Logarithmic Corrections in Quantum Impurity Problems

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The effect of a bulk marginal operator on boundary critical phenomena in two space-time dimensions is considered. The particular case of an open $S=1/2$ antiferromagnetic Heisenberg chain, corresponding to a Wess-Zumino-Witten non-linear $\sigma$ model, is solved. In this case, the needed renormalization group coefficient is associated with a novel operator product expansion in which three operators approach the same point. Resulting logarithmic corrections occurring in finite size calculations and nuclear magnetic resonance experiments are discussed.

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I. INTRODUCTION

Marginally irrelevant operators in two-dimensional conformal field theory lead to logarithmic corrections to scaling behaviour. Because the corresponding coupling constant, $g(l)$, renormalizes to 0 very slowly, as $1/\ln l$ where $l$ is a characteristic length or energy scale, logarithmic corrections occur to virtually all quantities which can be measured experimentally or simulated numerically. These create grave difficulties in obtaining agreement between analytical theory and numerical simulations or experiment. The particular case of the $S=1/2$ Heisenberg antiferromagnetic chain has been discussed extensively. The correlation function, initially predicted to decay as $1/r$, instead decays as $2/\sqrt{3} \ln(1/r)$ to make matters worse, the corrections to this result are only suppressed by additional powers of $1/\ln r$ and are highly sensitive to finite-size effects. Similarly, the energy gap between the ground state and the first excited (triplet) state behaves as

$$\Delta E = \frac{2\pi v}{l} \left[ \frac{1}{2} - \frac{\pi g(l)}{\sqrt{3}} \right]$$

where $v$ is the spin-wave velocity. At very long lengths,

$$g(l) \rightarrow \frac{\sqrt{3}}{4\pi \ln l},$$

giving an additive logarithmic correction to the finite-size energy gap. It is generally very hard to actually observe this logarithmic behaviour unless chains of length several thousand can be studied. Fortunately, this is possible for Bethe ansatz integrable models like the $S=1/2$ Heisenberg chain. For shorter chains it is generally better to regard $g(l)$ as a free parameter. Because Eq. (1.1) has been generalized to many other energy levels, all of which receive corrections linear in $g$, this still has considerable predictive power. Indeed, fitting to expressions of this sort, which effectively subtracts off the leading logarithmic correction to scaling, provides a practical method for numerically determining the universality class of a Hamiltonian. There are analogous finite temperature corrections (for infinite length systems). These include an additive $1/\ln T$ correction to the susceptibility and a multiplicative $(\ln T)^{1/2}$ correction to the spin relaxation rate, $1/T_1$. Although experimental data has been fit to these forms with apparent success, there is very little difficulty in the slow variation and the presence of various other types of corrections in any real material.

Another subject of current experimental and theoretical interest is the general area of quantum impurity problems (QIP’s). In the context of $S=1/2$ Heisenberg antiferromagnetic chains, such a problem occurs for a semi-infinite chain, associated with the dynamics at the chain end. This model can be realized experimentally by dilute substitution of the magnetic ion by a non-magnetic one, eg. Zn substitution for Cu. Related QIP’s involve the Kondo problem and tunneling through a single impurity in a quantum wire (or quantum Hall effect edge states). The general renormalization group (RG) treatment of these problems gives fixed points corresponding to conformally invariant boundary conditions imposed on a given bulk conformal field theory. In general, in such a theory, the effective Hamiltonian contains both bulk and boundary operators. The bulk terms contain integrals over the half-line whereas the boundary terms occur at the impurity location, $x = 0$. Bulk behaviour is unaffected by boundary dynamics, although it must be appreciated that the decay of Green’s functions away from the boundary is itself part of the
boundary critical phenomena. Time correlation functions at the boundary also involve exponents which characterize the boundary condition, as does the finite size spectrum with non-periodic boundary conditions. Boundary interactions cannot affect the renormalization of bulk coupling constants. In most treatments of these problems so far, any renormalization of boundary interactions by bulk interactions has also been ignored. The justification for this is that the bulk system has been assumed to be at a bulk RG fixed point. Any bulk operators present, apart from the fixed point Hamiltonian itself, are irrelevant and can be ignored at low energies. Thus, at least in principle, crossover between boundary fixed points can be treated independently of bulk renormalization. Strictly speaking, this is only justified when the energy scales associated with the boundary renormalization are much smaller than those associated with the bulk irrelevant couplings. This approximation is particularly bad when there are marginally irrelevant bulk interactions present since they renormalize to 0 logarithmically slowly. When marginally irrelevant bulk operators are present we should expect logarithmic corrections to exponents and finite-size scaling. However, the detailed form of these corrections is characteristic of the boundary condition and is not simply related to the log corrections in the bulk theory, nor to the finite-size scaling with periodic boundary conditions.

It is the purpose of this note to consider these logarithmic corrections to boundary critical exponents and finite-size scaling with non-periodic boundary conditions arising from a marginal bulk operator. In the next section we calculate general formulas for the logarithmic corrections using conformal field theory. In Section 3 we compare these formulas to results on the finite size spectrum for an S=1/2 chain with open boundary conditions, for lengths up to 2,000, obtained from the Bethe ansatz. In the final section we comment on the log corrections to correlation functions and the NMR relaxation rate.

