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LETTER TO THE EDITOR

Finite-size scaling of the quantum Ising chain with periodic, free, and antiperiodic boundary conditions

Theodore W Burkhardt† and Ihnsouk Guim‡
Institut Laue-Langevin, 156X, F-38042 Grenoble Cédex, France

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Abstract. We give exact results for the energy spectrum of a chain of N Ising spins in a transverse field with periodic, free, and antiperiodic boundary conditions. The dependence of the energy gaps on boundary conditions is compatible with predictions of conformal invariance for correlation lengths in two-dimensional strips. The feasibility of calculating surface critical indices using phenomenological renormalisation with free boundary conditions and the convergence for large N are discussed.

Consider the inverse correlation length $\kappa_\omega(N)$ associated with the two-point correlations of an operator $\hat{\omega}$ in a two-dimensional spin system with isotropic interactions defined on a strip with infinite length and a width of N lattice spacings. In a recent letter Cardy (1984a) proved that conformal invariance of the correlation functions at the critical point implies the relations

$$\lim_{N\to\infty} N\kappa_\omega(N) = \begin{cases} 2\pi x_\omega^{(\mathrm{bulk})}, & \text{periodic boundary conditions} \quad (1a) \\ \pi x_\omega^{(\mathrm{surf})}, & \text{free boundary conditions.} \quad (1b) \end{cases}$$

Here $x_\omega^{(\mathrm{bulk})}$ and $x_\omega^{(\mathrm{surf})}$ are the bulk and surface scaling dimensions§ of the operator $\hat{\omega}$. The first of these relations was known previously from exact calculations and numerical studies (Luck 1982, Derrida and de Seze 1982, Nightingale and Blöte 1983, Privman and Fisher 1984, and references therein) on a variety of models. The second relation has recently been verified numerically for Ising strips (Burkhardt and Guim 1985). The two relations are of considerable importance in finite-size scaling (Barber 1983), as they enable one to determine the scaling dimensions $x_\omega^{(\mathrm{bulk})}, x_\omega^{(\mathrm{surf})}$ directly from $\kappa_\omega(N)$ without introducing a perturbing field conjugate to $\hat{\omega}$.

In this letter we discuss the influence of periodic, free, and antiperiodic boundary conditions on the finite-size scaling properties of the two-dimensional Ising model in the extreme anisotropic or quantum-Hamiltonian limit (Suzuki 1971, Scalapino *et al* 1972, Fradkin and Susskind 1978, Kogut 1979, Hamer and Barber 1981). In this limit

† Permanent address: Department of Physics, Temple University, Philadelphia, PA 19122, USA.
‡ Present address: Department of Chemistry, Columbia University, New York, NY 10027, USA.
§ In an infinite bulk system, $\hat{\omega}$ scales as

$$\hat{\omega}(r, t) = b^{-x_\omega^{(\mathrm{bulk})}}\hat{\omega}(b^{-1}r, b, t)^{y_t}, \qquad t = T - T_c,$$

in thermal averages (Kadanoff 1976, Patashinskii and Pokrovskii 1979). At the free surface of a semi-infinite system, $x_\omega^{(\mathrm{surf})}$ replaces $x_\omega^{(\mathrm{bulk})}$ (Binder 1983).

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the transfer matrix T takes the form

$$T = 1 - \tau H + O(\tau^2) \tag{2}$$

where τ is an infinitesimal and H is the Hamiltonian of a one-dimensional chain of quantum spins in a transverse field. From (2), it follows that the inverse correlation length $\kappa_\omega(N)$ is given by

$$\kappa_\omega(N) = \tau \Delta_\omega(N) \tag{3}$$

where Δ_ω is the energy gap between the ground state $|\psi_0\rangle$ and the first excited state $|\psi\rangle$ with non-vanishing matrix element $\langle\psi|\hat{\omega}|\psi_0\rangle$.

