Ising model with mixed boundary conditions:
universal amplitude ratios.

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Abstract

In the vicinity of boundaries the bulk universality class of critical phenomena splits into several boundary universality classes, depending upon whether the tendency to order in the boundary is smaller or larger than in the bulk. For Ising universality class there are five different boundary universality classes: periodic, antiperiodic, free, fixed and mixed (mixture of the last two). In this paper we present the new set of the universal amplitude ratios for the mixed boundary universality class. The results are in perfect agreement with a perturbated conformal field theory scenario proposed by Cardy [2].

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A central element of the modern theory of bulk critical phenomena is the division into (bulk) universality classes. As is well known, the critical behavior near boundaries normally differs from the bulk behavior. In general, each bulk universality class of critical phenomena splits into several surface universality classes.

The criteria by which the critical systems can be classified into different universality classes is a problem of much academic interest. Two-dimensional critical systems are parameterized by the conformal anomaly $c$ which is the central charge in the Virasoro algebra \[ [3, 4] \]. The conformal anomaly $c$ can be obtained directly from the finite size corrections to the free energy for a two-dimensional classical system on infinitely long but finitely wide strip at a conformally invariant critical point.

The asymptotic finite-size scaling behavior of the critical free energy $f_M$ and the critical inverse correlation length $\xi_i$ associated with the two-point correlations of in a two-dimensional spin system on a strip with infinite length and a width of $M$ lattice spacings has the form

$$\lim_{M \to \infty} M^2 (f_M - f_\infty) - 2M f_{surf} = A,$$

$$\lim_{M \to \infty} M \xi_i^{-1} = D_i,$$

where $f_\infty$ is the bulk free energy, $f_{surf}$ is the surface free energy and $A$ and $D_i$ are the universal constants, but may depend on the boundary conditions (BCs). The index $i$ distinguishes different correlation lengths: for example, $i = s$ for the spin-spin correlation length or $i = e$ for the energy-energy correlation length. In some two-dimensional geometries, the values of $A$ and $D_i$ is known \[ [5, 6] \], to be related to the conformal anomaly number ($c$), the highest conformal weight ($\Delta$), and the scaling dimensions of the $i$-th scaling field ($x_i$) of the theory

$$A = -4\pi \left( \Delta - \frac{c}{24} \right), \quad D_i = 2\pi x_i \quad \text{for periodic or antiperiodic BCs},$$

$$A = -\pi \left( \Delta - \frac{c}{24} \right), \quad D_i = \pi x_i \quad \text{for free, fixed and mixed BCs},$$

The principle of unitarity of the underlying field theory restricts through the Kac formula the possible values of $c$ and for each value of $c$ only permits a finite number of possible values of $\Delta$. For the 2D Ising model, we have $c = 1/2$ and the only possible values are $\Delta = 0, 1/16, 1/2$. The highest conformal weight $\Delta$, and the scaling dimension $x_i$ depends on the BCs. For the Ising model on infinitely long cylinder there are two different boundary
universal classes: periodic and antiperiodic with
\[ \Delta = 0, \quad x_s = \frac{1}{8}, \quad x_e = 1 \] for periodic BCs,  
(5)  
\[ \Delta = \frac{1}{16}, \quad x_s = \frac{3}{8}, \quad x_e = 1 \] for antiperiodic BCs.  
(6)  
For the Ising model on infinitely long strip there are three different boundary universal classes: free, fixed (+−) and mixed with
\[ \Delta = 0, \quad x_s = \frac{1}{2}, \quad x_e = 2 \] for free and fixed (++) BCs,  
(7)  
\[ \Delta = \frac{1}{2}, \quad x_s = 2, \quad x_e = 2 \] for fixed (+−) BCs,  
(8)  
\[ \Delta = \frac{1}{16}, \quad x_s = 1, \quad x_e = 2 \] for mixed BCs.  
(9)  
For fixed ++ (or +−) boundary conditions the spins are fixed to the same (or opposite) values on two sides of the strip. The mixed boundary conditions corresponds to free boundary conditions on one side of the strip, and fixed boundary conditions on the other.

