

# Local magnetization in the boundary Ising chain at finite temperature

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**Abstract.** We study the local magnetization in the 2D Ising model at its critical temperature on a semi-infinite cylinder geometry, and with a nonzero magnetic field  $h$  applied at the circular boundary of circumference  $\beta$ . This model is equivalent to the semi-infinite quantum critical 1D transverse field Ising model at temperature  $T \propto \beta^{-1}$ , with a symmetry-breaking field proportional to  $h$  applied at the point boundary. Using conformal field theory methods we obtain the full scaling function for the local magnetization analytically in the continuum limit, thereby refining the previous results of Leclair, Lesage and Saleur. The validity of our result as the continuum limit of the 1D lattice model is confirmed numerically, exploiting a modified Jordan–Wigner representation. Applications of the result are discussed.

**Keywords:** conformal field theory, spin chains, ladders and planes (theory), renormalization group, surface effects (theory)

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**Contents**

<b>1. Introduction</b>	<b>2</b>
<b>2. Refinement of earlier results</b>	<b>3</b>
<b>3. Determination of the scaling function <math>f(2\beta h^2)</math></b>	<b>5</b>
3.1. Perturbation theory in the boundary field $h$ . . . . .	6
<b>4. Demonstration with numerical solution</b>	<b>8</b>
4.1. Modified Jordan–Wigner transformation and construction of the magnetization determinant . . . . .	9
<b>5. Conclusions</b>	<b>13</b>
<b>Acknowledgments</b>	<b>13</b>
<b>References</b>	<b>13</b>

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**1. Introduction**

The Ising model is a classic paradigm of statistical mechanics, and continues to find powerful application in diverse areas of modern physics [1]–[3]. It also reveals unique and generic universal behavior associated with boundaries [4]–[6]. In its quantum 1D chain version, the critical boundary Ising model (BIM) reads

$$H = - \sum_{i=0}^{\infty} [\sigma_i^z \sigma_{i+1}^z + \sigma_i^x] - h_B \sigma_0^z. \quad (1)$$

The uniform field along  $x$  is fixed such that the bulk system is at the critical point between Ising order and the disordered phase. The symmetry  $\sigma^z \leftrightarrow -\sigma^z$  is broken when a finite magnetic field  $h_B \neq 0$  is applied at the point boundary. Such a boundary field cannot lead to a finite *bulk* magnetization. Importantly however, it does cause a renormalization group flow from a free boundary condition  $h_B = 0$  to a fixed boundary condition  $h_B \rightarrow \pm\infty$ .

The renormalization group flow associated with this BIM has been shown to be at the heart of boundary critical phenomena occurring in a surprising variety of low-dimensional correlated electron systems, such as Luttinger liquids containing an impurity [7], coupled bulk and edge states in non-Abelian fractional quantum Hall states [8, 9], and quantum dots near the two-impurity Kondo [10, 11] or the two-channel Kondo [12, 13] critical points.

In the continuum, the BIM is in fact integrable [14], both in the massless bulk critical case, and also in the massive regime away from the critical point. Certain correlation functions can then be calculated exactly using form factor methods [15]–[17], although in the bulk critical case relevant to equation (1) many important quantities cannot be easily obtained due to the proliferation of many-particle excitations. On the other hand, Chatterjee and Zamolodchikov [18] (CZ) showed that conformal field theory imposes linear differential equations which fully determine correlation functions in this limit. Of course, conformal field theory has been used previously for systems with conformal invariant boundary conditions [5, 6]. The remarkable feature of the result of CZ is that the

correlation functions are still determined by differential equations even for nonconformal invariant boundary conditions obtained at finite boundary field.

The method of CZ was applied to the calculation of the local magnetization as a function of distance from the boundary,  $x$ . On the semi-infinite plane, equivalent to the quantum 1D model, equation (1), at zero temperature, their result reads [18]

$$\langle \sigma(x) \rangle_h = 2^{13/8} \sqrt{\pi} h x^{3/8} \Psi(1/2, 1; 8\pi h^2 x), \quad (2)$$

where  $\Psi$  is a degenerate hypergeometric function. Here  $\langle \sigma(x) \rangle$  has the standard field theory normalization, which we emphasize is only *proportional* to  $\langle \sigma_j^z \rangle$  of a particular lattice model, such as equation (1). Indeed,  $x \propto j$ , and  $h \propto h_B$  provided that  $h_B \ll 1$ . At short distance one thus obtains

$$\langle \sigma(x) \rangle = -2^{13/8} h x^{3/8} [\ln(x) + \mathcal{O}(1)] + \mathcal{O}(x^{7/8}) \quad \text{for } x \ll h^{-2}, \quad (3)$$

and at long distances  $\langle \sigma(x) \rangle \rightarrow (2/x)^{1/8}$ , corresponding exactly to the result for fixed boundary condition, obtained from boundary conformal field theory [19]. As such, the exact function, equation (2), captures the full crossover behavior between two fixed points where conformal invariant boundary conditions do hold.

Since the problem for finite  $h$  does not in general possess conformal invariance at the boundary, it is not possible to generalize equation (2) to other geometries by means of a simple conformal mapping. However the method of CZ can be applied directly to other geometries, yielding a new set of differential equations (this was demonstrated explicitly for the 2D disk geometry by CZ [18]). Similarly, Leclair, Lesage and Saleur [7] (LLS) applied the method to the geometry of a semi-infinite cylinder. In the present paper we shall be concerned with this semi-infinite cylinder geometry, whose boundary consists of a circle with circumference  $\beta$ , at which the boundary field  $h$  is applied. This classical 2D Ising model is equivalent to the *quantum* chain model equation (1) at *finite* temperature  $T \propto \beta^{-1}$  (see e.g. [20]).