II. CONFORMAL FIELD THEORY RESULTS

As observed by Cardy, such logarithmic corrections generally result from corrections to the anomalous dimensions of the various operators, \( \phi_n \), which are linear in \( g \). The associated coupling constants, \( u_n \), obey an renormalization group (RG) equation:

\[
du_n/d \ln L = (2 - \gamma_n)g,
\]

where:

\[
\gamma_n = x_n + 2\pi b_n g + \ldots
\]

Here the \( \ldots \) represents terms of higher order in \( g \) or in other irrelevant operators. Taking into account the fact that \( g \) itself also renormalizes leads to predictions of the various logarithmic corrections. In particular, the finite-size states are in one to one correspondence with the operators and their energy gaps are proportional to \( \gamma_n \). The coefficients, \( b_n \), can be conveniently determined from the operator product expansion (OPE) of the operator \( \phi_n \) with the marginal operator, \( \phi \):

\[
\phi(z)\phi_n(z') \rightarrow -b_n\phi_n(z)/|z-z'|^2.
\]

A calculation of any Green’s function involving \( \phi_n \), to the first order in \( g \), encounters a logarithmic ultraviolet divergence upon integrating \( z \) near \( z' \). This implies the correction to the anomalous dimension in Eq. (2.2). The finite size spectrum is given by:

\[
E_n - E_0 \approx \frac{2\pi v}{l}[x_n + 2\pi b_ng(l)].
\]

The scaling dimension \( x_n \) of the corresponding operator is simply corrected by the anomalous dimension term of first order in \( g \) which is replaced by the effective coupling at scale \( l \).

In the presence of a boundary, this calculation takes a rather unfamiliar turn because the local marginal bulk operator in general becomes bilocal in the presence of a boundary condition. This follows from Cardy’s general approach to conformally invariant boundary conditions, which are always assumed to obey:

\[
T_L(t, 0) = T_R(t, 0),
\]

where \( T_{L,R} \) are the left and right moving terms in the energy momentum tensor. Since \( T_{L,R} \) is a function of \( (t - x) [(t + x)] \) only, it then follows that we may regard the right-movers on the original physical space, \( x > 0 \) as the continuation of the left-movers to the negative axis,
Thus, the factor of $8\pi$ transforms under the irreducible spin representation then there will be a multiplet of $(2S + 1)$ operators, $\Phi_A$ and $\Phi_B$, which may transform under an arbitrary representation of $SU(2)_L \times SU(2)_R$. The finite dimensional matrices, $S^L_A$ are simply the representation of SU(2) under which $\Phi$ transforms. Explicitly, if $\Phi$ transforms under the irreducible spin $S$ representation then there will be a multiplet of $(2S + 1)$ operators, $\Phi_A$ and $\Phi_B$, which may transform under an arbitrary representation of $SU(2)_L \times SU(2)_R$.

Here the spin densities are normalized as:

$$< J^b_L(z)J^b_L(0) > = \frac{\delta^{ab}}{8\pi^2 z^2}.$$  

The factor of $8\pi^2/\sqrt{3}$ is inserted so that the operator multiplied by $g$ in the Hamiltonian has a unit-normalized 2-point function, following the convention of Cardy. The needed OPE’s in this case follow from the basic one of the WZW model:

$$\bar{J}^i_L(z)\phi(z') = \frac{\bar{S}_L^i(z)}{2\pi(z-z')} + \ldots$$

Here the general Virasoro primary operator, $\phi$, may transform under an arbitrary representation of $SU(2)_L \times SU(2)_R$. The finite dimensional matrices, $S^L_A$ are simply the representation of SU(2) under which $\phi$ transforms. Explicitly, if $\phi$ transforms under the irreducible spin $S$ representation then there will be a multiplet of $(2S + 1)$ operators, $\phi_A$ and $\phi_B$, and:

$$(\bar{S}_L^i)A = \sum_B \bar{S}_L^{iB} \phi_B.$$  

Thus,

$$\bar{J}^i_L(z) \cdot \bar{J}^i_R(z') = \frac{\bar{S}_L^i \cdot \bar{S}_R^i}{4\pi^2 |z-z'|^2} \phi(z) + \ldots$$

and we see that the coefficient $b_n$ defined in Eq. (2.3) takes the value:

$$b_n = -\frac{2 \bar{S}_L \cdot \bar{S}_R}{\sqrt{3}}.$$  

Now consider a semi-infinite chain with a free boundary condition at the origin. This boundary condition was treated using bosonization in Ref. [8]. The boundary condition not only is consistent with Eq. (2.6) but also with its Kac-Moody generalization:

$$\bar{J}_R(x) = \bar{J}_L(-x).$$

Eq. (2.6) and (2.14) imply that the correlation function of $T(t, x)$ and $\bar{J}(t, x)$ are simply the chiral correlation functions in the free WZW model. The boundary has no affect on them apart from identifying left with right. The operator

$$T_R(x) = T_L(-x), \quad (x > 0).$$  

This observation allows the Hamiltonian to be written in terms of left movers only, but defined on the entire real line. In particular, it implies that a generic local bulk operator, which can be factorized into its left-moving and right-moving parts, $O^1(t-x)$ and $O^2_R(t+x)$ respectively, becomes bilocal:

$$O(t, x) = O^1_L(t, x)O^2_R(t, x) \rightarrow O^1_L(t, x)O^2_L(t, -x).$$

In particular, the bulk marginal operator becomes bilocal, introducing a novel complication in calculating its effects perturbatively. Boundary operators are also drawn from the left-moving sector only. We may determine the correction to the anomalous dimension of an arbitrary boundary operator, $\Phi$, to first order in $g$, from the 3-point function $< \Phi \Phi^\dagger >$, where $O$ is the marginal bulk operator. However, this 3-point function must be calculated in the presence of the boundary condition, upon which it depends. Furthermore, we see from Eq. (2.7) that this 3-point function effectively becomes a 4-point function of left-moving operators.

In general, some data about the boundary condition will be needed to calculate this 4-point function. As will be seen from the example considered below, it is sufficient to know the OPE of the chiral part of the bulk marginal operator, $O(z)$ with general boundary operators. We consider a special case here, of some importance, for which this OPE can be readily calculated.

Let us consider the problem of an $S=1/2$ Heisenberg chain with an open boundary condition. The bosonized form of this model, applicable at low energies, is the $k=1$ Wess-Zumino-Witten non-linear $\sigma$ model. The marginal operator is quadratic in the chiral spin densities, $\vec{J}_L, \vec{J}_R$, and is written:

$$H = H_0 - g (8\pi^2/\sqrt{3}) \vec{J}_L \cdot \vec{J}_R.$$  

(2.8)

Here the spin densities are normalized as:

$$< J^j_L(z)J^j_L(0) > = \frac{\delta^{ab}}{8\pi^2 z^2}.$$  

(2.9)

The factor of $8\pi^2/\sqrt{3}$ is inserted so that the operator multiplied by $g$ in the Hamiltonian has a unit-normalized 2-point function, following the convention of Cardy. The needed OPE’s in this case follow from the basic one of the WZW model:

$$\vec{J}_L(z)\phi(z') = \frac{\vec{S}_L \phi(z)}{2\pi(z-z')} + \ldots$$

(2.10)

Here the general Virasoro primary operator, $\phi$, may transform under an arbitrary representation of $SU(2)_L \times SU(2)_R$. The finite dimensional matrices, $S^L_A$ are simply the representation of SU(2) under which $\phi$ transforms. Explicitly, if $\phi$ transforms under the irreducible spin $S$ representation then there will be a multiplet of $(2S + 1)$ operators, $\phi_A$ and $\phi_B$, and:

$$(\vec{S}_L^i)A = \sum_B (\vec{S}_L^{iB}) \phi_B.$$  

(2.11)

Thus,

$$\vec{J}_L(z) \cdot \vec{J}_R(z') = \frac{\vec{S}_L \cdot \vec{S}_R}{4\pi^2 |z-z'|^2} \phi(z) + \ldots$$

(2.12)

and we see that the coefficient $b_n$ defined in Eq. (2.3) takes the value:

$$b_n = -\frac{2 \vec{S}_L \cdot \vec{S}_R}{\sqrt{3}}.$$  

(2.13)

Now consider a semi-infinite chain with a free boundary condition at the origin. This boundary condition was treated using bosonization in Ref. [8]. The boundary condition not only is consistent with Eq. (2.6) but also with its Kac-Moody generalization:

$$\vec{J}_R(x) = \vec{J}_L(-x).$$

(2.14)

Eq. (2.6) and (2.14) imply that the correlation function of $T(t, x)$ and $\vec{J}(t, x)$ are simply the chiral correlation functions in the free WZW model. The boundary has no affect on them apart from identifying left with right. The operator
content and finite size spectrum are drawn from conformal towers of the left-moving Kac-Moody algebra only. It was shown in [3] that, for an even length chain, the spectrum consists of the identity conformal tower only. In particular, the spin operator at the boundary becomes the (left-moving) spin density, \( \vec{J}_L(t, 0) \) of the WZW model with correlation function, \( \propto 1/t^2 \). The finite-size spectrum, with free boundary conditions at both ends of a chain of length \( l \) is given by:

\[
E - E_0 = \frac{\pi v}{l} x_L, \tag{2.15}
\]

where \( x_L \) is the scaling dimension of the corresponding (left-moving) operator. This differs from the formula with periodic boundary conditions, Eq. (2.3), by the replacement of \( l \) by \( 2l \) corresponding to doubling the system size due to the identification of Eq. (2.4) at \( x = 0 \) and \( x = l \) and to the replacement of the scaling dimension \( x = x_L + x_R \) by a left-moving scaling dimension \( x_L \) only.

