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Logarithmic corrections in quantum impurity problems

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Abstract. The effect of a *bulk* marginal operator on *boundary* critical phenomena in two space–time dimensions is considered. The particular case of an open $S = \frac{1}{2}$ antiferromagnetic Heisenberg chain, corresponding to a Wess–Zumino–Witten nonlinear σ model, is solved. In this case, the required 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.

1. Introduction

Marginally irrelevant operators in two-dimensional conformal field theory (CFT) [1] lead to logarithmic corrections to scaling behaviour. Because the corresponding coupling constant, $g(l)$, renormalizes to zero 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 $S = \frac{1}{2}$ Heisenberg antiferromagnetic chain has been discussed extensively. The correlation function, initially predicted to decay as $1/r$, instead decays as $(\ln r)^{1/2}/r$ [2,3]. 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 [1]:

$$\Delta E = \frac{2\pi v}{l}\left[\frac{1}{2} - \frac{\pi g(l)}{\sqrt{3}}\right] \tag{1.1}$$

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

$$g(l) \rightarrow \frac{\sqrt{3}}{4\pi \ln l} \tag{1.2}$$

giving an additive logarithmic correction to the finite-size energy gap. It is generally very hard to actually observe this logarithmic behaviour unless chains with length of several thousand can be studied. Fortunately, this is possible for Bethe ansatz integrable models like the $S = \frac{1}{2}$ Heisenberg chain. For shorter chains it is generally better to regard $g(l)$ as a free parameter. Because equation (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 [2]. There are analogous finite-temperature corrections (for infinite-length systems). These include an additive $1/\ln T$ correction to the susceptibility [4] and a multiplicative $(\ln T)^{1/2}$ correction to the nuclear magnetic resonance (NMR) relaxation rate, $1/T_1$ [5]. Although experimental data have been fitted to these forms with apparent success [6, 7] this is a very difficult exercise due to 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 (QIPs). In the context of $S = \frac{1}{2}$ Heisenberg antiferromagnetic chains, such a problem occurs for a semi-infinite chain, associated with the dynamics at the chain end [8]. This model can be realized experimentally by dilute substitution of the magnetic ion by a non-magnetic one, e.g. Zn substitution for Cu. Related QIPs involve the Kondo problem and tunnelling 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 CFT (for a review see [9]). 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 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 zero 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 (PBCs).

It is the purpose of this paper to consider these logarithmic corrections to boundary critical exponents and finite-size scaling with non-PBCs arising from a marginal bulk operator. In the next section we calculate general formulae for the logarithmic corrections using CFT. In section 3 we compare these formulae to results on the finite-size spectrum for an $S = \frac{1}{2}$ chain with open boundary conditions (OBCs), for lengths up to 2000, obtained from the Bethe ansatz. In the final section we comment on the log corrections to correlation functions and the NMR relaxation rate.

2. Conformal field theory results

As observed by Cardy [1], such logarithmic corrections generally result from corrections to the anomalous dimensions of the various operators, ϕ_n, which are linear in g. The associated coupling constants, u_n, obey RG equations:

$$\mathrm{d}u_n/\mathrm{d}\ln L = [2-\gamma_n]u_n + \mathrm{O}(u_n^2) \tag{2.1}$$

where

$$\gamma_n = x_n + 2\pi b_n g + \cdots. \tag{2.2}$$

Here the $\cdots$ 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 γ_n. The coefficients, b_n can be conveniently determined from the operator product expansion (OPE) of the operator ϕ_n with the marginal operator, ϕ:

$$\phi(z)\phi_n(z') \to \frac{-b_n\phi_n(z)}{|z-z'|^2}. \tag{2.3}$$

A calculation of any Green function involving ϕ_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 equation (2.2). The finite-size spectrum is given by

$$E_n - E_0 \approx \frac{2\pi v}{l}[x_n + 2\pi b_n g(l)]. \tag{2.4}$$

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

$$T_L(t,0) = T_R(t,0) \tag{2.5}$$

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,

$$T_R(x) = T_L(-x) \qquad (x>0). \tag{2.6}$$

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, $O_L^1(t-x)$ and $O_R^2(t+x)$ respectively, becomes *bilocal*:

$$O(t,x) = O_L^1(t,x)O_R^2(t,x) \to O_L^1(t,x)O_L^2(t,-x). \tag{2.7}$$

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, Φ, to first order in g, from the three-point function $\langle\Phi O \Phi^\dagger\rangle$, where O is the marginal bulk operator. However, this three-point function must be calculated in the presence of the boundary condition, upon which it depends. Furthermore, we see from equation (2.7) that this three-point function effectively becomes a four-point function of left-moving operators.