Relations (1) are applicable to strips with isotropic interactions. (See Nightingale and Blöte 1983, Burkhardt and Guim 1984 for generalisations to anisotropic couplings.) Equation (3), on the other hand, holds in the extreme anisotropic limit. Penson and Kolb (1984a, b) have presented evidence that the inverse correlation lengths $\kappa_\omega(N)$ at criticality in the limit $N \to \infty$ in the isotropic and extreme anisotropic cases differ by a proportionality constant independent of the particular operator $\hat{\omega}$. Our results (see also Burkhardt and Guim 1985) suggest that the proportionality constant is also independent of the boundary conditions. (This also follows from intuitive arguments (Fradkin and Susskind 1978, Barber *et al* 1984) in which the lattice constants of the anisotropically coupled system are rescaled to restore isotropy of the correlations.) For Ising strips in the extreme anisotropic limit, we find that

$$\lim_{N\to\infty} N\Delta_\omega(N) = c \times \begin{cases} 2\pi x_\omega^{(\text{bulk})}, & \text{periodic boundary conditions} \quad (4a) \\ \pi x_\omega^{(\text{surf})}, & \text{free boundary conditions} \quad (4b) \end{cases}$$

with the same proportionality constant c for spin–spin and energy–energy correlations with both periodic and free boundary conditions.

Hamer and Barber (1981) have calculated the energy gap of the quantum Ising chain (corresponding to spin–spin correlations in the Ising strip) with periodic boundary conditions and discussed the finite-size scaling properties. As mentioned above, we consider periodic, free, and antiperiodic boundary conditions and both spin–spin and energy–energy correlations. Gehlen *et al* (1984) have recently reported results for the energy gaps of the quantum Ising chain and the Z_3 Potts chain with different boundary conditions. Their numerical results for the Z_3 model agree with our own, but we disagree with their statement that the energy gap in the Ising case is independent of boundary conditions to order N^{-1}.

The chain of N Ising spins in a transverse field λ with free boundary conditions has the Hamiltonian

$$H_F = -\lambda \sum_{n=1}^{N} S_n^z - 2 \sum_{n=1}^{N-1} S_n^x S_{n+1}^x. \tag{5}$$

Here S_n^x, S_n^z are spin-$\frac{1}{2}$ angular momentum operators. For periodic and antiperiodic boundary conditions an extra term $H_1 = \mp 2 S_N^x S_1^x$ is included in the Hamiltonian. In the limit $N \to \infty$, the ground state is singular at $\lambda = 1$, with $\lambda > 1$ and $\lambda < 1$ corresponding to strips with temperatures $T > T_c$ and $T < T_c$, respectively.

The Ising chain in a transverse field has been studied in great detail (see e.g. Katsura 1962, Pfeuty 1970, Boccara and Sarma 1974). The model can be solved by introducing fermion creation and annihilation operators and diagonalising the resultant quadratic form by a canonical transformation. A useful discussion of the general procedure has been given by Lieb *et al* (1961).

In terms of fermion creation and annhilation operators c_n, $c_n^\dagger$, equation (5) becomes (Lieb *et al* 1961)

$$H_F = \lambda \sum_{n=1}^{N} (c_n^\dagger c_n - \tfrac{1}{2}) - \tfrac{1}{2} \sum_{n=1}^{N-1} [(c_n^\dagger c_{n+1} + c_n^\dagger c_{n+1}^\dagger) + \text{HC}]. \tag{6}$$

The extra term $H_1 = \mp 2S_N^x S_1^x$ to be included for periodic and antiperiodic boundary conditions takes the form (Lieb *et al* 1961)

$$H_1 = \pm \tfrac{1}{2}[(c_N^\dagger c_1 + c_N^\dagger c_1^\dagger) + \text{HC}] \exp(\mathrm{i}\pi\mathcal{N}) \tag{7}$$

$$\mathcal{N} = \sum_{n=1}^{N} c_n^\dagger c_n. \tag{8}$$

Since $\exp(\mathrm{i}\pi\mathcal{N})$ commutes with $H_F + H_1$, $H_F + H_1$ is effectively quadratic in the fermion operators in the subspaces $\mathcal{N}$ even and $\mathcal{N}$ odd, but with different quadratic forms in each subspace.

