Excitation Spectrum at the Yang-Lee Edge
Singularity of the 2D Ising model with boundaries

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Abstract. The presence of the boundaries imposes severe constraints on the possible Conformal Field Theories (CFTs). Special physical boundary conditions are compatible with CFT and define Boundary Conformal Field Theories (BCFTs). This presentation contains a study of the Yang-Lee edge singularity (YLS) of the two dimensional (2D) Ising model on the infinite strip. At the 2D Ising model’s YLS, several potential BCFTs are identified. Based on numerical calculations on an Ising quantum chain at YLS, the measurements are used to identify one of potential BCFTs.

This presentation is organized as follows. The section titled "1" briefly introduces the subject of the boundary conformal field theories (BCFTs). The section titled "2" briefly introduces methods used to identify the BCFT for the Yang-Lee singularity in 2D Ising model with free boundaries. The YLS is described by variants of $(A_4, A_1)$ minimal CFTs. The section titled "3" lists the possible lowest lying spectra of candidate BCFTs. Finally, the section titled "4" presents our numerical data for the quantum chain realization of the YLS in 2D Ising model with free boundaries and identifies this critical statistical model with one of the candidate BCFTs associated with the $(A_4, A_1)$ minimal CFT.

1. Boundary Conformal Field Theories

Conformal field theories were first constructed for the unbounded geometry of the Euclidean plane [3]. New, interesting problems arise when the conformal theory is constructed in constrained geometry. One such geometry is an infinite strip geometry, which can be mapped into the upper half plane.

One common belief is that boundaries only influence the physical behavior in their neighborhood. That is, the influence of boundaries vanishes as the bulk grows. In CFTs, this will not be true, because CFTs are critical theories in which the correlation length is infinite. This fact makes the influence of boundaries significant whatever the size of the bulk. For example, the excitation spectrum of a CFT on the strip will be different than the excitation spectrum on the entire plane. The spectra of CFTs carry complete information about the irreducible representations of the conformal symmetry entering therein.
One theoretical approach to study of boundary CFTs consists of starting with CFTs on the plane and then asking what changes in the presence of boundaries. In the presence of boundaries, one can ask the following questions about CFT:

- What boundary conditions do not destroy conformal symmetry?
- What conformal symmetry survives the surgery associated with boundaries?
- What are the possible operator spectra of CFTs with boundaries?

The above questions have been studied, and some answers to these questions have been obtained [9, 10]. The answers follow from a constraint on admissible conformal symmetries in bounded geometries. On the geometry of the upper half plane, the constraint is that conformal transformations preserve the real axis. This constraint breaks the independence of the holomorphic and the anti-holomorphic symmetries of CFTs. As a result, only one of these symmetries typically has to be considered, e.g., the holomorphic symmetries. For this reason, the partition function, which is sesquilinear in characters \( \chi \) of Virasoro algebra on the plane, as follows:

\[
Z = \sum_{i,j} N_{i,j} \chi_i(q) \bar{\chi}_j(q) \quad (1)
\]

becomes linear in these characters on the half plane, as follows:

\[
Z^{(\alpha,\beta)} = \sum_i n_i^{(\alpha,\beta)} \chi_i(q). \quad (2)
\]

In these equations, the indices \( i \) and \( j \) run over all characters of the Virasoro algebra, and the positive integer coefficients \( N_{i,j} \) and \( n_i^{(\alpha,\beta)} \) give the operator content of CFT on the full plane and on the half plane, respectively. In the later case, the indices \( \alpha \) and \( \beta \) index the left-hand boundary condition and the right-hand boundary condition, respectively. Due to the dependence on the indices \( \alpha \) and \( \beta \), several different BCFTs can be generated from the original Virasoro algebra. For the unitary minimal CFTs, the coefficients \( n_i^{(\alpha,\beta)} \) are defined by the CFT’s fusion coefficients [9, 10].