We re-examine the result of LLS for the local magnetization in section 2. Whereas these nonperturbative results give the full  $x$  dependence of the local magnetization for any  $h$  and  $\beta$ , we find that a more general ansatz for the local magnetization allows for an additional multiplicative factor  $f(2\beta h^2)$ . The physical meaning of this missing factor is then explained. The full scaling function for the local magnetization is determined in section 3; while the lattice model equation (1) is studied directly in section 4. The local magnetization on the lattice is calculated numerically, and the results compared with the refined analytic solution, showing excellent agreement. The paper ends with a short summary, where implications and applications of the results are discussed.

## 2. Refinement of earlier results

LLS considered a classical Ising model on the half-cylinder in the continuum limit [7]. They calculated the local magnetization as a function of the distance  $x$  from the circular boundary of circumference  $\beta$ , which was conveniently written in the form [7]

$$\langle \sigma(x) \rangle = \left( \frac{1}{\sinh(2\pi x/\beta)} \right)^{1/8} g(X), \quad (4)$$

with  $X = (1 - \coth(2\pi x/\beta))/2$  and where  $\langle \sigma(x) \rangle$  is independent of  $\tau \in (0, \beta)$  due to translation symmetry along the boundary. LLS derived a linear differential equation for  $g(X)$ , which reads [7]

$$\left( (X - X^2) \frac{d^2}{(dX)^2} + \left( 1 + \frac{\Lambda}{2} - 2X \right) \frac{d}{dX} - \frac{1}{4} \right) g(X) = 0, \quad (5)$$

parametrized in terms of  $\Lambda = 2\beta h^2$ . Their solution is [7]

$$\langle \sigma(x) \rangle_{\text{LLS}} = \left( \frac{4\pi/\beta}{\sinh(2\pi x/\beta)} \right)^{1/8} {}_2F_1 \left( \frac{1}{2}, \frac{1}{2}; 1 + 2\beta h^2, \frac{1 - \coth(2\pi x/\beta)}{2} \right), \quad (6)$$

where  ${}_2F_1(a, b, c, z)$  is the Gauss hypergeometric function. Below we will use its integral representation

$${}_2F_1(a, b, c, z) = \frac{\Gamma[c]}{\Gamma[b]\Gamma[c-b]} \int_0^1 dt \frac{t^{b-1}(1-t)^{c-b-1}}{(1-tz)^a}, \quad (7)$$

where  $\Gamma(y)$  is the gamma function. This result is normalized with an overall constant such that at long distances  $\langle \sigma(x) \rangle \rightarrow ((4\pi/\beta)\sinh(2\pi x/\beta))^{1/8}$  recovers the expected result for fixed boundary conditions (taking  $\beta \rightarrow \infty$  then yields  $\langle \sigma(x) \rangle \rightarrow (2/x)^{1/8}$ , consistent with [19]).

In this paper we point out that the differential equation (5) leaves a freedom which goes beyond an overall normalization constant. Unlike the zero-temperature case (corresponding to the semi-infinite plane,  $\beta \rightarrow \infty$ ), here the normalization of equation (6) can itself be a scaling function of  $\Lambda$ . We thus replace equation (6) by the more general ansatz,

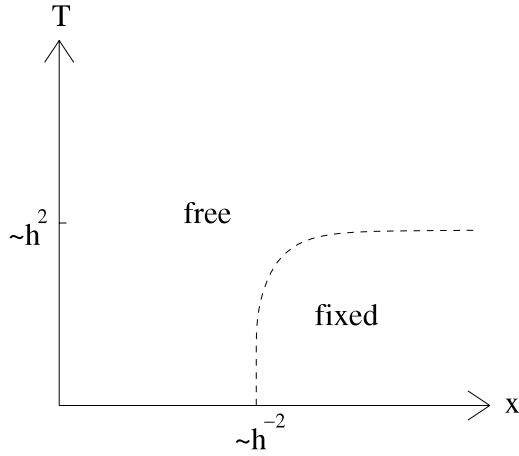
$$\langle \sigma(x) \rangle_{h,\beta} = f(2\beta h^2) \times \left( \frac{4\pi/\beta}{\sinh(2\pi x/\beta)} \right)^{1/8} {}_2F_1 \left( \frac{1}{2}, \frac{1}{2}; 1 + 2\beta h^2, \frac{1 - \coth(2\pi x/\beta)}{2} \right), \quad (8)$$

which depends explicitly on the function  $f(2\beta h^2)$ , determined in section 3, below. Equation (8) implies  $f(\infty) = 1$ , so that  $\langle \sigma(x) \rangle_{h,\beta}$  recovers asymptotically the behavior of the fixed boundary condition fixed point.

We note that the same subtlety occurs with other geometries, as highlighted by CZ in the case of the disk [18]. In that case, the additional scale in the problem is the disk radius  $R$ ; and an additional scaling function of  $Rh^2$  (analogous to our  $\Lambda = 2\beta h^2$ ) appears in the expression for the local magnetization. As in the present case, this function is not fixed by the linear differential equations [18].

Finally, we comment briefly upon the physical significance of the scaling function  $f(2\beta h^2)$ . It describes the dependence on the additional thermal scale influencing the renormalization group flow at  $T \neq 0$ . In accord with physical expectation, the renormalization group flow is cut off at the external scale given by  $\max\{T, x^{-1}\}$ . Since  $h$  grows under renormalization (and has scaling dimension 1/2) [5, 6], we should consider two regimes depending on the ratio between this external scale and the field-induced scale  $\sim h^2$ :

$$\begin{aligned} \max\{T, x^{-1}\} \gg h^2: & \quad \text{free boundary condition,} \\ \max\{T, x^{-1}\} \ll h^2: & \quad \text{fixed boundary condition.} \end{aligned} \quad (9)$$



**Figure 1.** Schematic phase diagram of the BIM as a function of temperature and distance from the boundary. The dashed line denotes the crossover between free and fixed boundary conditions occurring when  $\max\{T, x^{-1}\} \sim h^2$ .