The Hamiltonians H_F and $H_F + H_1$ may be re-expressed in the diagonal form

$$H = \sum_k \Lambda(k)(\eta_k^\dagger \eta_k - \tfrac{1}{2}) \tag{9a}$$

$$\Lambda(k) = [(\lambda - 1)^2 + 4\lambda \sin^2(k/2)]^{1/2} \tag{9b}$$

by a canonical transformation (Lieb *et al* 1961)

$$\eta_k = \sum_n (g_{kn} c_n + h_{kn} c_n^\dagger) \tag{10}$$

to quasiparticle (fermion) operators η_k, $\eta_k^\dagger$.

For free boundary conditions one finds that the allowed values of k are determined by the secular equation (Pfeuty 1970, Boccara and Sarma 1974)

$$\lambda^{-1} = \sin[(N+1)k]/\sin(Nk). \tag{11}$$

At the critical field $\lambda = 1$, equation (11) reduces to $\tan kN = \cot(k/2)$, so that

$$|k| = [(2m+1)/(2N+1)]\pi, \qquad m = 0, 1, \ldots, N-1. \tag{12}$$

From equations (9) and (12) one sees that the ground-state energy corresponds to the quasiparticle vacuum and at $\lambda = 1$ has the value

$$E_0^{(F)} = -\frac{1}{2} \sum_{m=0}^{N-1} \Lambda\left(\frac{2m+1}{2N+1}\pi\right) = \frac{1}{2}\left(1 - \operatorname{cosec} \frac{\pi}{2(2N+1)}\right). \tag{13}$$

Since $\exp(\mathrm{i}\pi\mathcal{N})$ anticommutes with the x-component of the spin density but commutes with the energy density, these operators only couple the ground state to states with odd and even numbers of quasiparticle excitations, respectively. Thus for the case of free boundaries, the energy gaps $\Delta_s^{(F)}$ and $\Delta_e^{(F)}$ that determine the spin-spin and energy-energy correlation lengths according to (3) are given by

$$\Delta_s^{(F)} = \Lambda\left(\frac{\pi}{2N+1}\right) = 2 \sin \frac{\pi}{2(2N+1)} \tag{14a}$$

$$\Delta_e^{(F)} = \Lambda\left(\frac{\pi}{2N+1}\right) + \Lambda\left(\frac{3\pi}{2N+1}\right) = 2\left(\sin \frac{\pi}{2(2N+1)} + \sin \frac{3\pi}{2(2N+1)}\right). \tag{14b}$$

For periodic boundary conditions with $\mathcal{N}$ even or antiperiodic boundary conditions with $\mathcal{N}$ odd, the allowed k are

$$k = [(2m+1)/N]\pi, \qquad m = 0, 1, \ldots, N-1 \tag{15}$$

while for periodic boundary conditions with $\mathcal{N}$ odd or antiperiodic boundary conditions with $\mathcal{N}$ even

$$k = (2m/N)\pi, \qquad m = 0, 1, \ldots, N-1. \tag{16}$$

The two sets of k's yield two different quasiparticle vacuum states. At $\lambda = 1$, $\mathcal{N}$ is even for both of these states (see Lieb *et al* 1961, appendix F). Thus the ground-state energies for periodic and antiperiodic boundary conditions, respectively, are given by

$$E_0^{(\mathrm{P})} = -\frac{1}{2}\sum_{m=0}^{N-1} \Lambda\left(\frac{2m+1}{N}\pi\right) = -\operatorname{cosec}\frac{\pi}{2N} \tag{17a}$$

$$E_0^{(\mathrm{A})} = -\frac{1}{2}\sum_{m=0}^{N-1} \Lambda\left(\frac{2m}{N}\pi\right) = -\cot\frac{\pi}{2N}. \tag{17b}$$