In the terminology of surface critical phenomena these three boundary universal classes: free, mixed and fixed (+−) correspond to "ordinary", "special" and "extraordinary" surface critical behavior, respectively.

Quite recently, Izmailian and Hu \[7, 8\] studied the finite size correction terms for the free energy per spin and the inverse correlation length of critical two-dimensional (2D) Ising models on \( M \times \infty \) lattice and one-dimensional quantum spin model with periodic, antiperiodic and free BCs. They obtain analytic expressions for the finite-size correction coefficients \( a_k, b_k \) and \( c_k \) in the expansions
\[ \mathcal{M} (f_M - f_\infty) = 2f_{surf} + \sum_{k=1}^{\infty} \frac{a_k}{M^{2k-1}}, \]  
(10)  
\[ \xi_s^{-1} = \sum_{k=1}^{\infty} \frac{b_k}{M^{2k-1}}, \]  
(11)  
\[ \xi_e^{-1} = \sum_{k=1}^{\infty} \frac{c_k}{M^{2k-1}}, \]  
(12)  
and find that although the finite-size correction coefficients \( a_k, b_k \) and \( c_k \) are not universal, the amplitude ratios for the coefficients of these series are universal and given by
\[ r_s(k) = \frac{b_k}{a_k} = \frac{2^{2k} - 1}{2^{2k-1} - 1}; \quad r_s(1) = 3, \quad r_s(2) = \frac{15}{7}, \ldots \]  
(13)  
\[ r_e(k) = \frac{c_k}{a_k} = \frac{4k}{(2^{2k-1} - 1)B_{2k}}; \quad r_e(1) = 24, \quad r_e(2) = -\frac{240}{7}, \ldots \]  
(14)
for periodic BCs, where $B_n$ is the $n$-th Bernoulli number ($B_2 = 1/6, B_4 = -1/30, \ldots$),

$$r_s(k) = \frac{b_k}{a_k} = \frac{(2^{2k} - 1)B_{2k} - 2k}{2^{2k-1}B_{2k}}; \quad r_s(1) = -\frac{9}{2}, \quad r_s(2) = \frac{135}{8}, \ldots$$

$$r_e(k) = \frac{c_k}{a_k} = \frac{-2^k}{B_{2k}}; \quad r_e(1) = -12, \quad r_e(2) = 120, \ldots$$

for antiperiodic BCs,

$$r_s(k) = \frac{b_k}{a_k} = \frac{4k}{(2^{2k-1} - 1)B_{2k}}; \quad r_s(1) = 24, \quad r_s(2) = -\frac{240}{7}, \ldots$$

$$r_e(k) = \frac{c_k}{a_k} = \frac{4k(3^{2k-1} + 1)}{(2^{2k-1} - 1)B_{2k}}; \quad r_e(1) = 96, \quad r_e(2) = -960, \ldots$$

for free BCs.

In this paper we present exact calculations for a set of universal amplitude ratios for the two-dimensional (2D) Ising models on $\mathcal{M} \times \infty$ lattice with the special boundary conditions studied by Brascamp and Kunz (BK) [9]. They considered a lattice with $2\mathcal{N}$ sites in the $x$ direction and $\mathcal{M}$ sites in the $y$ direction. The boundary conditions are periodic in the $x$ direction; in the $y$ direction, the spins are up ($+1$) along the upper border of the resulting cylinder and have the alternative values along the lower border of the resulting cylinder. It was shown [10] that the asymptotic finite-size scaling behavior of the critical free energy $f_\mathcal{M}$ of the Ising model on infinitely long strip with Brascamp-Kunz boundary condition has the form

$$\lim_{\mathcal{M} \to \infty} \mathcal{M}^2(f_\mathcal{M} - f_\infty) - 2\mathcal{M}f_{surf} = -\frac{\pi}{24},$$

which is consistent with the conformal field theory prediction for the mixed boundary condition (see Eqs. (1), (4) and (9)) although the mixed boundary condition and the BK boundary condition are different on one side of the long strip.