These regimes are illustrated in figure 1. The important consequence following from this is that, at finite temperatures, the fixed boundary condition fixed point is not always reached on taking  $x \rightarrow \infty$ . The single scaling function  $f(2\beta h^2)$  thus describes the crossover from free to fixed boundary condition at a given  $x$ , upon decreasing temperature. Obviously its effect is most apparent at large  $x$ , since there is no crossover at small  $x$ . However, as suggested by figure 1, the system is always close to the free boundary condition fixed point at small  $x$ , and this fact will prove useful in determining  $f(2\beta h^2)$ , as considered in section 3.

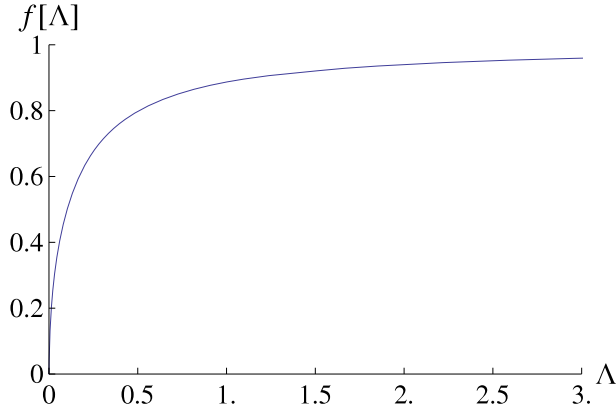
### 3. Determination of the scaling function $f(2\beta h^2)$

In this section we find the function  $f(2\beta h^2)$  appearing in equation (8). Since this function is a scaling function of  $\beta h^2$  and does not depend on distance  $x$ , it could in principle be determined at any given  $x$ . While its influence is most pronounced at large  $x$ , where the system undergoes a crossover as a function of  $T$  (see figure 1), here we determine  $f(2\beta h^2)$  by exploring the small  $x$  behavior, where the system remains close to the free boundary condition fixed point. Importantly, the resulting behavior at small  $x$  is *perturbative* in  $h$  regardless of  $\beta h^2$ , as shown explicitly below.

First we note that at both large and small  $\Lambda$ , the short distance behavior of  $\langle \sigma(x) \rangle$  is linear in  $h$ . As  $\Lambda \rightarrow \infty$ , one sees this directly from the small  $x$  expansion of the exact  $T = 0$  result of CZ, equation (3). In the opposite limit  $\Lambda \rightarrow 0$ , the behavior is by definition perturbative in  $h$ , and so the leading correction to magnetization is of course also linear in  $h$ . In section 3.1, we perform first-order perturbation theory in the boundary field  $h$ , with respect to the free boundary condition fixed point. The key point is that its short distance behavior yields *precisely* equation (3), implying that

$$\langle \sigma(x) \rangle_{h,\beta} = -2^{13/8} h x^{3/8} [\ln(x) + \mathcal{O}(1)] + \mathcal{O}(x^{7/8}) \quad \text{for } x \ll \beta, h^{-2} \quad (10)$$

holds at short distances  $x \ll \beta, h^{-2}$  for *any*  $\Lambda$ . Naively, one might think that the coefficient of the  $x^{3/8} [\ln(x) + \mathcal{O}(1)]$  term could be renormalized by higher orders in  $h$ . But the scaling



**Figure 2.** Plot of equation (12).

form of the problem implies that every power of  $h$  is accompanied by a power of  $\sqrt{\beta}$  (or  $\sqrt{x}$ , which gives a subleading  $x$  dependence to equation (10)). Such terms diverge as  $T \rightarrow 0$ , and so this renormalization is not consistent with the exact nonperturbative  $T = 0$  result, equation (2), which is well behaved at short distances, equation (3).

Finally, we consider the short distance expansion of our ansatz equation (8), which using equation (7) is found to be

$$\langle \sigma(x) \rangle_{h,\beta} = -f(2\beta h^2) \frac{2^{9/8}}{\sqrt{\beta}} \frac{\Gamma[1 + 2\beta h^2]}{\Gamma[1/2 + 2\beta h^2]} x^{3/8} [\ln(x) + \mathcal{O}(1)] + \mathcal{O}(x^{7/8}) \quad \text{for } x \ll \beta, h^{-2}. \quad (11)$$

Comparing equations (10) and (11) we now obtain the scaling function

$$f(\Lambda) = \sqrt{\Lambda} \frac{\Gamma[1/2 + \Lambda]}{\Gamma[1 + \Lambda]}. \quad (12)$$

This function increases monotonically as shown in figure 2, and has asymptotic limits  $f(\Lambda \ll 1) \approx \sqrt{\pi\Lambda}$  and  $f(\Lambda \gg 1) \approx 1 - 1/8\Lambda$ .

We note that a similar perturbative method was used by CZ to fix the scaling function of  $Rh^2$  for the disk geometry [18].

### 3.1. Perturbation theory in the boundary field $h$

In this subsection we show that the form of equation (10) indeed follows from perturbation theory around the free boundary condition fixed point. We obtain the full  $x/\beta$  dependence of the magnetization at small  $h$ , recovering perturbatively the  $\Lambda \rightarrow 0$  limit of equation (8).