Let us now consider the logarithmic corrections to this formula for open boundary conditions. The problem again reduces to finding the correction to the anomalous dimension of a given operator, \( \phi_n \), to first order in \( g \) where \( \phi_n \) is now a boundary operator. We might again attempt to obtain this from an OPE but we must deal with the fact that the marginal operator is now bilocal. The obvious generalization of Eq. (2.12) is:

\[
\vec{J}_L(z) \cdot \vec{J}_L(z^*) \phi(0) \approx \frac{\vec{S}_L \cdot \vec{S}_L}{2\pi z^2} \phi. \tag{2.16}
\]

However, this is not a conventional OPE because we are bringing three operators to the same point rather than just two. However, as will be argued below, it is nonetheless correct. It is now easy to calculate the correction to the anomalous dimension of a boundary operator. The obvious generalization of Eq. (2.12) is:

\[
b_n = -\frac{\vec{S}_L \cdot \vec{S}_L}{\sqrt{3}}. \tag{2.17}
\]

This differs from the bulk formula Eq. (2.13) only by the identification of \( \vec{S}_R \) with \( \vec{S}_L \) and by the extra factor of \( 1/2 \) arising from the different integration region.

To complete our derivation we just need to justify the rather unorthodox 3-operator OPE occurring in Eq. (2.16). The validity of this formula can be understood by considering the more general connected 4-point function:

\[
G^{AB} = \langle \vec{J}_L(z_1) \cdot \vec{J}_L(z_2) \phi^A(0) \phi^B(\tau) \rangle_{\text{connected}}. \tag{2.18}
\]

We normalize the Virasoro primary boundary operator, \( \phi^A \) so that its two point function is given by:

\[
\langle \phi^A(0) \phi^B(\tau) \rangle = \frac{\delta^{AB}}{(-\tau)^{2x_L}}. \tag{2.19}
\]

We wish to consider the short-distance singularity in \( G^{AB} \) when \( z_1, z_2 \to 0 \). We claim that this is given by:

\[
G^{AB} \to \frac{\vec{S}_L \cdot \vec{S}_L}{4\pi^2 z_1 z_2 (-\tau)^{2x_L}} \delta^{AB}. \tag{2.20}
\]

The correctness of this result can be seen by considering the three different limits \( |z_1| \ll |z_2|, |z_1 - z_2| \) and \( |z_2| \ll |z_1|, |z_1 - z_2| \) and \( |z_1 - z_2| \ll |z_1|, |z_2| \). In the first case, we can obtain the leading singularity by using the OPE of \( \vec{J}_L(z_1) \) with \( \phi^A(0) \) and then the OPE of the result with \( \vec{J}_L(z_2) \). This gives Eq. (2.20). The same singularity is obtained in the second case. In the third case there should be no singularity of the form \( 1/(z_1 - z_2) \) because there is no singular term in the OPE \( \vec{J}_L(z_1) \cdot \vec{J}_L(z_2) \) away from the trivial one which doesn’t contribute to the connected Green’s function. These considerations uniquely fix all singularities in \( G^{AB} \) at \( z_1, z_2 \to 0 \). Note that the crucial property of the boundary condition that is being used is that the OPE of the spin density operators \( \vec{J}_L \) with arbitrary (Virasoro primary) boundary operators has the same form as in the bulk. Now letting \( z_1 = z, z_2 = z^* \) gives Eq. (2.16).
In the particular case where the $φ_A$ are the spin-density operators, $J^a_L$, we have calculated $G^{ab}$ exactly and verified the form of the singularity. In this case we find:

$$< \vec{J}_L(z_1) \cdot \vec{J}_L(z_2)J^a_L(0)J^b_L(\tau) > = \frac{\delta^{ab}}{(2\pi)^4 z_1 z_2 (\tau - z_1)(\tau - z_2)}.$$  \hspace{1cm} (2.21)

We see from Eq. (2.14) that the unit normalized operator is $\phi^a = 2\pi \sqrt{2} J^a$. Also using the fact that $\vec{J}$ has $S_L = 1$ and therefore $\vec{S}_L \cdot \vec{S}_L = S_L(S_L + 1) = 2$, we see that, in the limit $z_1 \to 0$, Eq. (2.21) agrees with Eq. (2.20).

Now let us consider the finite size spectrum, examining the lowest energy excited state of spin $S$. This is given by Eq. (2.13) except that the dimension of the (left-moving) field, $x_L$, must be replaced by the anomalous dimension, $\gamma_n$. This is given by Eq. (2.3) with $b_n$ now given by Eq. (2.17). Thus we obtain:

$$E_S^{\text{open}} - E_0^{\text{open}} \approx \frac{\pi v}{l} \left[ S^2 - \frac{2\pi S(S + 1)(g/\sqrt{3})}{4\ln l} \right].$$  \hspace{1cm} (2.22)

For exponentially long chains we may use the asymptotic form of $g(l)$: $g(l) \to \sqrt{3}/(4\pi \ln l)$, giving:

$$E_S^{\text{open}} - E_0^{\text{open}} \approx \frac{\pi v}{l} \left[ S^2 - \frac{S(S + 1)}{2\ln l} \right].$$  \hspace{1cm} (2.23)

It is interesting to compare Eq. (2.23) to the corresponding result for periodic boundary conditions. If we again consider the lowest energy state of given spin $S$, this has $S_L = S_R = S/2$ and hence:

$$E_S^{\text{per}} - E_0^{\text{per}} \approx \frac{2\pi v}{l} \left[ \frac{S^2}{2} - \frac{S^2}{4\ln l} \right].$$  \hspace{1cm} (2.24)

The $1/l$ terms are the same for open and periodic boundary conditions but the $1/\ln l$ terms are not. (We note that the logarithmic corrections for open boundary conditions were assumed to be same as the ones for periodic boundary conditions in [10]).