In general, some data about the boundary condition will be needed to calculate this four-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 $S = \frac{1}{2}$ Heisenberg chain with an OBC. The bosonized form of this model, applicable at low energies, is the $k = 1$ Wess–Zumino–Witten (WZW) nonlinear σ model. The marginal operator is quadratic in the chiral spin densities, $\vec{J}_{L,R}$, and is written as

$$H = H_0 - g(8\pi^2/\sqrt{3})\vec{J}_L \cdot \vec{J}_R. \tag{2.8}$$

Here the spin densities are normalized as

$$\langle J_L^a(z) J_L^b(0)\rangle = \frac{\delta^{ab}}{8\pi^2 z^2}. \tag{2.9}$$

The factor of $8\pi^2/\sqrt{3}$ is inserted so that the operator multiplied by g in the Hamiltonian has a unit-normalized two-point function, following the convention of Cardy [1]. The required OPEs in this case follow from the basic one of the WZW model:

$$\vec{J}_L(z)\phi(z') = \frac{\vec{S}_L\phi(z)}{2\pi(z - z')} + \cdots. \tag{2.10}$$

Here the general Virasoro primary operator, ϕ, 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 ϕ transforms. Explicitly, if ϕ transforms under the irreducible spin S representation then there will be a multiplet of $(2S + 1)$ operators, ϕ_A and

$$(\vec{S}_L\phi)^A \equiv \sum_B \vec{S}_L^{AB}\phi^B. \tag{2.11}$$

Thus,

$$\vec{J}_L(z) \cdot \vec{J}_R(z)\phi(z') = \frac{\vec{S}_L \cdot \vec{S}_R}{4\pi^2|z - z'|^2}\phi(z) + \cdots \tag{2.12}$$

and we see that the coefficient b_n defined in equation (2.3) takes the value

$$b_n = -\frac{2\vec{S}_L \cdot \vec{S}_R}{\sqrt{3}}. \tag{2.13}$$

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

$$\vec{J}_R(x) = \vec{J}_L(-x). \tag{2.14}$$

Equations (2.6) and (2.14) imply that the correlation functions of $T(t, x)$ and $\vec{J}(t, x)$ are simply the chiral correlation functions in the free WZW model. The boundary has no effect 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 [8] 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 PBCs, equation (2.4), by the replacement of l by $2l$ corresponding to doubling the system size due to the identification of equation (2.6) 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 OBCs. The problem again reduces to finding the correction to the anomalous dimension of a given operator, ϕ_n, to first order in g where ϕ_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 equation (2.12) is

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

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. A logarithmic ultraviolet divergence is again encountered for any Green function involving the operator ϕ, to first order in g from integrating over z near zero. However, this is reduced by a factor of two relative to the bulk case because z is only integrated over the half-plane rather than the entire plane. A convenient ultraviolet cut-off is given by restricting the z integral to $|z| > a$. In the bulk case the excluded region is a circle of radius a around the origin but in the boundary case it is only a semi-circle of radius a. Our conclusion is thus that the anomalous dimension of a boundary operator is given by equation (2.2) but with the coefficient b_n now given by

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

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

To complete our derivation we just need to justify the rather unorthodox three-operator OPE occurring in equation (2.16). The validity of this formula can be understood by considering the more general connected four-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, ϕ^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

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

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 equation (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 $\vec{J}_L(z_1) \cdot \vec{J}_L(z_2)$ apart from the trivial one which does not contribute to the connected Green 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 J_L^z with arbitrary (Virasoro primary) boundary operators has the same form as in the bulk. Now letting $z_1 = z$, $z_2 = z^*$ gives equation (2.16).

In the particular case where the ϕ_A are the spin-density operators, J_L^a, we have calculated G^{ab} exactly and verified the form of the singularity. In this case we find

$$\langle \vec{J}_L(z_1)\cdot\vec{J}_L(z_2)J_L^a(0)J_L^b(\tau)\rangle = \frac{\delta^{ab}}{(2\pi)^4 z_1 z_2(\tau - z_1)(\tau - z_2)}. \tag{2.21}$$

We see from equation (2.9) 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 $z_i \to 0$, equation (2.21) agrees with equation (2.20).