The continuum limit of the critical classical 2D Ising model is described by a  $c = 1/2$  conformal field theory, which admits a Lagrangian formulation in terms of the free massless Majorana Fermi field  $(\psi, \bar{\psi})$ , with the action

$$S_0 = \frac{1}{2\pi} \int d^2z [\psi \partial_{\bar{z}} \psi + \bar{\psi} \partial_z \bar{\psi}]. \quad (13)$$

Here  $(z, \bar{z}) = (\tau + ix, \tau - ix)$  are complex coordinates and  $d^2z = d\tau dx$ . In the presence of a boundary  $\mathcal{B}$  with a magnetic field  $h$ , the action can be decomposed into a bulk part

and a boundary part,

$$S = \frac{1}{2\pi} \int_{\mathcal{D}} d^2z [\psi \partial_z \psi + \bar{\psi} \partial_z \bar{\psi}] + h \int_{\mathcal{B}} \sigma_B. \quad (14)$$

The boundary operator  $\sigma_B$  was identified in [5, 6] with a dimension 1/2 operator  $\sigma_B(\tau) \sim \psi(\tau, x = 0)$ , associated with the fermion field at the boundary. In our case  $\mathcal{B} = \partial\mathcal{D}$  is a circle parametrized by  $\tau \in [0, \beta]$  and  $\mathcal{D}$  is the semi-infinite cylinder. Following Cardy's method of images [5] the one point function of the magnetization is  $\sigma(z_1, z_2) = \langle \sigma_L(z_1) \sigma_L(z_2) \rangle$ , where  $\sigma_L(z)$  is a dimension 1/16 left moving field living in the geometry of the *infinite* cylinder. We then obtain conformal invariant boundary conditions, with the 'boundary' at  $x = 0$ . The boundary field  $h$  is now considered as a perturbation to the free boundary condition fixed point. To first order in  $h$ ,

$$\sigma^{(1)}(z_1, z_2) = h \int_0^\beta d\tau \langle \sigma(z_1) \sigma_B(0, \tau) \sigma(z_2) \rangle. \quad (15)$$

The three-point function appearing in the integrand is fully determined by conformal invariance, and one obtains up to a normalization constant  $N$

$$\begin{aligned} \sigma^{(1)}(z_1, z_2) &= hN \left( \frac{\sin(\pi/\beta)(z_1 - z_2)}{\pi/\beta} \right)^{3/8} \\ &\times \int_0^\beta d\tau \frac{(\pi/\beta)}{[\sin((\pi/\beta)(\tau - z_1)) \sin((\pi/\beta)(\tau - z_2))]^{1/2}}. \end{aligned} \quad (16)$$

The physical magnetization is obtained by setting  $\langle \sigma(x) \rangle = \langle \sigma(z_1 = ix, z_2 = -ix) \rangle$ . We now take  $z_1 = ix, z_2 = -ix$  in equation (16) and use the trigonometric identity,

$$2 \sin\left(\frac{\pi}{\beta}(\tau - z_1)\right) \sin\left(\frac{\pi}{\beta}(\tau - z_2)\right) = \cos\left(\frac{2i\pi x}{\beta}\right) - \cos\left(\frac{2\pi\tau}{\beta}\right). \quad (17)$$

The integral in equation (16) then becomes

$$\int_0^{2\pi} \frac{d\theta}{\sqrt{(w^{1/2} + w^{-1/2})/2 - \cos\theta}} = \frac{2\pi}{\sqrt{\sinh(2\pi x/\beta)}} {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1, \frac{1 - \coth(2\pi x/\beta)}{2}\right), \quad (18)$$

in terms of  $w = e^{-4\pi x/\beta}$  and  $\theta = 2\pi\tau/\beta$ . The constant  $N$  was carefully accounted for by CZ [18]. Using this and equation (18), first-order perturbation theory in the boundary field  $h$  yields

$$\langle \sigma(x) \rangle_\beta^{(1)} = h\sqrt{2\pi\beta} ((4\pi/\beta)\sinh(2\pi x/\beta))^{1/8} {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1, \frac{1 - \coth(2\pi x/\beta)}{2}\right) + \mathcal{O}(h^2). \quad (19)$$

It is interesting to compare this with the full result of LLS, equation (6). At small  $h$ , both carry the same  $x/\beta$  dependence; however, LLS miss the overall *linear* dependence on  $h$ , accounted for by the function  $f(2\beta h^2)$  in equation (8).

The short distance behavior of equation (19) is precisely equation (10).



#### 4. Demonstration with numerical solution

In this section we demonstrate the validity of equation (8) as the continuum limit of the lattice magnetization

$$\langle \sigma(j, h_B, T) \rangle \equiv \frac{\text{Tr}(e^{-H/T} \sigma_j^z)}{\text{Tr}(e^{-H/T})}, \quad (20)$$

where  $H$  is the Hamiltonian of the lattice model, equation (1). The quantum boundary Ising chain can be solved by applying a Jordan–Wigner transformation, which yields a quadratic fermionic Hamiltonian. The magnetization is nonlocal in terms of these fermions: calculation of  $\langle \sigma(j, h_B, T) \rangle$  is then equivalent to evaluation of the determinant of a matrix whose elements are fermionic correlation functions [21]. We construct these analytically, but ultimately evaluate them numerically. Details of this calculation follow in section 4.1. Here we pre-empt that discussion and present our numerical results, comparing to the refined exact expression, equation (8).

The continuum limit expression equation (8) admits the scaling form

$$\langle \sigma(x, h, T) \rangle = T^{1/8} \mathcal{F}[x/\beta, 2\beta h^2]. \quad (21)$$

For this function to be a continuum limit of the lattice magnetization, there should exist nonuniversal constants  $c, c_x, c_h$  such that

$$\langle \sigma(j, h_B, T) \rangle = c T^{1/8} \mathcal{F}[c_x j/\beta, 2c_h \beta h_B^2] \quad (22)$$

is satisfied for all  $j, h_B$  and  $T$ , as long as distances are large compared to the lattice constant,  $j \gg 1$ , and the energy scales  $h_B$  and  $T$  are small compared to the lattice cutoff scale,  $h_B, T \ll 1$ .