2. Methods

We used quantum Ising spin chains with free boundary conditions to determine the low lying excitation spectrum at special scaling values \( h = iB_{YL}(N) \) of magnetic field. The phenomenological renormalization group (PRG) determined the special imaginary values of the magnetic field that define the YLS. Numerical measurements of the spectrum of such chains for different chain lengths organize themselves into series that correspond to different excited states in the thermodynamic limit. Indeed, fitting each series to leading scaling behavior enables one obtain the spectrum in the thermodynamic limit from measurements on finite-length quantum Ising spin chains. These steps of our methods are briefly described in this section.

The hamiltonian limit of the statistical 2D Ising model provides a quantum spin chain model having the same critical behavior as the 2D Ising model. This paper focuses on Yang-Lee singularity of such a quantum spin chain model.

The quantum spin chain model corresponding to the 2D Ising model has a Hamiltonian that is given by [4]:

\[
H_{Ising} = -t \sum_{n=1}^{N-1} \sigma_z(n)\sigma_z(n+1) + \sum_{n=1}^{N} (-h \sigma_z(n) + \sigma_x(n)). \quad (3)
\]

In eq. (3), \( N \) is the number of sites in the chain, \( \sigma_x(n) \) and \( \sigma_z(n) \) are 2x2 Pauli spin matrices at site “\( n \)”, ”\( h \)” is an external magnetic field, and ”\( t \)” is a ferromagnetic spin-spin coupling, i.e.,
$t > 0$. In our studies, the quantum spin chain is open and does not include a special boundary magnetic fields at the first and the last sites. That is, free-free boundary conditions are imposed on the quantum spin chain.

At the Yang-Lee edge singularity, the external magnetic field, $h$, is purely imaginary, i.e., $h = iB$ for real values of $B$. On a quantum spin chain of length, $N$, the phenomenological renormalization group (PRG) defines special values, $iB_{Y\text{L}}(N)$, of the magnetic field. For a chain length of $N$, the special value $iB_{Y\text{L}}(N)$ satisfies the PRG equation [5, 6]:

$$[N - 1]m(iB_{Y\text{L}}(N), N - 1) = [N]m(iB_{Y\text{L}}(N), N).$$  \hspace{1cm} (4)

In eq. (4), $m(iB, N)$ is the energy gap, which is equal to $[E_i(iB, N) - E_0(iB, N)]$. Here, $E_0(iB, N)$ and $E_1(iB, N)$ are the energies of the respective ground state "0" and the first excited state "1" for the Ising quantum spin chain of length $N$. As $N \rightarrow \infty$, the special magnetic values, $iB_{Y\text{L}}(N)$, converge to the magnetic field at the Yang-Lee edge singularity.

For these special magnetic field values and temperatures greater than the ordinary critical temperature, the low-lying excitation spectrum was measured for the chain lengths of 6 to 12. The measured spectra were organized into series of eigenstates, wherein each series corresponds to one excitation state in the thermodynamic limit. For low-lying eigenstates, an identification of corresponding eigenstate for adjacent chain lengths was possible, because the energies of corresponding states vary smoothly and monotonically with $N$, and the correspondences between eigenstates for different chain lengths properly accounts for degeneracies as $N$ increases.

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BCFT predicts that the leading scaling behavior of actual excitation energies with the chain-length, $N$, will be [8]:

$$E_i(N) - E_0(N) = \xi 2\pi \Delta_i / N.$$  \hspace{1cm} (5)

Here, $\Delta_i$ is the conformal dimension of the field $i$, and $\xi$ is a non-universal constant that depends on the normalization of the Hamiltonian for the Ising quantum spin chain. In eq. (5), the excitation energies depend only on one conformal weight, because the presence of physical boundaries reduces the conformal symmetry to a single Virasoro algebra.

Normalizing the spectrum for each chain-length $N$ by the first gap eliminates the non-universal constant. Such normalized excitation energies, i.e., $\tilde{E}_i(N) = (E_i(N) - E_0(N))/|E_1(N) - E_0(N)|$, were then, fitted to an equation of the following form:

$$\tilde{E}_i(N) = \tilde{E}_0(\infty) + A_iN^{p_i} \quad \text{with} \quad p_i < 0.$$  \hspace{1cm} (6)

In eq. (6), $\tilde{E}_i(\infty) = \tilde{E}_0(\infty)$ is the thermodynamic limit of the $i$-th normalized excitation energy as $N \rightarrow \infty$, and $A_iN^{p_i}$ is a correction term representing the leading scaling correction.