We obtain analytic equations for $a_k, b_k$ and $c_k$ in the expansions given by Eqs. (10), (11) and (12) and find that universal amplitude ratios the two-dimensional (2D) Ising models on $\mathcal{M} \times \infty$ lattice with mixed BCs are given by

$$r_s(k) = \frac{b_k}{a_k} = \frac{-4k}{B_{2k}}; \quad r_s(1) = -24, \quad r_s(2) = 240, \ldots$$

$$r_e(k) = \frac{c_k}{a_k} = \frac{-2^{2k+1}k}{B_{2k}}; \quad r_e(1) = -48, \quad r_e(2) = 1920, \ldots$$

As far as we know, no previous RG arguments, analytic calculations, or numerical studies predict the existence of this whole set of universal amplitude ratios.
Consider an Ising ferromagnet on an $N \times M$ lattice. The Hamiltonian of the system is

$$\beta H = -J \sum_{\langle ij \rangle} s_i s_j,$$

where $\beta = (k_B T)^{-1}$, the Ising spins $s_i = \pm 1$ are located at the sites of the lattice and the summation goes over all nearest-neighbor pairs of the lattice. There are a few boundary conditions for which the Ising model has been solved exactly. Among them is the special boundary conditions studied by Brascamp and Kunz (BK) \[9\]. We consider a transfer matrix acting along the $M$ direction. If $\Lambda_0$, $\Lambda_1$ and $\Lambda_2$ are the largest, the second-largest and the third-largest eigenvalues of the transfer matrix, in the limit $N \to \infty$ the free energy per spin,

$$f_M = \lim_{N \to \infty} F/2N,$$

and the inverse spin-spin correlation length, $\xi_s^{-1}$, and the inverse energy-energy correlation length, $\xi_e^{-1}$, are

$$f_M = \frac{1}{M+1} \ln \Lambda_0, \quad \xi_s^{-1} = \ln (\Lambda_0/\Lambda_1) \quad \text{and} \quad \xi_e^{-1} = \ln (\Lambda_0/\Lambda_2). \quad (23)$$

where $F$ is the total free energy. The three leading eigenvalues of the transfer matrix ($\Lambda_0$, $\Lambda_1$ and $\Lambda_2$) can be obtained from exact expression for the partition function of the Ising model on a $2N \times M$ rectangular lattice under under Brascamp-Kunz BCs \[9\]:

$$\Lambda_0 = C_\mu \exp \left\{ \frac{1}{2} \sum_{m=0}^{2M+1} \omega_\mu \left( \frac{\pi m}{2(M+1)} \right) \right\}, \quad (24)$$

$$\Lambda_1 = C_\mu \exp \left\{ -2\omega_\mu \left( \frac{\pi}{2(M+1)} \right) + \frac{1}{2} \sum_{m=0}^{2M+1} \omega_\mu \left( \frac{\pi m}{2(M+1)} \right) \right\}, \quad (25)$$

$$\Lambda_2 = C_\mu \exp \left\{ -2\omega_\mu \left( \frac{\pi}{M+1} \right) + \frac{1}{2} \sum_{m=0}^{2M+1} \omega_\mu \left( \frac{\pi m}{2(M+1)} \right) \right\}, \quad (26)$$

where

$$C_\mu = \left( \sqrt{2e^\mu} \right)^M \frac{1}{4 \cosh (2N \omega_\mu(0)) \cosh (2N \omega_\mu(\pi/2))} \left( \frac{1}{\pi^\gamma} \right)$$

and a lattice dispersion relation $\omega_\mu(x)$ is implicitly given by

$$\omega_\mu(x) = \operatorname{arcsinh} \sqrt{2 \sinh^2 \mu + \sin^2 x}$$

with $\mu = \frac{1}{2} \ln \sinh 2J$. At the critical point $\mu = \mu_c = 0$ ($J_c = \frac{1}{2} \ln (1 + \sqrt{2})$) one then obtains

$$\omega_0(x) = \operatorname{arcsinh} \sin x$$
and

\[ C_0 = \left( \sqrt{2} \right)^M \left( \frac{1}{4 \cosh \left( 2N \arcsinh 1 \right)} \right)^{1/4} \]