The constant  $c_x$  is related to the velocity  $v$  of bulk excitations via  $c_x = v^{-1}$ . This follows from the requirement that the exponential decay at long distances  $j \gg \beta$  is given by [22]  $\langle \sigma(x=j) \rangle = \langle \sigma(z_1=ix)\sigma(z_2=-ix) \rangle \rightarrow e^{-(2\nu)\pi(2j)/(v\beta)}$ , with  $\nu = 1/16$  being the scaling dimension of the chiral  $\sigma$  field. In our model we obtain  $c_x = 1/2$  exactly.  $c$  is an overall factor relating the lattice magnetization to the field theory one, and  $c_h$  relates the (squared) boundary field,  $h_B$ , in the lattice model to  $h$  appearing in the continuum action, equation (14). We determine  $c$  and  $c_h$  by demanding that the ratio

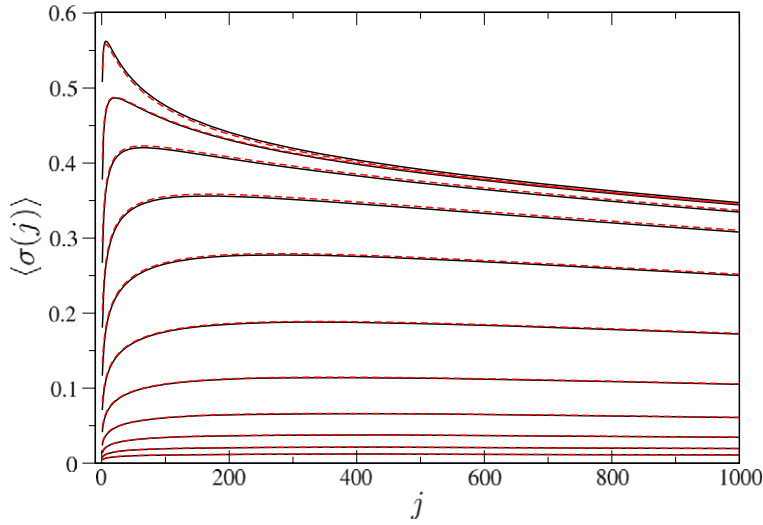
$$\frac{\langle \sigma(j, h_B, T) \rangle}{c T^{1/8} \mathcal{F}[c_x j/\beta, 2c_h \beta h_B^2]} \quad (23)$$

is equal to unity for all  $h_B$ . The best fit from our numerical data was obtained for  $c_h \simeq 0.161$  and  $c \simeq 0.729$ .

As shown in figure 3, we obtain essentially perfect agreement between numerical calculations and field theoretical predictions for the magnetization as a full function of distance, over a wide range of  $2h^2/T = 2c_h h_B^2/T$ .

Figure 3 should be seen as confirmation that the  $x$  dependence of the magnetization is described by the LLS result, equation (6). However, the full dependence on  $h, x$  and  $T$ —capturing the evolution from the  $T \ll h^2$  result of CZ, equation (2), to the perturbative  $T \gg h^2$  result, equation (19)—is only recovered on inclusion of the factor  $f(2\beta h^2)$  appearing in equation (8).





**Figure 3.** Comparison of analytical results using equation (8) (full lines) and numerical results (dashed lines) for fixed temperature  $T = 0.5 \times 10^{-3}$  and varying boundary field  $h_B = 10^{-3+n/4}/\sqrt{2}$ ,  $n = 0, 1, \dots, 10$  increasing from bottom to top (explicitly  $h_B = 0.000\,707, 0.001\,25, 0.002\,23, 0.003\,97, 0.007\,07, 0.0125, 0.0223, 0.0397, 0.0707, 0.125, 0.223$ ).

#### 4.1. Modified Jordan–Wigner transformation and construction of the magnetization determinant

We now describe the calculation of the magnetization using a fermionic representation of the transverse field quantum Ising chain, equation (1). We start from a finite lattice with  $L$  sites,

$$H_L = - \sum_{i=0}^{L-2} \sigma_i^z \sigma_{i+1}^z - \sum_{i=0}^{L-1} \sigma_i^x - h_B \sigma_0^z, \quad (24)$$

with boundary field  $h_B$  at site  $j = 0$ , and with free boundary conditions at site  $j = L - 1$ . Ultimately, we will take the  $L \rightarrow \infty$  limit to avoid finite size effects.

Consider first the usual Jordan–Wigner representation of the Pauli matrices  $\tau_j$  ( $j = 0, \dots, L - 1$ ),

$$\tau_j^x = i\gamma_{B,j}\gamma_{A,j}, \quad \tau_j^z = - \left( \prod_{\ell=0}^{j-1} i\gamma_{A,\ell}\gamma_{B,\ell} \right) \gamma_{B,j}, \quad (25)$$

in terms of self-Hermitian (Majorana) lattice fermions  $\gamma_{A(B),j}$ , satisfying  $\{\gamma_{A,j}, \gamma_{A,j'}\} = 2\delta_{jj'}$ ,  $\{\gamma_{B,j}, \gamma_{B,j'}\} = 2\delta_{jj'}$ ,  $\{\gamma_{A,j}, \gamma_{B,j'}\} = 0$ . Here,  $\tau_j^y$  can be obtained from  $i\tau_j^y = \tau_j^z \tau_j^x$ . Employing this representation for equation (24), one obtains a linear term involving a single fermionic operator representing the boundary spin operator,  $\tau_0^z = -\gamma_{B,0}$ . This proves to be inconvenient in the following, and so we use a modified fermionic representation of the spins to eliminate this linear term from the Hamiltonian. Specifically, we introduce an extra boundary Majorana fermion  $\gamma$  (with  $\gamma^2 = 1$ ), which anticommutes with all other fermions  $\gamma_{A,j}$  and  $\gamma_{B,j}$ . It can be checked that, if  $[\tau_j^a, \tau_{j'}^b] = 2i\epsilon^{abc}\delta_{jj'}\tau_j^c$ , then