Now let us consider the finite-size spectrum, examining the lowest energy excited state of spin S. This is given by equation (2.15) except that the dimension of the (left-moving) field, x_L must be replaced by the anomalous dimension, γ_n. This is given by equation (2.2) with b_n now given by equation (2.17). Thus we obtain

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

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

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

It is interesting to compare equation (2.23) with the corresponding result for PBCs [2]. If we again consider the lowest energy state of given spin S, this has $S_L = S_R = S/2$ and hence

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

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

We have also calculated the logarithmic correction to the ground state energy for OBCs. Ignoring the irrelevant operator, the ground state energy for any one-dimensional Hamiltonian which renormalizes to a CFT, defined on an interval of length l with generic boundary conditions at zero and l consistent with equation (2.6), is

$$E_0(l) = e_0 l + e_1 - (\pi v/24l)c \tag{2.25}$$

where c is the central charge [11]. Note that the coefficient of $1/l$ is $\frac{1}{4}$ times the value for PBCs. 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 PBCs, this leading correction was found to be $O(g^3)$. By contrast, in the case of OBCs we find that it is $O(g^2)$.

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

$$\delta E_0^{(1)} = \frac{-8\pi^2 g}{\sqrt{3}}\int_0^l \mathrm{d}x\,\langle \vec{J}_L(x)\cdot\vec{J}_L(-x)\rangle. \tag{2.26}$$

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

$$(\tau' + \mathrm{i}x') = \mathrm{e}^{(\pi/l)(\tau+\mathrm{i}x)} \tag{2.27}$$

giving

$$\langle J_L^a(x) J_L^b(-x)\rangle = \frac{\delta^{ab}}{8\pi^2[\frac{l}{\pi}\sin\frac{\pi x}{l}]^2}. \tag{2.28}$$

The integral of equation (2.26) 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:

$$\delta E_0^{(1)} = -2g\sqrt{3}\frac{\pi}{l}\cot\frac{\pi a}{l}. \tag{2.29}$$

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 equation (2.25), together with corrections of $\mathrm{O}(1/l^2)$:

$$\delta E_0^{(1)} \approx \frac{-2g\sqrt{3}}{a} + \mathrm{O}(a/l^2). \tag{2.30}$$

Importantly, there is no term of $\mathrm{O}(1/l)$.

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

$$\delta E_0^{(2)} = -\frac{1}{2}\left[\frac{8\pi^2}{\sqrt{3}}g\right]^2 \int_{-\infty}^{\infty}\mathrm{d}\tau \int_0^l \mathrm{d}x_1 \int_0^l \mathrm{d}x_2 \langle \vec{J}_L(\tau, x_1)\cdot\vec{J}_L(\tau,-x_1)\vec{J}_L(0,x_2) \cdot\vec{J}_L(0,-x_2)\rangle. \tag{2.31}$$

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

$$\delta E_0^{(2)} \to -\left[\frac{8\pi^2}{\sqrt{3}}g\right]^2 \frac{3}{(2\pi)^4}\int_{-\infty}^{\infty}\mathrm{d}\tau \int_0^{\infty}\frac{\mathrm{d}x_1\,\mathrm{d}x_2}{[\tau^2+(x_1-x_2)^2][\tau^2+(x_1+x_2)^2]}. \tag{2.32}$$

Note that we have inserted a factor of two here because equal contributions arise from x near zero and x near l. The x-integrals can be calculated exactly and are ultraviolet finite, for non-zero τ:

$$\delta E_0^{(2)} \to -\frac{g^2\pi^2}{2}\int_{-\infty}^{\infty}\frac{\mathrm{d}\tau}{\tau^2}. \tag{2.33}$$