Then the critical free energy \( f_M \), critical spin-spin correlation length \( \xi_s \) and critical energy-energy correlation length \( \xi_e \) of Eq. (23) can be written as

\[ f_M = \frac{M}{2(M+1)} \ln 2 - \frac{1}{2(M+1)} \ln (1 + \sqrt{2}) + \frac{1}{2(M+1)} \sum_{m=0}^{2M+1} \omega_0 \left( \frac{\pi m}{2(M+1)} \right), \quad (27) \]

\[ \xi_e^{-1} = 2\omega_0 \left( \frac{\pi}{2(M+1)} \right), \quad (28) \]

\[ \xi_s^{-1} = 2\omega_0 \left( \frac{\pi}{M+1} \right), \quad (29) \]

Using the Euler-Maclaurin summation formula [11] the asymptotic expansion of the critical free energy \( f_M \) can be written in the following form

\[ (M+1)(f_M - f_\infty) = 2f_{surf} - \sum_{k=0}^{\infty} \frac{\lambda_{2k} B_{2k+2}}{(2k)!(2k+2)} \left( \frac{\pi}{2(M+1)} \right)^{2k+1}, \quad (30) \]

\[ = 2f_{surf} - \frac{\pi}{24(M+1)} - \frac{1}{2880} \left( \frac{\pi}{M+1} \right)^3 - \frac{1}{4384} \left( \frac{\pi}{M+1} \right)^5 + \ldots, \]

where

\[ f_\infty = \frac{1}{2} \ln 2 + \frac{2G}{\pi} \quad (31) \]

\[ f_{surf} = -\frac{1}{4} \ln (2 + 2\sqrt{2}) \quad (32) \]

and \( \lambda_{2k} \) is the coefficients in the the Taylor expansion of the \( \omega_0(x) \):

\[ \omega_0(x) = \sum_{p=0}^{\infty} \frac{\lambda_{2p}}{(2p)!} x^{2p+1}, \quad \lambda_0 = 1, \lambda_2 = -\frac{2}{3}, \lambda_4 = 4, \ldots \quad (33) \]

Using the Taylor expansion of the \( \omega_0(x) \) given by Eq. (33) the asymptotic expansion of the critical spin-spin correlation length \( \xi_s \) and critical energy-energy correlation length \( \xi_e \) can be written as

\[ \xi_s^{-1} = \sum_{k=0}^{\infty} \frac{2\lambda_{2k}}{(2k)!} \left( \frac{\pi}{2(M+1)} \right)^{2k+1}, \quad (34) \]

\[ = \frac{\pi}{M+1} - \frac{1}{12} \left( \frac{\pi}{M+1} \right)^3 + \frac{1}{96} \left( \frac{\pi}{M+1} \right)^5 + \ldots, \]

\[ \xi_e^{-1} = \sum_{k=0}^{\infty} \frac{2\lambda_{2k}}{(2k)!} \left( \frac{\pi}{M+1} \right)^{2k+1}, \quad (35) \]

\[ = \frac{2\pi}{M+1} - \frac{2}{3} \left( \frac{\pi}{M+1} \right)^3 + \frac{1}{3} \left( \frac{\pi}{M+1} \right)^5 + \ldots, \]
Equations (30), (34), and (35) imply that the ratios of the amplitudes of the $(\mathcal{M} + 1)^{-(2k+1)}$ correction terms in the spin-spin correlation length, the energy-energy correlation lengths, and the free energy expansion, i.e. $b_k/a_k$ and $c_k/a_k$, should not depend in detail on the dispersion relation $(\omega_0(x))$ as given by Eqs. (20) and (21).