We have also calculated the logarithmic correction to the ground state energy for open boundary conditions. Ignoring the irrelevant operator, the ground state energy for any one dimensional Hamiltonian which renormalizes to a conformal field theory, defined on an interval of length $l$ with generic boundary conditions at 0 and $l$ consistent with Eq. (2.6) is:

$$E_0(l) = e_0 l + e_1 - (\pi v/24l)c,$$  \hspace{1cm} (2.25)

where $c$ is the central charge. Note that the coefficient of $1/l$ is $1/4$ times the value for periodic boundary conditions. Also note that an additional non-universal surface energy, $e_1$, appears when the boundary conditions are non-periodic. Logarithmic corrections to this formula can be calculated by doing perturbation theory in the marginally irrelevant coupling constant, $g(l)$ just as in the periodic case. One finds that the correction of $O(1/l)$ is universal. This must be separated from various non-universal corrections to $e_0$ and $e_1$. Once the correction to the $1/l$ term of leading order in $g$ is calculated, $g$ may be replaced by the effective coupling constant at scale $l$, $g(l)$, resulting in logarithmic corrections. In the case of periodic boundary conditions, this leading correction was found to be $O(g^3)$. By contrast, in the case of open boundary conditions we find that it is $O(g^2)$.

Let us first consider the correction of $O(g)$. From Eq. (2.8) this gives a correction to the ground state energy:

$$\delta E^{(1)}_0 = -\frac{8\pi^2 g}{\sqrt{3}} \int_0^l dx < \vec{J}_L(x) \cdot \vec{J}_L(-x) >.$$  \hspace{1cm} (2.26)

This Green’s function is given in Eq. (2.9) for the case $l \to \infty$. We may obtain the Green’s function for finite length by a conformal transformation:

$$e^{(\pi/l)(\tau + ix)} = e^{(\pi/l)(\tau - ix)},$$  \hspace{1cm} (2.27)

giving:

$$< J^a_L(x) J^b_L(-x) > = \frac{\delta^{ab}}{8\pi^2 \left( \frac{1}{\pi} \sin \frac{\pi x}{l} \right)^2}.$$  \hspace{1cm} (2.28)
The integral of Eq. (2.20) is ultraviolet divergent both at \( x = 0 \) and \( x = l \). We may insert an ultraviolet cut-off on the integration region, \( x > a, \ l - x > a \) where \( a \) is of order the lattice spacing. This gives the ground state energy correction of first order in \( g \):

\[
\delta E_0^{(1)} = -2 a \sqrt{\frac{\pi}{3}} \cot \frac{\pi a}{l}.
\]  

(2.29)

Now Taylor expanding in powers of \( a/l \), we see that we obtain a cut-off dependent contribution to the non-universal surface energy, \( e_1 \) in Eq. (2.23) together with corrections of \( O(1/l^2) \):

\[
\delta E_0^{(1)} \approx -2 g \sqrt{\frac{3}{a}} + O(a/l^2).
\]  

(2.30)

Importantly, there is no term of \( O(1/l) \).

We now push this calculation to second order in \( g \). This term is given by:

\[
\delta E_0^{(2)} = -\frac{1}{2} \left[ \frac{8\pi^2}{\sqrt{3}} g \right]^2 \int_{-\infty}^{\infty} d\tau \int_{0}^{l} dx_1 \int_{0}^{l} dx_2 < \mathcal{J}_L(\tau, x_1) \cdot \mathcal{J}_L(\tau, -x_1) \mathcal{J}_L(0, x_2) \cdot \mathcal{J}_L(0, -x_2) > .
\]

(2.31)

Let us first evaluate this expression in the limit \( l \to \infty \). Using Eq. (2.21), we obtain:

\[
\delta E_0^{(2)} \to -\frac{g^2 \pi^2}{2} \int_{-\infty}^{\infty} d\tau \frac{dx_1 dx_2}{\tau^2}.
\]  

(2.32)

Note that we have inserted a factor of 2 here because equal contributions arise from \( x \) near 0 and \( x \) near \( l \). The \( x \)-integrals can be done exactly and are ultraviolet finite, for non-zero \( \tau \):

\[
\delta E_0^{(2)} \to -\frac{g^2 \pi^2}{\tau_0},
\]  

(2.33)

another cut-off dependent contribution to the surface energy, \( e_1 \) in Eq. (2.25). To obtain \( \delta E_0^{(2)} \) at finite \( l \), we again use the conformal transformation of Eq. (2.27) to obtain:

\[
\delta E_0^{(2)} = -2 g^2 \int_{-\infty}^{\infty} d\tau \int_{0}^{l} dx_1 dx_2 (\pi/2l)^4 \frac{dx_1 dx_2}{\left| \sin(\pi/2l)(x_1 - x_2)^2 + i\tau \right|^2 \sin(\pi/2l)(x_1 + x_2)^2 + i\tau \right|^2}.
\]  

(2.35)