Bearing in mind that $\exp(\mathrm{i}\pi\mathcal{N})$ undergoes a change in sign for each quasifermion excitation, we find the following spin-spin and energy-energy gaps in the periodic and antiperiodic cases

$$\Delta_\mathrm{s}^{(\mathrm{P})} = \Lambda(0) + E_0^{(\mathrm{A})} - E_0^{(\mathrm{P})} = \tan(\pi/4N) \tag{18a}$$

$$\Delta_\mathrm{e}^{(\mathrm{P})} = \Lambda(\pi/N) + \Lambda[(2N-1)\pi/N] = 4\sin(\pi/2N) \tag{18b}$$

$$\Delta_\mathrm{s}^{(\mathrm{A})} = \Lambda(\pi/N) + E_0^{(\mathrm{P})} - E_0^{(\mathrm{A})} = 2\sin(\pi/2N) - \tan(\pi/4N) \tag{18c}$$

$$\Delta_\mathrm{e}^{(\mathrm{A})} = \Lambda(0) + \Lambda(2\pi/N) = 2\sin(\pi/N). \tag{18d}$$

We have confirmed the analytic expressions (13), (14), (17), (18) for the ground-state energies and energy gaps by calculating the excitation spectrum of the Ising chain in the spin representation of (5) numerically for $N = 2, 3, \ldots, 8$.

From the analytical expessions for the energy gaps one finds

$$\lim_{N\to\infty} N\Delta_\mathrm{s}(N) = \begin{cases} \pi/4, & \text{periodic boundary conditions} \\ \pi/2, & \text{free boundary conditions} \\ 3\pi/4, & \text{antiperiodic boundary conditions} \end{cases} \tag{19a}$$

$$\lim_{N\to\infty} N\Delta_\mathrm{e}(N) = 2\pi, \qquad \text{all three boundary conditions.} \tag{19b}$$

We now compare these results with (4). The well known critical behaviour (McCoy and Wu 1973) $m \sim t^{1/8}$, $m_1 \sim t^{1/2}$ for the bulk and surface magnetisations of the two-dimensional Ising model and $g(r) \sim r^{-1/4}$, $g_{\|}(r) \sim r^{-1}$ for the bulk and surface pair correlation functions implies (see footnote on title page)

$$x_\mathrm{s}^{(\mathrm{bulk})} = \tfrac{1}{8}, \qquad x_\mathrm{s}^{(\mathrm{surf})} = \tfrac{1}{2}. \tag{20a}$$

From the singular behaviour $\varepsilon \sim t \ln t$, $\varepsilon_1 \sim t^2 \ln t$ for the bulk and surface energy densities†, one obtains

$$x_\mathrm{e}^{(\mathrm{bulk})} = 1, \qquad x_\mathrm{e}^{(\mathrm{surf})} = 2. \tag{20b}$$

† The result $\varepsilon_1 \sim t^{2-\alpha} = t^{d\nu}$, established for the n-vector model to all orders in $\varepsilon = 4-d$ by Dietrich and Diehl (1981), implies $x_\mathrm{e}^{(\mathrm{surf})} = d$. See also Cardy (1984b).

These four scaling dimensions are entirely consistent with equations (4) and (19) and the proportionality constant $c=1$.

Assuming that equations (4) hold for other two-dimensional models besides the Ising model and their one-dimensional quantum analogues, we estimate the surface critical exponent $\eta_{\|}=2x_s^{(\mathrm{surf})}$ with which surface pair correlations decay in the two-dimensional three-state Potts model from the numerical results of Gehlen *et al* (1984) for the Z_3 chain. These authors find that $\Delta_s^{(\mathrm{P})}/\Delta_s^{(\mathrm{F})}\to\frac{2}{5}$ as $N\to\infty$. Setting $2x_s^{(\mathrm{bulk})}/x_s^{(\mathrm{surf})}=2\eta/\eta_{\|}=\frac{2}{5}$ and making use of the known value $\eta=\frac{4}{15}$ (Nienhuis *et al* 1980, Pearson 1980), we obtain $\eta_{\|}=\frac{4}{3}$. This value agrees with the exact result recently obtained by Cardy (1984b) with conformal-invariance methods.

Phenomenological renormalisation (Nightingale 1982, Barber 1983) has proved to be an extremely reliable method for determining the bulk critical properties of low-dimensional systems. In two-dimensional strips the predictions often converge toward limiting values, as the strip width N increases, more rapidly than one would expect on general grounds (Privman and Fisher 1984). Derrida and de Seze (1982) have studied the convergence analytically in two-dimensional Ising strips with periodic boundary conditions. Equation (1*b*) provides a way to determine surface critical exponents using phenomenological renormalisation with free boundary conditions. We now make use of our analytical results to study the convergence of phenomenological renormalisation in Ising strips with free boundaries in the extreme anisotropic or quantum-Hamiltonian limit.