The τ integral is ultraviolet divergent. We cut off the integral, $|\tau| > \tau_0$, where τ_0 is of $\mathrm{O}(a/v)$. This gives the second-order ground state energy correction:

$$\delta E_0^{(2)} \to -\frac{g^2\pi^2}{\tau_0} \tag{2.34}$$

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

$$\delta E_0^{(2)} = -2g^2\int_{-\infty}^{\infty}\mathrm{d}\tau\int_0^l \frac{\mathrm{d}x_1\,\mathrm{d}x_2\,(\pi/2l)^4}{|\sin(\pi/2l)[(x_1-x_2)^2+\mathrm{i}\tau]|^2|\sin(\pi/2l)[(x_1+x_2)^2+\mathrm{i}\tau]|^2}. \tag{2.35}$$

The x_i integrals are again finite for non-zero τ. We again cut off the τ 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_i integrals from $-l$ to l and reduce the τ integral from τ_0 to ∞. This introduces a net factor of $\frac{1}{2}$. It is now convenient to change the variables to

$$z_j \equiv \mathrm{e}^{\mathrm{i}\pi x_j/l} \tag{2.36}$$

and

$$u \equiv \pi\tau/l. \tag{2.37}$$

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

$$\delta E_0^{(2)} = -\frac{g^2\pi}{l}\int_{u_0}^{\infty} \mathrm{d}u \int_C \mathrm{d}z_1 \int_C \mathrm{d}z_2 \frac{z_1}{z_2(z_1 - z_2\mathrm{e}^{u})(z_1 - z_2\mathrm{e}^{-u})(z_1 - z_2^{-1}\mathrm{e}^{u})(z_1 - z_2^{-1}\mathrm{e}^{-u})} \tag{2.38}$$

where $u_0 \equiv \pi\tau_o/l$ and C denotes the unit circle integration contour. The z_1 integral can now be calculated by the standard contour integration method, with contributions from the poles at $z_2^{\pm 1}\mathrm{e}^{-u}$. The result is

$$\delta E_0^{(2)} = -2\pi\mathrm{i}g^2\frac{\pi}{l}\int_{u_0}^{\infty} \mathrm{d}u \coth u \int_C \mathrm{d}z_2 \frac{z_2}{(z_2^2 - \mathrm{e}^{2u})(z_2^2 - \mathrm{e}^{-2u})}. \tag{2.39}$$

Also calculating the z_2 integral by contour methods gives

$$\delta E_0^{(2)} = -\pi^2 g^2(\pi/l)\int_{u_0}^{\infty} \frac{\mathrm{d}u}{\sinh^2(u)}. \tag{2.40}$$

Finally, performing this elementary integration gives

$$\delta E_0^{(2)} = -2\pi^2 g^2(\pi/l)\frac{1}{\mathrm{e}^{2u_0} - 1} \approx -\frac{\pi^2 g^2}{\tau_0} + \pi^2 g^2\frac{\pi}{l} + \mathrm{O}(\tau_0/l^2). \tag{2.41}$$

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

$$E_0^{\mathrm{open}}(l) \approx e_0 l + e_1 - \frac{\pi v}{24l}[1 - 24\pi^2 g(l)^2]. \tag{2.42}$$

For exponentially large l we may use equation (1.2) to write

$$E_0^{\mathrm{open}}(l) \approx e_0 l + e_1 - \frac{\pi v}{24l}\left[1 - \frac{9/2}{(\ln l)^2}\right]. \tag{2.43}$$

As usual, the corrections to these formulae are only down by additional powers of $g(l)$, that is $1/\ln l$. The corresponding formula for PBCs is

$$E_0^{\mathrm{per}}(l) \approx e_0 l - \frac{\pi v}{6l}[1 + (2\pi)^3 g(l)^3/\sqrt{3}] \approx e_0 l - \frac{\pi v}{6l}\left[1 + \frac{3/8}{(\ln l)^3}\right]. \tag{2.44}$$

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

3. 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 equations (2.22) and (2.42) from the energies of finite-size spin-$\frac{1}{2}$ antiferromagnetic Heisenberg open chains. The Hamiltonian is

$$H = \sum_{i=1}^{l-1} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} \tag{3.1}$$

where the $\boldsymbol{S}_i$ are spin-$\frac{1}{2}$ operators. The Bethe ansatz equations [13] for the Hamiltonian of equation (3.1) are

$$\left(\frac{\Lambda_k + \mathrm{i}/2}{\Lambda_k - \mathrm{i}/2}\right)^{2l} = \prod_{j\neq k}^{M} \frac{\Lambda_k - \Lambda_j + \mathrm{i}}{\Lambda_k - \Lambda_j - \mathrm{i}}\frac{\Lambda_k + \Lambda_j + \mathrm{i}}{\Lambda_k + \Lambda_j - \mathrm{i}} \tag{3.2}$$