The \( x \)-integrals are again finite for non-zero \( \tau \). We again cut off the \( \tau \) integral at \( |\tau| > \tau_0 \). Noting that the integrand is symmetric under \( x_1 \to -x_1 \) or \( x_2 \to -x_2 \) and also \( \tau \to -\tau \), it is convenient to extend the \( x \)-integrals from \(-l\) to \( l \) and reduce the \( \tau \) integral from \( \tau_0 \) to \( \infty \). This introduces a net factor of 1/2. It is now convenient to change variables to:

\[
z_j = e^{i\pi x_j/l},
\]  

(2.36)

and

\[
u \equiv \pi \tau/l.
\]  

(2.37)

The complex variables, \( z_j \) are integrated around the unit circle. This expression now becomes:

\[
\delta E_0^{(2)} = -\frac{g^2 \pi}{l} \int_{u_0}^{\infty} du \int_{C} dz_1 \int_{C} dz_2 \frac{z_1}{z_2(z_1 - z_2 e^u)(z_1 - z_2 e^{-u})(z_1 - z_2^{-1} e^u)(z_1 - z_2^{-1} e^{-u})}.
\]  

(2.38)

where \( u_0 \equiv \pi \tau_0/l \) and \( C \) denotes the unit circle integration contour. The \( z_1 \) integral can now be done by the standard contour integration method, with contributions from the poles at \( z_2^{\pm 1} e^{-u} \). The result is:
\[
\delta E_0^{(2)} = -2\pi i g^2 \frac{\pi}{l} \int_{u_0}^{\infty} du \coth u \int_C dz_2 \frac{z_2}{(z_2^2 - e^{2u})(z_2^2 - e^{-2u})}. 
\]

(2.39)

Also doing the \(z_2\) integral by contour methods gives:

\[
\delta E_0^{(2)} = -\pi^2 g^2 (\pi/l) \int_{u_0}^{\infty} \frac{du}{\sinh^2(u)}. 
\]

(2.40)

Finally, performing this elementary integration gives:

\[
\delta E_0^{(2)} = -2\pi^2 g^2 (\pi/l) \frac{1}{e^{2u_0} - 1} \approx -\frac{\pi^2 g^2}{\tau_0} + \frac{\pi^2 g^2 \pi}{l} + O(\tau_0/l^2). 
\]

(2.41)

We have recovered the same cut off dependent to the surface energy, \(e_1\) as in Eq. (2.34). More importantly, we have also obtained a term of \(O(1/l)\) which is cut off independent and therefore is expected to be universal. Thus, we obtain the log correction to the ground state energy with open boundary conditions:

\[
E_0^{\text{open}}(l) = e_0 l + e_1 - \frac{\pi v}{24l} \left[1 - 24\pi^2 g(l)^2\right]. 
\]

(2.42)

For exponentially large \(l\) we may use Eq. (1.2) to write:

\[
E_0^{\text{open}}(l) \approx e_0 l + e_1 - \frac{\pi v}{24l} \left[1 - \frac{9/2}{(\ln l)^2}\right]. 
\]

(2.43)

As usual, the corrections to these formulas are only down by additional powers of \(g(l)\), that is \(1/\ln l\). The corresponding formula for periodic boundary conditions is:

\[
E_0^{\text{per}}(l) \approx e_0 l - \frac{\pi v}{6l} [1 + (2\pi)^3 g(l)^3/\sqrt{3}] \approx e_0 l - \frac{\pi v}{6l} \left[1 + \frac{3/8}{(\ln l)^3}\right]. 
\]

(2.44)

Among other differences, note that the log corrections decrease the apparent value of \(c\) for open boundary conditions but increase it for periodic boundary conditions. The fact that the correction to \(c\) goes like \(1/(\ln l)^2\) was obtained from the Bethe ansatz in Ref. [12], although the coefficient was not obtained.

**III. NUMERICAL RESULTS ON FINITE SIZE SPECTRUM**

One application of the above results for boundary critical phenomena is to the numerical study of finite size scaling. We extract estimates of \(g(l)\) defined in Eq. (2.22) and Eq. (2.42) from the energies of finite size spin 1/2 antiferromagnetic Heisenberg open chains. The Hamiltonian is

\[ H = \sum_{i=1}^{l-1} S_i \cdot S_{i+1}, \]

(3.1)

where the \(S_i\)'s are spin 1/2 operators. The Bethe ansatz equations\(^4\) for the Hamiltonian of Eq. (3.1) are

\[
\left(\frac{\Lambda_k + i/2}{\Lambda_k - i/2}\right)^{2l} = \prod_{j \neq k}^{M} \frac{\Lambda_k - \Lambda_j + i}{\Lambda_k - \Lambda_j - i} \frac{\Lambda_k + \Lambda_j + i}{\Lambda_k + \Lambda_j - i}, 
\]

(3.2)

where \(l\) is the number of sites in the open chain. The roots can be numerically calculated\(^4\) The number of roots, \(M\) determines the total \(S^z\) component through the relation \(S^z = L/2 - M\). In terms of the solutions, \(\Lambda_k\), to the Bethe ansatz equations, Eq. (3.2), the energy is given by

\[
E = \frac{l - 1}{4} - \frac{1}{2} \sum_{k=1}^{M} \frac{1}{\Lambda_k^2 + 1/4}. 
\]