3. **BCFTs generated by $(A_4, A_1)$ minimal CFT**

The simplest non-unitary minimal CFT, is known as the $(A_4, A_1)$ in the ADE classification [7]. Cardy identified this minimal CFT with the Yang-Lee singularity of the 2D Ising model on plane [1].

On the 1/2-plane, BCFTs have a partition function that is a linear combination of the Virasoro characters appearing in the partition function of the corresponding CFT on the plane [9, 10]. On the plane, the partition function of the $(A_4, A_1)$ minimal CFT is constructed from $(c = -22/5, \Delta = 0)$ and $(c = -22/5, \Delta = -1/5)$ Verma modules. Here, each Verma module has been labeled by the central charge $c$ of the CFT, and the field dimension $\Delta$ of the corresponding primary field. Thus, the BCFT of the Yang-Lee edge singularity on the infinite strip should have the states of the $(c = -22/5, \Delta = 0)$ Verma module and/or the states of the $(c = -22/5,$
\[ \Delta = -1/5 \] Verma module. That is, there are three types of candidate BCFT for the Yang-Lee edge singularity of the 2D Ising model on the infinite strip with free boundary conditions. The candidate BCFTs have the states of the \( c = -22/5, \Delta = 0 \) Verma module, the states of the \( (c = -22/5, \Delta = -1/5) \) Verma module, or the states of both these Verma modules. For each of these candidate BCFTs, Table [1] shows the low-lying excitation spectrum. In Table

| Strip Boundary Conditions | CFT of \((-22/5, 0)\) Verma module | CFT of \((-22/5, -1/5)\) Verma module | CFT of \((-22/5, 0)\) and \((-22/5, -1/5)\) modules |
|---------------------------|-------------------------------------|--------------------------------------|-----------------------------------------|
| Excitation Energy         | 2 3 4 5 6 7                        | 2 4 6 8 10 12                       | 2 10 20 22 30 32                        |
| Degeneracy                | 1 1 1 1 2 2                        | 1 1 1 2 2 3                        | (A_4, A_1) CFT on \(\infty\)-long cylinder |
| Excitation Energy         | 2 5 10 12 15                       |                                      |                                        |
| Degeneracy                | 1 2 3 2 4                         |                                      |                                        |

Table 1. Low-Lying Excitation spectra of candidate BCFTs

[1], the BCFT predictions for the excitation energies have been normalized so that the lowest excitation energy is two. For the candidate BCFT that combines both Verma modules, Table [1] does not list state degeneracies, because these degeneracies will depend on the number of copies of each Verma modules in the BCFT. For comparison, Table [1] also lists the low-lying excitation spectrum of the \((A_4, A_1)\) minimal CFT describing the Yang-Lee edge singularity on the infinitely long cylinder. From Table [1], one sees that low-lying excitation spectra distinguish the candidate CFTs for the Yang-Lee edge from each other.

4. Numerical results for the spectrum

For a spin-spin coupling \(t\) of 0.1, Table [2] shows our measurements of the special values of the magnetic field that solve the PRG eq. (4).

| \( N \) | \( B_{YL}(N) \) |
|--------|-----------------|
| 6      | 0.64452828      |
| 7      | 0.64155254      |
| 8      | 0.63986508      |
| 9      | 0.63884984      |
| 10     | 0.63820860      |
| 11     | 0.63778681      |
| 12     | 0.63749969      |
| \( \infty \) | —                |

Table 2. PRG values of \( B_{YL}(N) \) when \( t = 0.1 \).