where l is the number of sites in the open chain. The roots can be numerically calculated [16]. The number of roots, M, determines the total S^z component through the relation $S^z = L/2 - M$. In terms of the solutions, Λ_k, to the Bethe ansatz equations (3.2), the energy is given by

$$E = \frac{l-1}{4} - \frac{1}{2}\sum_{k=1}^{M}\frac{1}{\Lambda_k^2 + 1/4}. \tag{3.3}$$

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 (3.2) for the ground state of the open chain are all bigger than zero. Let us order Λ_k so that $\Lambda_1 > \Lambda_2 > \cdots > \Lambda_{l/2-1} > \Lambda_{l/2} > 0$. We can construct another set of rapidities $\{\Lambda'_k, k = 1, l\}$:

$$\Lambda'_j = -\Lambda_j \qquad \Lambda'_{l+1-j} = \Lambda_j \qquad \text{for} \quad j = 1 \text{ to } l/2 \tag{3.4}$$

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

$$\left(\frac{\Lambda'_k + \mathrm{i}/2}{\Lambda'_k - \mathrm{i}/2}\right)^{2l+1} = \prod_{j\neq k}^{l}\frac{\Lambda'_k - \Lambda'_j + \mathrm{i}}{\Lambda'_k - \Lambda'_j - \mathrm{i}}. \tag{3.5}$$

The energy for the periodic chain is given by

$$E' = \frac{2l+1}{4} - \frac{1}{2}\sum_{k=1}^{l}\frac{1}{\Lambda'^2_k + \frac{1}{4}}. \tag{3.6}$$

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 $\{I'_k, k = 1, l\}$:

$$\begin{aligned} &I'_j = j - (l/2+1) \qquad I'_{l+1-j} = j \qquad \text{for} \quad j = 1 \text{ to } l/2 \\ &\text{i.e.} \quad -l/2, -l/2+1, \ldots -2, -1 \qquad 1, 2, \ldots l/2-1, l/2. \end{aligned} \tag{3.7}$$

The ground state of the open chain corresponds to an excited state of the periodic chain with a hole exactly at $I_i = 0$ in the connected integer set $\{I_i, i = 1, l+1\}$ for the ground state of the periodic chain [17]. While the ground states of the periodic chain of odd length have spin $S^z = \pm\frac{1}{2}$ and momentum $\pm\pi/2$, the state of the odd-length periodic chain corresponding to the ground state of the even-length open chain has $S^z = -\frac{1}{2}$ and momentum zero. From its momentum, and from the fact that it has one hole we expect its energy, in the large l limit, to be the ground state energy of the periodic chain plus the excitation energy for a magnon of momentum $\pi/2$: $E' = e_0(2l+1) + v_s \sin(k)$, $v_s = \pi/2$, and $e_0 = \frac{1}{4} - \ln 2$ for the spin-$\frac{1}{2}$ chain. Comparing the expressions for E and E', we can eliminate the summation over Λ and obtain $E = e_0 l + e_1$ 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 six decimal places. This result was derived earlier from the Bethe ansatz equations by a somewhat different method [12, 14, 15].

To test the CFT predictions, we extract three estimates of $g(l)$ using equation (2.22) for the $S = 1$ and $S = 2$ excited states and equation (2.42) for the ground state for chains with up to 2000 sites with OBCs by solving equation (3.2) numerically. We show the three $g(l)$ completely determined by the energies of these three states, respectively, in figure 1. The reason that these three estimates of $g(l)$ do not 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 $g(l) \to 0$. We see that the coupling constants indeed collapse into one value which approaches zero as the chain length increases, thus verifying the CFT predictions. Previous numerical studies for PBCs have verified finite-size scaling obtained by CFT [2, 10, 16]. We

