$

We will eventually integrate the flow up to  $B'$ , say, where  $x = -x_0$  and  $y = y_0$ . Hence, we obtain

$$Z_{B'} \approx \pi/\sqrt{t} - 2/x_0. \quad (3.24)$$

Let us revisit the Callan-Symanzik equation for the noncritical case, namely,

$$G_{ab}(R, g_0, t) = \exp \left[ - \int_0^{\ln R} \gamma_{ab}[x(z), y(z)] dz \right] F_{ab}[R/\xi(t)], \quad (3.25)$$

where, now,  $g_0 = (x_0 + y_0)/2$  and  $t \sim x_0 - y_0$  are the natural coordinates while  $F_{ab}$  is a smooth function of its argument. To lowest nontrivial order in  $x$  and  $y$ , we know from the earlier analysis (3.12) that

$$\gamma_{+-} = 1 - x/2. \quad (3.26)$$

We ignore the smoothly varying piece and concentrate on the prefactor

$$G_{+-}^{\text{pre}}(R, g_0, t) = \frac{1}{R} \exp \left[ \frac{1}{2} \sqrt{t} \int_0^{\ln R} \cot[Z\sqrt{t} + \sqrt{t}/x_0] dZ \right], \quad (3.27)$$

or,

$$G_{+-}^{\text{pre}}(R, g_0, t) \approx \frac{1}{R t^{1/4}} \sqrt{\sin[\sqrt{t}(\ln R + 1/x_0)]}. \quad (3.28)$$

In obtaining the prefactor we have used the fact that  $\sin(\sqrt{t}/x_0) \approx \sqrt{t}/x_0$ , since  $x_0$  is fixed and finite. We then proceed to calculate

$$S_{+-}(t) \sim \int_1^{\exp(\pi/\sqrt{t} - 2/x_0)} G_{+-}(R) dR = \frac{1}{t^{1/4} t^{1/2}} \int_0^{\pi - 2\sqrt{t}/x_0} dy \sqrt{[\sin(y + \sqrt{t}/x_0)]} \sim \frac{1}{t^{3/4}} \quad (3.29)$$

noting that the integral is, asymptotically, just a constant.

Now, returning to Eq. (3.14), we will compute  $G_{zz}$ . Keeping  $x$  and  $y$  as separate variables, we get to lowest order in  $x$  and  $y$

$$\gamma_{zz} = 1 - y + x/2, \quad (3.30)$$

which on using (3.20) in general form and (3.25) gives,

$$G_{zz}(R, g_0, t) = \frac{1}{R} \exp \left[ \int_0^{\ln R} (\sqrt{x^2 + t} - x/2) dz \right] G(R/\xi) \quad (3.31)$$

$$\approx \frac{1}{Rt^{1/4}} \frac{\tan \left[ \frac{\sqrt{t}}{2} (\ln R + 1/x_0) \right]}{\sqrt{\sin[\sqrt{t} (\ln R + 1/x_0)]}}. \quad (3.32)$$

Notice that for  $\sqrt{t} \ln R \ll \pi/2$  both  $G_{zz}$  and  $G_{+-}$  go as  $(\ln R)^{1/2}/R$ , but that later on their behavior is quite different. To compute  $S_{zz}(t)$ , all that remains is to integrate  $G_{zz}(R, g_0, t)$  between  $R = 1$  and  $R = e^{-2/x_0 \xi}$ , which yields

$$S_{zz}(t) \approx \int_1^{\exp(\pi/\sqrt{t} - 2/x_0)} dR \frac{1}{Rt^{1/4}} \frac{\tan \left[ \frac{\sqrt{t}}{2} (\ln R + 1/x_0) \right]}{\sqrt{\sin[\sqrt{t} (\ln R + 1/x_0)]}}. \quad (3.33)$$

Changing variables to  $z = \sqrt{t} \ln R$  gives

$$S_{zz}(t) \approx \frac{1}{t^{3/4}} \int_0^{\pi - 2\sqrt{t}/x_0} \frac{\tan[(z + \sqrt{t}/x_0)/2]}{\sqrt{[\sin(z + \sqrt{t}/x_0)]}} dz, \quad (3.34)$$

and, shifting variables to  $z' = z + \sqrt{t}/x_0$ , we get

$$S_{zz} \approx \frac{1}{t^{3/4}} \int_{\sqrt{t}/x_0}^{\pi - \sqrt{t}/x_0} \frac{\tan(z'/2)}{\sqrt{\sin z'}} dz'. \quad (3.35)$$

Here, unlike the situation in (3.29), the integrand is singular as  $t \rightarrow 0$ . The singular part of the integral is readily seen to be  $t^{-1/4}$  so that we finally obtain

$$S_{zz}(t) \approx t^{-1}. \quad (3.36)$$

This confirms and explains the numerical results quoted earlier for two different values of  $\sigma^{+-}$  and  $\sigma^{zz}$ .

#### IV. CONCLUSIONS

The study of the  $S = \frac{1}{2}$  critical chain is an old subject, but looking at it from a different point of view has still revealed novel and unexpected behavior. We have focused attention on the behavior of the longitudinal and transverse structure factors on approach to the isotropic criti-

cal point. Even though the correlations are isotropic at criticality, and there is only one correlation length in the problem, the two structure factors diverge with different exponents. This result has been confirmed by an exact renormalization-group argument. Our analysis shows that such a behavior is a general feature of problems with marginal variables or Kosterlitz-Thouless-type flows. We have also demonstrated that the mechanism for getting different exponents for the longitudinal and transverse correlation sums is related to the scaling function being singular.<sup>11</sup>

*Note added.* After completion of this work we received unpublished results from I. Affleck, D. Gepner, H. Shultz, and T. Ziman where the result (3.13) has been independently derived.

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