To check the applicability of these results, we study the anisotropic Ising model with coupling constant $J$ and $\gamma J$ along the horizontal and vertical directions, respectively, with $0 < \gamma < \infty$. At the critical point $J_c$, where $J_c$ is defined by $\sinh 2J_c \sinh 2\gamma J_c = 1$, we obtain that the dispersion relation for the anisotropic Ising model $\omega_0(\text{anysotrop})(x)$ is now given by

$$
\omega_0(\text{anysotrop})(x) = \text{arcsinh} (\sin x \sinh 2\gamma J_c)
$$

(36)

The asymptotic expansion of the critical free energy $f_{\mathcal{M}}$, the critical spin-spin correlation length $\xi_s$ and critical energy-energy correlation length $\xi_e$ is given by the first line in the Eqs. (30), (34), and (35), where $\lambda_{2k}$ is now the coefficients in the the Taylor expansion of the dispersion relation $\omega_0(\text{anysotrop})(x)$:

$$
\omega_0(\text{anysotrop})(x) = \sum_{p=0}^{\infty} \frac{\lambda_{2p}}{(2p)!} x^{2p+1},
$$

(37)

where

$$
\lambda_0 = \sinh 2\gamma J_c, \quad \lambda_2 = -\frac{1}{3} \sinh 2\gamma J_c \cosh^2 2\gamma J_c, \quad ...
$$

It is easy to see that the ratios $b_k/a_k$ and $c_k/a_k$ does not depend in detail on the dispersion relation $(\omega_0(\text{anysotrop})(x))$ and Eqs. (20) and (21) holds for all anisotropy $\gamma$.

In [7], we have shown that the Ising model on the square, honeycomb and plan-triangular lattices, and the quantum spin model have universal amplitude ratios, i.e. we confirmed that such models are in the same universality class. It is reasonable to expect that the ratios of Eqs. (20) and (21) are valid for the same universality class. The leading terms of Eqs. (30), (34) and (35) are consistent with Eqs. (1) - (4), i.e. $a_1$, $b_1$ and $c_1$ are universal. Equations (1) and (2) implies immediately that their ratio is also universal, namely $r_s(1) = D_1/A$ and $r_e(1) = D_2/A$, which is consistent with Eqs. (20) and (21) for the case $k = 1$

$$
 r_s(1) = \frac{D_1}{A} = -24
$$

(38)

$$
 r_e(1) = \frac{D_2}{A} = -48
$$

(39)
The finite-size corrections to Eqs. (1) and (2) can be calculated by the means of a perturbed conformal field theory \[2, 12\]. In general, any lattice Hamiltonian will contain correction terms to the critical Hamiltonian \(H_c\)

\[
H = H_c + \sum_p g_p \int_{-\mathcal{M}/2}^{\mathcal{M}/2} \phi_p(v) dv,
\]

where \(g_p\) is a non-universal constant and \(\phi_p(v)\) is a perturbative conformal field. Below we will consider the case with only one perturbative conformal field, say \(\phi_l(v)\). Then the eigenvalues of \(H\) are

\[
E_n = E_{n,c} + g_l \int_{-\mathcal{M}/2}^{\mathcal{M}/2} < n|\phi_l(v)|n > dv + \ldots,
\]

where \(E_{n,c}\) are the critical eigenvalues of \(H\). The matrix element \(< n|\phi_l(v)|n >\) can be computed in terms of the universal structure constants \((C_{nlm})\) of the operator product expansion \[2\]:

\[
<n|\phi_l(v)|n> = \frac{2\pi}{\mathcal{M}} x_l C_{nln},
\]

where \(x_l\) is the scaling dimension of the conformal field \(\phi_l(v)\). The energy gaps \((E_n - E_0)\) and the ground-state energy \((E_0)\) can be written as

\[
E_n - E_0 = \frac{2\pi}{\mathcal{M}} x_n + 2\pi g_l (C_{nlm} - C_{000}) \left(\frac{2\pi}{\mathcal{M}}\right)^{x_l-1} + \ldots,
\]

\[
E_0 = E_{0,c} + 2\pi g_l C_{000} \left(\frac{2\pi}{\mathcal{M}}\right)^{x_l-1} + \ldots.
\]