$\{\sigma_j^x, \sigma_j^y, \sigma_j^z\} \equiv \{\sigma_j^x, i\gamma\sigma_j^y, i\gamma\sigma_j^z\}$  also satisfy  $[\sigma_j^a, \sigma_{j'}^b] = 2i\epsilon^{abc}\delta_{jj'}\sigma_j^c$ . Thus we work with the modified Jordan–Wigner representation

$$\sigma_j^x = i\gamma_{B,j}\gamma_{A,j}, \quad \sigma_j^z = -i\gamma \left( \prod_{\ell=0}^{j-1} i\gamma_{A,\ell}\gamma_{B,\ell} \right) \gamma_{B,j}. \quad (26)$$

This is formally equivalent to embedding the spins in a larger Hilbert space. The model equation (24) now becomes a tight binding model of Majorana fermions, containing only *quadratic* terms:

$$H_L = \sum_{j=0}^{L-2} i\gamma_{A,j}\gamma_{B,j+1} + \sum_{j=0}^{L-1} i\gamma_{A,j}\gamma_{B,j} + h_B i\gamma_{B,0}. \quad (27)$$

The model can be straightforwardly diagonalized by introducing the fermionic modes

$$A_n = \frac{1}{2} \sum_{j=0}^{L-1} \left( g_n(j + \frac{1}{2})\gamma_{A,j} + i g_n(j)\gamma_{B,j} \right), \quad (n = 1, 2, \dots, L) \quad (28)$$

with

$$g_n(j) = \sqrt{\frac{2}{L+1/2}} \sin \left( \frac{\pi n}{L+1/2} \left( j + \frac{1}{2} \right) \right) \quad (29)$$

satisfying the completeness relation  $\sum_{n=1}^L g_n(j)g_n(j') = \sum_{n=1}^L g_n(j + \frac{1}{2})g_n(j' + \frac{1}{2}) = \delta_{jj'}$ . This gives  $\{A_n, A_{n'}\} = \delta_{n,n'}$ , and

$$\gamma_{A,j} = \sum_{n=1}^L g_n(j + \frac{1}{2})(A_n + A_n^\dagger), \quad i\gamma_{B,j} = \sum_{n=1}^L g_n(j)(A_n - A_n^\dagger). \quad (30)$$

The Hamiltonian thus becomes

$$H_L = \sum_{n=1}^L E_n A_n^\dagger A_n + h_B \sum_{n=1}^L g_n(0)\gamma(A_n - A_n^\dagger), \quad (31)$$

with  $E_n = 4 \cos(\pi n/(2L+1))$ , which consists of a band of fermionic levels coupled to a Majorana impurity.

Using equation (26), the magnetization is given by

$$\langle \sigma_j^z \rangle = -i^{j+1} \langle \gamma_{B,0}\gamma_{A,0}\gamma_{B,1}\gamma_{A,1} \cdots \gamma_{B,j-1}\gamma_{A,j-1}\gamma_{B,j} \rangle. \quad (32)$$

One proceeds using Wick's theorem [21], applicable for the quadratic Hamiltonian equation (31). Due to the bipartite structure in equation (27) it follows that  $\langle \gamma_{A,j}\gamma_{A,j'} \rangle = \langle \gamma_{A,j'} \rangle = \langle \gamma_{B,j}\gamma_{B,j'} \rangle = 0$ . All nonzero contractions, including relative signs, are then captured by the determinant

$$\langle \sigma_j^z \rangle = - \left| \begin{pmatrix} i\langle \gamma_{B,0} \rangle & i\langle \gamma_{B,1} \rangle & \cdots & i\langle \gamma_{B,j} \rangle \\ i\langle \gamma_{A,0}\gamma_{B,0} \rangle & i\langle \gamma_{A,0}\gamma_{B,1} \rangle & \cdots & i\langle \gamma_{A,0}\gamma_{B,j} \rangle \\ \vdots & \vdots & \ddots & \vdots \\ i\langle \gamma_{A,j-1}\gamma_{B,0} \rangle & i\langle \gamma_{A,j-1}\gamma_{B,1} \rangle & \cdots & i\langle \gamma_{A,j-1}\gamma_{B,j} \rangle \end{pmatrix} \right|. \quad (33)$$

The calculation of the fermionic correlators in equation (33) can be done by exact Green function resummation, treating the problem as a noninteracting impurity model [23]. In equation (31) we have a quasi-continuum of modes labeled by  $n$  coupled to a localized impurity state  $\gamma$ . The Green functions for  $n$ -modes and for the localized state are defined as

$$\hat{G}_{nn'}(\tau) = - \left\langle \mathcal{T} \begin{pmatrix} A_n(\tau) \\ A_n^\dagger(\tau) \end{pmatrix} \begin{pmatrix} A_{n'}^\dagger & A_{n'} \end{pmatrix} \right\rangle, \quad G_\gamma(\tau) = - \langle \mathcal{T} \gamma(\tau) \gamma \rangle, \quad (34)$$

where  $O(\tau) = e^{H_L \tau} O e^{-H_L \tau}$ , and  $\mathcal{T}$  is Wick's time-ordering operator. We now construct a perturbative expansion of the Green functions in  $h_B$ , with  $G(i\omega_m) = \int_0^\beta d\tau e^{i\omega_m \tau} G(\tau)$  in terms of the Matsubara frequencies  $\omega_m = \pi T(1 + 2m)$ . The zeroth-order Green functions are given by

$$\hat{G}_{nn'}^{(0)}(i\omega_m) = \delta_{nn'} \begin{pmatrix} i\omega_m - E_n & 0 \\ 0 & i\omega_m + E_n \end{pmatrix}^{-1}, \quad G_\gamma^{(0)}(i\omega_m) = \frac{2}{i\omega_m}. \quad (35)$$