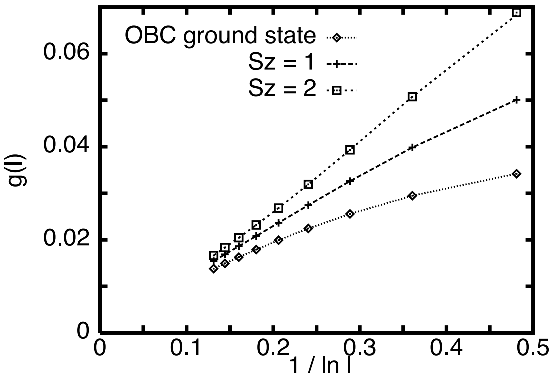

Figure 1. $g(l)$ calculated by equations (2.22) and (2.42) from Bethe ansatz energies of spin-$\frac{1}{2}$ antiferromagnetic Heisenberg open chain (OBC). The three $g(l)$ are obtained from energies of ground state, total spin $S = 1$ excited state and $S = 2$ excited state, respectively.

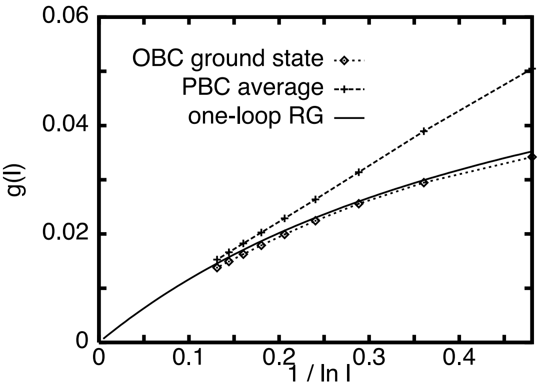

Figure 2. The $g(l)$ calculated from ground state of open chain (OBC) and the average $g(l)$ for periodic [16] chain (PBC), for spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model. The full curve is the one-loop RG prediction [2], $g(l) = g_0(l_0)/[1 + \pi b g_0(l_0)\ln(l/l_0)]$ with $b = 4/\sqrt{3}$. $g_0(l_0)$ is determined by the average of open chain ground state $g(l)$ and the periodic chain average $g(l)$ at the chain length $l_0 = 2048$.

then compare the $g(l)$ obtained from the OBCs with the one from PBCs in figure 2. We show the ground state $g(l)$ for OBCs and the average $g(l)$ given by the ground state, the singlet excitation, and the triplet excitation for PBCs. These data for PBCs were obtained in [16]. The two $g(l)$ approach each other in the large-length limit. The one-loop RG prediction for $g(l)$ given in [2], $g(l) = g_0(l_0)/[1 + \pi b g_0(l_0)\ln(l/l_0)]$, with $b = 4/\sqrt{3}$ is also drawn in figure 2. We use the average of the $g(l)$ for periodic and open chains at $l_0 = 2048$ to fix g_0. The one-loop RG prediction fits $g(l)$ at large l. So we see that the logarithmic corrections for Heisenberg chains have been successfully predicted by CFT.

4. Correlation functions and $1/T_1$

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

$$[\partial/\partial \ln\tau + \beta(g)\partial/\partial g + 2\gamma(g)]G(\tau, g) = 0 \tag{4.1}$$

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

$$\langle\phi(\tau, 0)\phi(0, 0)\rangle \to \frac{(\ln|\tau|)^{-4b_n/b}}{\tau^{2x_n}}. \tag{4.2}$$

Both the exponent, x_n, 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

$$\langle\vec{S}_0(\tau)\cdot\vec{S}_0(0)\rangle \to \text{constant}\frac{(\ln|\tau|)^2}{|\tau|^2}. \tag{4.3}$$

The imaginary part of the retarded Green function at zero frequency and finite T, obtained from the Fourier transform of equation (4.3), gives the NMR 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 the order of the exchange energy. The $1/\tau^2$ power law was first derived in [8], without consideration of logarithmic corrections. 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 of the pure system, in which $1/T_1 \propto [\ln(T/T_0)]^{1/2}$, constant up to a log correction [5].

Of course, an actual experiment on a doped $S = \frac{1}{2}$ 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 [8]

$$\langle\vec{S}_j(t)\cdot\vec{S}_j(0)\rangle \propto \frac{2x/v}{|t|\sqrt{t^2 - 4x^2/v^2}} \tag{4.5}$$

where v is the spin-wave velocity. At sufficiently long times this decays as $1/t^2$ for all x. However, for $t \ll x/v$ 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_2CuO_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 in which many of the results obtained here were derived independently.

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