Note, that the ground state energy \(E_0\), the first energy gap \((E_1 - E_0)\) and the second energy gap \((E_2 - E_0)\) of a quantum spin chain are, respectively, the quantum analogies of the free energy \(f(N)\), inverse spin-spin correlation length \(\xi_s^{-1}(N)\), and inverse energy-energy correlation length \(\xi_e^{-1}(N)\) for the Ising model; that is,

\[
\mathcal{M} f_M \Leftrightarrow -E_0, \quad \xi_s^{-1}(N) \Leftrightarrow E_1 - E_0 \equiv \Delta_s, \quad \text{and} \quad \xi_e^{-1}(N) \Leftrightarrow E_2 - E_0 \equiv \Delta_e.
\]

For the 2D Ising model, one finds \[13\] that the leading finite-size corrections \((1/\mathcal{M}^3)\) can be described by the Hamiltonian given by Eq. \[[10\] with a single perturbative conformal field \(\phi_l(v) = L^2_2(v)\) with scaling dimension \(x_l = 4\).

In order to obtain the corrections we need the matrix elements \(< n|L^2_2(v)|n >\), which have already been computed by Reinicke \[14\].

\[
<\Delta + r|L^2_2|\Delta + r> = \left(\frac{2\pi}{\mathcal{M}}\right)^4 \begin{pmatrix}
\frac{49}{11520} + (\Delta + r) \left(\Delta - \frac{5}{24} + \frac{r(2\Delta + r)(5\Delta + 1)}{(\Delta + 1)(2\Delta + 1)}\right)
\end{pmatrix}.
\]
The universal structure constants $C_{2l_2}, C_{1l_1}$ and $C_{0l_0}$ can be obtained from the matrix element $< n|L_{-2}^2(v)|n > = (2\pi/\mathcal{M})^{x_l} C_{nl_n}$, where $x_l = 4$ is the scaling dimension of the conformal field $L_{-2}^2(v)$.

At the critical point the spectra of the Hamiltonian with free, fixed and mixed BCs are built by the irreducible representation $\Delta$ of a single Virasoro algebra with possible values of $\Delta$ are $0, \frac{1}{2}, \frac{1}{16}$. We denote by $\Delta$ the highest weight, and by $\Delta + r$, the $r$-th level having degeneracy $d(\Delta, r)$ of irreducible representation of the Virasoro algebra. A state will be labeled by $|n > \sim |\Delta + r >$.

For mixed BCs the ground state $|0 >$, first excited state $|1 >$, and second excited state $|2 >$ are given by \[2, 15]:

\begin{align*}
|0 > &= |\Delta = \frac{1}{16}, r = 0 >, \\
|1 > &= |\Delta = \frac{1}{16}, r = 1 >, \\
|2 > &= |\Delta = \frac{1}{16}, r = 2 >.
\end{align*}

(46) (47) (48)

After reaching this point, one can easily compute the universal structure constants $C_{2l_2}, C_{1l_1}$ and $C_{0l_0}$ for mixed boundary conditions. The values of $C_{0l_0}, C_{1l_1}, C_{2l_2}$ can be obtained from Eqs. (45) - (48) and given by:

\begin{align*}
C_{0l_0} &= -7/1440, \\
C_{1l_1} &= 1673/1440, \\
C_{2l_2} &= 13433/1440.
\end{align*}

(49)

Equations (42) and (43) implies that the ratios of first-order corrections amplitudes for $E_n - E_0 (\xi_n^{-1})$ and $-E_0 (f_{\mathcal{M}})$ is universal and equal to $(C_{0l_0} - C_{nl_n})/C_{0l_0}$, which is consistent with Eq. (20) for the case $n = 1, k = 2$

\[r_s(2) = \frac{C_{0l_0} - C_{1l_1}}{C_{0l_0}} = 240 \quad \text{for mixed BCs}
\]

(50)

and with Eq. (21) for the case $n = 2, k = 2$

\[r_e(2) = \frac{C_{0l_0} - C_{2l_2}}{C_{0l_0}} = 1920 \quad \text{for mixed BCs}
\]

(51)

In this paper we present exact calculations for a set of universal amplitude ratios for the two-dimensional (2D) Ising models on $\mathcal{M} \times \infty$ lattice for mixed BCs universality class. We find that such result are in perfect agreement with a perturbated conformal field theory scenario proposed by Cardy \[2\].
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