The full impurity Green function can then be written as  $G_\gamma(i\omega_m) = [(G_\gamma^{(0)}(i\omega_m))^{-1} - \Sigma(i\omega_m)]^{-1}$ . Writing the boundary term in the Hamiltonian as  $H_L|_{h_B} = h_B \sum_{n=1}^L g_n(0) \gamma \begin{pmatrix} A_n^\dagger & A_n \end{pmatrix} \begin{pmatrix} -1 \\ 1 \end{pmatrix}$ , the exact self-energy follows as

$$\Sigma(i\omega_m) = h_B^2 \sum_{n=1}^L g_n^2(0) \begin{pmatrix} 1 & -1 \end{pmatrix} \hat{G}_{nn}^{(0)}(i\omega_m) \begin{pmatrix} 1 \\ -1 \end{pmatrix} = -h_B^2 \sum_{n=1}^L g_n^2(0) \frac{2i\omega_m}{(\omega_m)^2 + E_n^2}. \quad (36)$$

We can now calculate the fermionic correlators entering the determinant equation (33). With  $G(\tau) = T \sum_{\omega_m} e^{-i\omega_m \tau} G(i\omega_m)$ , the correlators involving the impurity fermion are given by

$$\begin{aligned} i \langle \gamma \gamma_{B,x} \rangle &= i \langle \mathcal{T} \gamma(\tau = 0^+) \gamma_{B,x} \rangle = iT \sum_{\omega_m} e^{-i\omega_m 0^+} \langle \gamma \gamma_{B,x} \rangle_{\omega_m} \\ &= T \sum_{\omega_m} e^{-i\omega_m 0^+} \sum_{n=1}^L g_n(x) \langle \gamma (A_n - A_n^\dagger) \rangle_{\omega_m}, \end{aligned} \quad (37)$$

where we used equation (30) in the last equality. Proceeding with first-order perturbation theory in  $h_B$ , we have

$$\begin{aligned} i \langle \gamma \gamma_{B,x} \rangle &= T \sum_{\omega_m} e^{-i\omega_m 0^+} \sum_{n=1}^L g_n(x) G_\gamma(i\omega_m) h_B g_n(0) \begin{pmatrix} 1 & -1 \end{pmatrix} \hat{G}_{nn}^{(0)}(i\omega_m) \begin{pmatrix} 1 \\ -1 \end{pmatrix} \\ &= -Th_B \sum_{\omega_m} G_\gamma(i\omega_m) e^{-i\omega_m 0^+} \sum_{n=1}^L g_n(x) g_n(0) \frac{2i\omega_m}{(\omega_m)^2 + E_n^2}. \end{aligned} \quad (38)$$

Using the exact expression for  $G_\gamma$ , this becomes

$$i \langle \gamma \gamma_{B,x} \rangle = -Th_B \sum_{\omega_m} e^{-i\omega_m 0^+} \frac{\sum_{n=1}^L (g_n(x) g_n(0) / ((\omega_m)^2 + E_n^2))}{1/4 + h_B^2 \sum_{n=1}^L ((g_n(0))^2 / ((\omega_m)^2 + E_n^2))}. \quad (39)$$

Similarly, the  $\langle \gamma_A \gamma_B \rangle$  correlators are given by

$$i\langle \gamma_{A,x} \gamma_{B,x'} \rangle = -T \sum_{\omega_m} e^{-i\omega_m 0^+} \sum_{n,n'=1}^L g_n(x + \frac{1}{2}) g_{n'}(x') (1 \quad 1) \hat{G}_{nn'}(i\omega_m) \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \quad (40)$$

Using standard impurity Green function methods, the full  $\hat{G}_{nn'}(i\omega_m)$  Green function is seen to contain two terms,

$$\hat{G}_{nn'}(i\omega_m) = \delta_{nn'} \hat{G}_{nn}^{(0)}(i\omega_m) + h_B^2 \hat{G}_{nn}^{(0)}(i\omega_m) \begin{pmatrix} -1 \\ 1 \end{pmatrix} g_n(0) G_\gamma(i\omega_m) g_{n'}(0) (1 \quad -1) \hat{G}_{n'n'}^{(0)}(i\omega_m). \quad (41)$$

Explicitly, the desired correlator can be expressed as

$$\begin{aligned} i\langle \gamma_{A,x} \gamma_{B,x'} \rangle &= \sum_{n=1}^L g_n \left( x + \frac{1}{2} \right) g_n(x') \tanh \left( \frac{E_n}{2T} \right) \\ &+ 2h_B^2 T \sum_{\omega_m} e^{-i\omega_m 0^+} \left[ \left( \sum_{n=1}^L \frac{g_n(x + 1/2) g_n(0) E_n}{(\omega_m)^2 + E_n^2} \right) \left( \sum_{n'=1}^L \frac{g_{n'}(x') g_{n'}(0)}{(\omega_m)^2 + E_{n'}^2} \right) \right] \\ &\times \left[ \frac{1}{4} + h_B^2 \sum_{n''=1}^L \frac{(g_{n''}(0))^2}{(\omega_m)^2 + E_{n''}^2} \right]^{-1}. \end{aligned} \quad (42)$$

All these expressions are exact for the model equation (24) containing two boundaries. We are interested in the effect of the boundary  $j = 0$ , but not on the boundary at  $j = L - 1$ . Thus we proceed by taking the limit  $L \rightarrow \infty$ , which reproduces the desired semi-infinite chain. Replacing discrete summations over  $n$  by integrals,  $(2/(L + 1/2)) \sum_{n=1}^L \rightarrow (4/\pi) \int_0^{\pi/2} d\theta$ , with  $\theta = (\pi n / (2L + 1))$ , equations (39) and (42) become

$$\begin{aligned} i\langle \gamma \gamma_{B,j} \rangle &= -T h_B \sum_{\omega_m} e^{-i\omega_m 0^+} \frac{\sigma_1(\omega_m, j)}{1/4 + h_B^2 \sigma_1(\omega_m, 0)}, \quad (j = 0, 1, 2, \dots) \\ i\langle \gamma_{A,j} \gamma_{B,j'} \rangle &= \sigma(j + j' + 1) - \sigma(j - j') + 2h_B^2 T \\ &\times \sum_{\omega_m} e^{-i\omega_m 0^+} \frac{\sigma_2(\omega_m, j) \sigma_1(\omega_m, j')}{1/4 + h_B^2 \sigma_1(\omega_m, 0)}, \quad (j, j' = 0, 1, 2, \dots) \end{aligned} \quad (43)$$