\(^1\) For this choice of normalization, the measured normalized excitation energies will also be actual conformal dimensions.
Table 3. Measured normalized low-lying excitation energies as a function of length, $N$, of the Ising quantum spin chain.

| $N$ | 6     | 7     | 8     | 9     | 10    | 11    | 12    | $\infty$ |
|-----|-------|-------|-------|-------|-------|-------|-------|---------|
| A   | 3.10970 | 3.08865 | 3.07468 | 3.06481 | 3.05748 | 3.05183 | 3.04732 | 3.02    |
| B   | 4.01911 | 4.01608 | 4.01552 | 4.01700 | 4.01801 | 4.01895 | 4.01855 | 4.00    |
| C   | 4.72083 | 4.77954 | 4.82010 | 4.85112 | 4.87569 | 4.89555 | 4.91182 | 5.05    |
| D1  | —     | 5.35658 | 5.47758 | 5.56177 | 5.62651 | 5.67802 | 5.71994 | 6.01    |
| D2  | 6.15534 | 6.12718 | 6.11081 | 6.09947 | 6.08136 | 6.08017 | 6.08176 | 6.06    |
| E1  | —     | —     | 5.95864 | 6.13662 | 6.26129 | 6.35878 | 6.43745 | 6.90    |
| E2  | 7.03192 | 7.02799 | 7.02804 | 7.03040 | 7.03483 | 7.03688 | 7.03914 | 7.03    |

Figure 1. Measured Low-Lying Normalized Excitation Energies for $N$ between 6 and 12.

For the special magnetic field values of Table [2] and $t = 0.1$, the measured low-lying excitation spectra of Ising quantum spin chains with 6 to 12 sites are given in Table [3] and are plotted in Figure (1). The excitation energies have again been normalized by dividing by $1/2$ times the lowest measured excitation energy.

This normalization enables a direct comparison between the measured excitation spectra of Table [3] and the predicted spectra of candidate CFTs as given in Table [1].

To compare the measured spectra of Fig.(1) to the predicted spectra of Table [1], it is necessary to determine the limit of the normalized excitation energies of states as the quantum spin chain’s length, $N$, becomes large. To find these limit values, one identifies corresponding

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$^2$ Figure (1) does not show the lowest excitation energy, which is exactly two in this normalization.
states in Ising quantum spin chains of different lengths, \( N \). In Fig.(1), these correspondences are indicated by lines between measured excitation energies for different inverse chain-lengths, \( 1/N \). The correspondences were found by assuming a smooth scaling behavior and by using the fact that level crossings should disappear as \( N \) grows.

In Fig.(1), it is easy to identify the sequences A, B, C, D1, D2, E1, E2, F, G, and H of normalized excitation energies. As expected, for low-lying sequences, crossings between different ones of these sequences disappear as \( N \) increases. The normalized excitation energies of the lowest sequences, which are labeled by A, B, C, D1, D2, E1, and E2, smoothly scale toward values of about 3 to 7 as \( N \to \infty \). The normalized excitation energies of the sequences labeled by F, G, and H smoothly scale towards higher values as \( N \to \infty \). For the states F, G, and H, the evaluation of these limits as \( N \to \infty \) is outside of our measurements on short Ising quantum spin chains.

The last column of Table [3] also shows the normalized excitation energies obtained by extrapolating the measured excitation energies to the limit where \( N \to \infty \). From the above-described extrapolations, we found that the low-lying excitation spectrum for the Ising quantum spin chain at the Yang-Lee edge singularity has the following sequence of normalized excitation energies (degeneracies): 2(1), 3(1), 4(1), 5(1), 6(2), and 7(2). By comparing these results with the CFT predictions of Table [1], it is readily seen that the measured low-lying excitation spectrum is the same as the low-lying excitation spectrum of the minimal CFT, which is based only on the \((c, \Delta) = (-22/5, 0)\) Verma module.

In conclusion, measured low-lying excitation spectra of the Ising quantum spin chain with free boundary conditions at the Yang-Lee edge singularity are in excellent agreement with the spectrum of the \((c, \Delta) = (-22/5, 0)\) Verma module. Thus, the \((c, \Delta) = (-22/5, 0)\) Verma module defines the CFT for the Yang-Lee edge singularity of the 2D Ising model on the infinite strip with free boundary conditions.

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No state has been double counted in identifying the sequences A - H.