(3.3)

The surface energy \(e_1 = (\pi - 1 - 2\ln 2)/4\) for the two ends of open chain can be exactly obtained. The rapidities \(\{\Lambda_k, k = 1, l/2\}\) solving the Bethe ansatz equations Eq. (3.2) for the ground state of the open chain are all bigger.
than zero. Let’s order \( \Lambda_k \) so that: \( \Lambda_1 > \Lambda_2 > \ldots > \Lambda_{l/2-1} > \Lambda_{l/2} > 0 \). We can construct another set of rapidities \( \{\Lambda'_k, k = 1, l\} \):

\[
\Lambda'_j = -\Lambda_j, \quad \Lambda'_{l+1-j} = \Lambda_j, \quad \text{for } j = 1 \text{ to } l/2,
\]

which solves exactly the following Bethe ansatz equations for a periodic chain of length \( 2l + 1 \):

\[
\left( \frac{\Lambda'_k + i/2}{\Lambda'_k - i/2} \right)^{2l+1} = \prod_{j \neq k} \frac{\Lambda'_k - \Lambda'_j + i}{\Lambda'_k - \Lambda'_j - i}.
\]

The energy for the periodic chain is given by

\[
E' = \frac{2l + 1}{4} - \frac{1}{2} \sum_{k=1}^{l} \frac{1}{\Lambda'^2_k + 1/4}.
\]

In the logarithmic form of the Bethe ansatz equations for the periodic chain, the set \( \{\Lambda'_k, k = 1, l\} \) corresponds to a set of integers \( \{I'_k, k = 1, l\} \):

\[
I'_j = j - (l/2 + 1), \quad I'_{l+1-j} = j, \quad \text{for } j = 1 \text{ to } l/2,
\]

\[\text{i.e.,} \quad -l/2, -l/2 + 1, \ldots -2, -1, 1, 2, \ldots l/2 - 1, l/2.\]

The groundstate of the open chain corresponds to an excited state of the periodic chain with a hole exactly at \( I = 0 \) in the connected integer set \( \{I_i, i = 1, l + 1\} \) for the ground state of the periodic chain.\(^4\) While the groundstates of the periodic chain of odd length have spin \( S^z = \pm 1/2 \) and momentum \( \pm \pi/2 \), the state of the odd length periodic chain corresponding to the groundstate of the even length open chain has \( S^z = -1/2 \) and momentum 0. From its momentum, and from the fact that it has one hole we expect its energy, in the large \( l \) limit, to be the groundstate energy of the periodic chain plus the excitation energy for a magnon of momentum \( \pi/2 \): \( E' = c_0(2l + 1) + \nu_s \sin(k) \), \( \nu_s = \pi/2 \), and \( c_0 = 1/4 - \ln 2 \) for the spin 1/2 chain. Comparing the expressions for \( E \) and \( E' \), we can eliminate the summation over \( \Lambda \) and obtain \( E = c_0l + e_1 \) for the ground state of the open chain with \( e_1 = (\pi - 1 - 2 \ln 2)/4 \). We have checked this result from our numerical solution of the Bethe ansatz equations for finite \( l \) obtaining agreement to at least 6 decimal places. This result was derived earlier from the Bethe ansatz equations by a somewhat different method.\(^4\)

To test the CFT predictions, we extract three estimates of \( g(l) \) using Eq. \((2.22)\) for the \( S = 1 \) and \( S = 2 \) excited states and Eq. \((2.12)\) for the groundstate for chains up to two thousands sites by solving Eq. \((3.2)\) numerically. We draw the three \( g(l) \) completely determined by the energies of these three states, respectively, in Fig. \(\text{4}\). The reason that these three estimates of \( g(l) \) don’t agree exactly is because of the various corrections to these energies of higher order in \( g(l) \). However, at large \( l \) these estimates should converge since \( g(l) \rightarrow 0 \). We see that the coupling constants indeed collapse into one value which approaches 0, as the chain length increases thus verifying the CFT predictions. Previous numerical studies for periodic boundary conditions have verified finite size scaling obtained by conformal field theory.\(^4\)\(^4\)\(^4\)\(^4\)\(^4\) We then compare the \( g(l) \) obtained from the open boundary conditions with the one from periodic boundary conditions in Fig. \(\text{5}\). We redraw the ground state \( g(l) \) for open boundary conditions and the average \( g(l) \) given by the ground state, the singlet excitation, and the triplet excitation for periodic boundary conditions. These data for periodic boundary conditions were obtained in Ref. \([10]\). The two \( g(l) \) approach each other in the large length limit. The one-loop renormalization group prediction for \( g(l) \) given in Ref. \([3]\), \( g(l) = g_0(l_0)/[1 + \pi \beta g_0(l_0) \ln(l/l_0)] \), with \( b = 4/\sqrt{3} \) is also drawn in Fig. \(\text{5}\). We use the average of the \( g(l) \) for periodic and open chains at \( l_0 = 2048 \) to fix \( g_0 \). The one-loop renormalization group prediction fits \( g(l) \) at large \( l \). So we see that the logarithmic corrections for Heisenberg chains have been successfully predicted by conformal field theory.
FIG. 1. \( g(l) \) calculated by Eq. (2.22) and Eq. (2.42) from Bethe ansatz energies of spin 1/2 antiferromagnetic Heisenberg open chain (OBC). The three \( g(l) \) are obtained from energies of ground state, total spin \( S = 1 \) excited state and \( S = 2 \) excited state, respectively.