where

$$\begin{aligned} \sigma_1(\omega, j) &= \frac{4}{\pi} \int_0^{\pi/2} d\theta \frac{\sin(\theta) \sin[(2j + 1)\theta]}{\omega^2 + (4 \cos \theta)^2}, \\ \sigma_2(\omega, j) &= \frac{4}{\pi} \int_0^{\pi/2} d\theta \frac{4 \sin(\theta) \sin[(2j + 2)\theta] \cos(\theta)}{\omega^2 + (4 \cos \theta)^2}, \\ \sigma(j) &= -\frac{2}{\pi} \int_0^{\pi/2} d\theta \cos[(1 + 2j)\theta] \tanh \left( \frac{4 \cos(\theta)}{2T} \right). \end{aligned} \quad (44)$$

The magnetization due to a field  $h_B$  applied at the single boundary of a semi-infinite chain at finite temperatures is thus given exactly by equations (33) and (43). In practice

we evaluate the integrals in equation (44) numerically, yielding the results presented in figure 3. It would be interesting to rederive the field theoretical results by analytic evaluation of the determinant equation (33) in the continuum limit following the methods of [4].

## 5. Conclusions

The crossover physics evinced by the boundary Ising model has been shown to play a key role in a surprisingly diverse range of physical problems [7]–[13]. Analysis of the exact universal crossover from free to fixed boundary conditions in such problems at finite temperatures thus requires the corresponding scaling functions of the boundary Ising model to be known exactly. In this paper we obtained the full scaling function for the magnetization of the boundary Ising chain at finite temperature. Among the potential applications of our results, one example is calculation of finite-temperature conductance crossovers in two-channel or two-impurity Kondo quantum dot systems [24]. The crossover from non-Fermi-liquid to Fermi liquid physics in such systems is characterized by the same renormalization group flow as occurs in the boundary Ising chain [10]. We plan to extend our earlier work [12] at  $T = 0$  in this area to finite temperatures, employing the results of this paper [24]. We note in this regard that without the function  $f(2\beta h^2)$ , the conductance near the non-Fermi-liquid fixed point is unphysical [24]; but using the main result of this paper, equation (8), exact results [10] at both non-Fermi-liquid and Fermi liquid fixed points are recovered precisely.

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## References

- [1] Lenz W, 1920 *Phys. Z.* **21** 613
- [2] McCoy B M and Wu T T, 1967 *Phys. Rev.* **162** 436  
McCoy B M and Wu T T, 1968 *Phys. Rev.* **174** 546
- [3] McCoy B M and Wu T T, 1973 *The Two-Dimensional Ising Model* (Cambridge, MA: Harvard University Press)
- [4] Bariev R Z, 1979 *Teor. Mat. Fiz.* **40** 40  
Bariev R Z, 1980 *Teor. Mat. Fiz.* **42** 262  
Bariev R Z, 1988 *Teor. Mat. Fiz.* **77** 1090
- [5] Cardy J L, 1984 *Nucl. Phys. B* **240** 514
- [6] Cardy J L, 1989 *Nucl. Phys. B* **324** 581
- [7] Lesage F, Leclair A and Saleur H, 1996 *Phys. Rev. B* **54** 13597
- [8] Rosenow B, Halperin B I, Simon S H and Stern A, 2009 *Phys. Rev. B* **80** 155305
- [9] Bishara W and Nayak C, 2009 *Phys. Rev. B* **80** 155304
- [10] Affleck I and Ludwig A W W, 1992 *Phys. Rev. Lett.* **68** 1046  
Affleck I, Ludwig A W W and Jones B A, 1995 *Phys. Rev. B* **52** 9528
- [11] Sela E and Affleck I, 2009 *Phys. Rev. Lett.* **102** 47201  
Sela E and Affleck I, 2009 *Phys. Rev. Lett.* **103** 087204  
Sela E and Affleck I, 2009 *Phys. Rev. B* **79** 125110
- [12] Sela E, Mitchell A K and Fritz L, 2011 *Phys. Rev. Lett.* **106** 147202
- [13] Mitchell A K, Becker M and Bulla R, 2011 *Phys. Rev. B* **84** 115120
- [14] Ghoshal S and Zamolodchikov A, 1994 *Int. J. Mod. Phys. A* **9** 3841  
Ghoshal S and Zamolodchikov A, 1994 *Int. J. Mod. Phys. A* **9** E4353

- [15] Konik R, LeClair A and Mussardo G, 1996 *J. Mod. Phys. A* **11** 2765
- [16] De Martino A, Moriconi M and Mussardo G, 1998 *Nucl. Phys. B* **509** 615
- [17] Schuricht D and Essler F H L, 2007 *J. Stat. Mech.* [P11004](#)
- [18] Chatterjee R and Zamolodchikov A, 1994 *Mod. Phys. Lett. A* **9** 2227
- [19] Cardy J and Lewellen D, 1991 *Phys. Lett. B* **259** 274
- [20] Cardy J, 1996 *Scaling and Renormalization in Statistical Physics* (Cambridge: Cambridge University Press)
- [21] Sachdev S, 1999 *Quantum Phase Transitions* (Cambridge: Cambridge University Press)
- [22] Giamarchi T, 2004 *Quantum Physics in One Dimension* (New York: Oxford University Press)
- [23] Hewson A C, 1993 *The Kondo Problem to Heavy Fermions* (Cambridge: Cambridge University Press)
- [24] Mitchell A K and Sela E, 2012 arXiv:[1203.4456](#)