Expressed in terms of the energy gap $\Delta_s(N,\lambda)$ corresponding to the spin–spin correlation length via (3), the fundamental equation of phenomenological renormalisation takes the form (Barber 1983)

$$N\Delta_s(N,\lambda)=N'\Delta_s(N',\lambda'). \tag{21}$$

For free boundary conditions $\Delta_s^{(\mathrm{F})}(N,\lambda)=\Lambda(k_1(N,\lambda))$, where $\Lambda(k)$ is given by (9*b*) and $k_1(N,\lambda)$ is the smallest positive value of k that satisfies (11). At $\lambda=1$, $k_1(N,1)=\pi/(2N+1)$, in agreement with (14*a*). Expanding $\Delta_s^{(\mathrm{F})}(N,\lambda)$ about $\lambda=1$, one finds

$$\begin{aligned}\Delta_s^{(\mathrm{F})}(N,\lambda)=&\frac{A_0}{N+1/2}\left(1+\frac{A_2}{(N+1/2)^2}+\ldots\right)+B_0\left(1+\frac{B_1}{N+1/2}+\ldots\right)(\lambda-1)\\&+\tfrac{1}{2}C_0(N+1/2)\left(1+\frac{C_2}{(N+1/2)^2}+\ldots\right)(\lambda-1)^2+\ldots\end{aligned} \tag{22}$$

with $A_0=\pi/2$, $A_2=-\pi^2/96$, $B_0=2/\pi$, $B_1=\pi^2/8$, and $C_0=2/\pi-16/\pi^3$.

Setting $N'=N-1$ in equation (21), we obtain estimates $\lambda_c(N)$ and $y_t(N)$ for the critical field and thermal scaling index, respectively, from the fixed point and the linearised form of the equation at the fixed point. An estimate for the surface magnetic scaling index $y_{h_1}=d-1-x_s^{(\mathrm{surf})}$ is given by $y_{h_1}(N)=1-\pi^{-1}N\Delta_s^{(\mathrm{F})}(N,\lambda_c(N))$, in accordance with (4*b*) and $c=1$. Making use of the expansion (22), we find the following behaviour in the large-N limit

$$\lambda_c(N)=1-(A_0/2B_0)N^{-2}+\ldots \tag{23a}$$

$$y_t(N)=1-[(A_0C_0/2B_0^2)+B_1]N^{-1}+\ldots \tag{23b}$$

$$y_{h_1}(N)=\tfrac{1}{2}+\tfrac{1}{2}N^{-1}+\ldots. \tag{23c}$$

Recent numerical results (Burkhardt and Guim 1985) for Ising strips with isotropic interactions and free boundary conditions are consistent with leading corrections to the exact values of K_c (critical coupling), y_t, and y_{h_1} of order N^{-2}, N^{-1}, and N^{-1}, as in equations (23). For Ising strips with isotropic interactions and periodic boundary conditions, there is faster convergence, the leading corrections to K_c and y_t varying as N^{-3} and N^{-2}, respectively (Derrida and de Seze 1982). Despite the slower convergence with free boundaries, it is possible to determine critical properties with high precision (see e.g. Barber *et al* 1984, Burkhardt and Guim 1985, Gehlen *et al* 1984) by considering sequences of N values and extrapolating to $N=\infty$.

That N in equation (22) always occurs in the combination $N+\frac{1}{2}$ suggests replacing (21) by $(N+1/2)\Delta_s(N, \lambda)=(N'+1/2)\Delta_s(N', \lambda')$. The fixed point of this equation approaches the exact value $\lambda_c=1$ with a deviation of order N^{-3}, instead of N^{-2} as in (23*a*). The deviation from the exact scaling index $y_t=1$ is again of order N^{-1}, as in (23*b*).

Equations (1*b*) and (4*b*) should prove very useful in determinations of surface scaling indices with finite-size scaling. An interesting open question concerns the extension of equations (1) to antiperiodic boundary conditions.

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