FIG. 2. The \( g(l) \) calculated from ground state of open chain (OBC) and the average \( g(l) \) for periodic chain (PBC), for spin 1/2 antiferromagnetic Heisenberg model. The full line is the one-loop renormalization group (RG) prediction \( g(l) = g_0(l_0)/[1 + \pi bg_0(l_0) \ln(l/l_0)] \) with \( b = 4/\sqrt{3} \). \( g_0(l_0) \) is determined by the average of open chains ground state’s \( g(l) \) and the periodic chain’s average \( g(l) \) at the chain length \( l_0 = 2048 \).

**IV. CORRELATION FUNCTIONS AND \( 1/T_1 \)**

Another application of the anomalous dimension of boundary operators is to Green’s functions for a semi-infinite system. A time-dependent Green’s function at the boundary, for obeys the RG equation:

\[
\frac{\partial}{\partial \ln \tau} \gamma + \frac{\partial}{\partial \gamma} \beta + 2\gamma g) G(\tau, g) = 0,
\]

where \( \gamma \) is the anomalous dimension of the boundary operator whose Green’s function is being calculated. This is given, to \( O(g) \), by Eq. (2.2). \( g(\tau) \) in Eq. (4.1) is the effective coupling constant at scale \( \tau \). Solving this equation we obtain:

\[
< \phi(\tau, 0) \phi(0, 0) > \rightarrow \frac{(\ln |\tau|)^{-4b_0/b}}{\tau^{2x_n}}.
\]
Both the exponent, \(x\), and the power of the logarithm are different than what occurs in the bulk. For the lowest dimension boundary operator of spin \(S\) the factor of \(\ln|\tau|\) is raised to the power \(S_L(S_L + 1)\). In particular, for the spin operator at the boundary in the lattice Heisenberg model, the correlation function behaves as:

\[
< \vec{S}_0(\tau) \cdot \vec{S}_0(0) > \approx \text{constant} \frac{\ln|\tau|^2}{|\tau|^2}. \tag{4.3}
\]

The imaginary part of the retarded Green’s function at zero frequency and finite \(T\), obtained from the Fourier transform of Eq. (4.3), gives the nuclear magnetic resonance relaxation rate, \(1/T_1\) for a chain with non-magnetic impurities. This behaves as:

\[
1/T_1 \propto T[\ln(T_0/T)]^2, \tag{4.4}
\]

for some temperature scale \(T_0\) of order the exchange energy. The \(1/\tau^2\) power law was first derived in [8], without consideration of logarithmic corrections. The discussion of the linear power-law in \(1/T_1\), resulting from performing the Fourier transform, was first discussed, as far as we know, in [18]. These authors also attempted to calculate the logarithmic correction. However, their result, for which no derivation was given, differs from ours, containing \([\ln(T_0/T)]^4\) rather than \([\ln T_0/T]^2\). This behaviour is to be contrasted with that for the pure system, in which \(1/T_1 \propto [\ln(T/T_0)]^{1/2}\), constant up to a log correction.

Of course, an actual experiment on a doped \(S=1/2\) chain compound would presumably average over all distances from the chain ends. (This is related both to the fact that the relaxing nuclei can be at arbitrary locations and that even a nucleus near the end of a chain will have a transferred hyperfine interaction with spins further away from the chain end.) We note that, at \(T = 0\) and ignoring log corrections, the spin self-correlation for a spin a distance \(x\) from the chain end is given by:

\[
< \vec{S}_j(t) \cdot \vec{S}_j(0) > \propto \frac{2x/v}{|t| \sqrt{t^2 - 4x^2/v^2}}, \tag{4.5}
\]

where \(v\) is the spin-wave velocity. At sufficiently long times this decays as \(1/t^2\) for all \(x\). However, for \(t << x/v\) it exhibits the bulk behaviour, decaying as \(1/t\). Thus we expect that the zero frequency finite \(T\) Fourier transform, which determines \(1/T_1\), will be essentially constant (ignoring log corrections) down to a temperature of order \(v/x\), below which it will vanish essentially linearly in \(T\).

\(1/T_1\) has been measured\(^{19}\) for the quasi one dimensional antiferromagnetic compound Sr\(_2\)CuO\(_3\) obtaining apparent agreement with the field theory prediction\(^{5}\) \((\ln T)^{1/2}\). Broad shoulders observed in the NMR intensity\(^{21}\) were interpreted as resulting from the distribution of local susceptibilities predicted by field theory methods\(^{20}\) for chains with free ends. Possibly such data will also verify the distribution of relaxation rates resulting from impurities.

After this work was completed we managed to obtain a copy of a three year old preprint\(^{22}\) which was never published nor available on the xxx archive, and which derived many of the results obtained here.

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