Finite-Size scaling at Yang-Lee singularities of 2D discrete spin models

Tomasz Wydro(1) and John F McCabe(2)

(1) Laboratoire de Physique Moléculaire et des Collisions Université de Metz 1 bvd Arago, 57078 Metz, France
(2) 412 Morris Ave., # 34, Summit, NJ 07901, USA

E-mail: wydro@sciences.univ-metz.fr
E-mail: jfmccabe2@earthlink.net

Abstract. We numerically study the Hamiltonian limits of the two dimensional (2D) Ising and 3-state Potts models in complex magnetic fields. From the Phenomenological Renormalization Group, we find the critical field values associated with the Yang-Lee singularity (YLS) in these models. We also determine the low-lying part of the excitation spectrum at the YLS. Finally, we compare the resulting patterns of energy levels to predictions for conformal non-unitary minimal models.

1. Introduction

In their seminal papers [1, 2], Yang and Lee related the analytical properties of the partition function to phase properties of statistical systems. Yang and Lee showed that grand canonical partition functions of lattice gases have zeros at complex fugacities $z$. Yang and Lee also showed that these zeros become dense at edges of a gap about the positive $z$ axis and that the gap disappears at the transition temperature. The edges of this gap have become known as the Yang–Lee edge singularities (YLSs).

While Yang and Lee showed that the zeros of the partition function have a role in ordinary phase transitions, it has also become clear that YLSs themselves are critical points [3]. Thus, YLSs became other critical points of interest in studies of statistical systems. Indeed, YLSs appear in many magnetic systems for complex values of the magnetic field. Furthermore, it is now clear that the effects of YLSs are directly accessible via experiments [4].

The critical nature of YLSs has raised considerable interest. The interest is even larger in 2D where there is a classification of many critical points. A large class of 2D statistical models have critical points that are described by the conformal field theories (CFTs) of the ADE classification[8], i.e., the minimal CFTs [6, 7].

Cardy identified the YLS of the 2D Ising model with the $(A_4, A_1)$ minimal CFT [5]. Indeed, some properties of this YLS have been studied numerically [9, 10]. Nevertheless, other properties of this YLS had not been studied prior to our work. Also, the YLS of the next simplest 2D spin model, i.e., the 3-state Potts model, had not been studied at all prior to our work.

In this paper, we review our numerical studies of the YLSs of the 2D Ising and 3-state Potts models. In particular, we discuss numerical determinations of the low-lying excitation spectrum at these YLSs and compare our numerical determinations with predictions from CFT.
This paper is organized as follows. In section 2, we introduce the quantum spin chains for the 2D Ising and 3-state Potts models. Via universality, the criticality of a 2D model is equivalent to that of its quantum spin chain, which is more convenient for numerical studies. In the section 3, we provide a list of candidate CFTs for the YLS of the 2D 3-state Potts model based on the ADE classification.[7, 8, 6] In section 4, we review finite-size scaling [11], and provide predictions for low-energy excitation spectra from CFT. In section 5, we comment on numerical methods herein. In section 6, we report our measurements of the low-lying excitation spectrum at the YLS of the 2D Ising model. In section 7, we report our measurements of the low-lying excitation spectrum and the exponent \( \nu \) at the YLS of the 2D 3-state Potts model and determine the associated CFT. In section 8, we summarize our results.

2. Quantum spin chain for the Ising and 3-state Potts models

We will consider the Hamiltonian limit of the transfer matrix for 2D discrete spin models on a square lattice [12, 13].

For the 2D Ising model, the associated \( N \)-site, quantum spin chain has the Hamiltonian given by [14]

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

Here, \( \sigma_x(n) \) and \( \sigma_z(n) \) are 2x2 Pauli spin matrices at site \( n \).

For the 2D 3-state Potts model, the associated \( N \)-site, quantum spin chain has the Hamiltonian given by:[14, 13]

\[
H_{\text{Potts chain}} = -\sum_{n=1}^{N} \{ t[W(n)W(n+1) + H.C.] + L(n) + BD(n) \} .
\]

Here, \( t \) is a positive coupling associated with same row ferromagnetic spin-spin interactions, and \( B \) is an external magnetic field. \( W(n), L(n), \) and \( D(n) \) are 3x3 matrices associated with intra-row spin-spin interactions, single inter-row spin flips, and the external magnetic field interaction, respectively. These matrices are given by:

\[
W = \begin{pmatrix} \omega & 0 & 0 \\ 0 & \omega^2 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad L = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \quad \text{and} \quad D = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}
\]

Here, \( \omega \) is the 3rd root of unity, i.e., \( \omega = \exp(i2\pi/3) \).

Quantum chains have sparse Hamiltonian matrices and can be studied with powerful numerical matrix techniques, e.g., the Lanczos algorithm [15]. Both the quantum spin chain and its associated 2D spin model have the same critical points via universality.

3. Candidate Conformal Field Theories

The YLS of the 2D Ising model is described by a conformal minimal model [5, 10]. This suggests that the YLS of the 2D 3-state Potts model is also described by one of the conformal minimal models.

Each conformal minimal model is classified by a central charge and a primary field content. The central charges of the conformal minimal models satisfy [6, 7, 8]

\[
c = 1 - \frac{6(p-p')^2}{pp'} ,
\]
where \( p \) and \( p' \) are coprime integers that are greater than 1. The primary fields are denoted by pairs of conformal dimensions \((h_{r,s}, \bar{h}_{r',s'})\), given by:

\[
h_{r,s} = h_{p'-r,p-s} = \frac{(rp - sp')^2 - (p - p')^2}{4pp'}
\]

\[
\bar{h}_{r',s'} = \bar{h}_{p'-r',p-s'} = \frac{(r'p - s'p')^2 - (p - p')^2}{4pp'}.
\]

Here, \( s, r, s', r' \) are integers satisfying: \( 1 \leq r, r' \leq p' - 1 \) and \( 1 \leq s, s' \leq p - 1 \). When \(|p - p'| > 1\), the associated conformal minimal model is non-unitary.

The YLSs are described by non-unitary CFTs, because they occur at complex values of magnetic fields. These singularities are associated with non-Hermitian transfer matrices. For this reason, we assumed that the Yang-Lee edge singularity of the 2D 3-state Potts model would be described by a conformal minimal model in which \(|p - p'| > 1\).

Since we expected that the YLS of the 2D 3-state Potts model would be described by a relatively simple CFT, we searched for candidate CFTs among conformal minimal models with small values of \( p \) and \( p' \).

The conformal minimal models are described by the ADE classification. The ADE classification lists the sets of \((h_{r,s}, \bar{h}_{r',s'})\) of the conformal minimal models as being in an \((A_{p'-1}, A_{p-1})\) series; two \((D_{p'/2+1}, A_{p-1})\) series; and a \((E_n, A_{p-1})\) series [8]. For each series, the ADE classification provides the primary field content. The simplest models of the \((A_{p'-1}, A_{p-1})\) and \((D_{p'/2+1}, A_{p-1})\) series are listed in Table 1.

| \((p', p)\) | Central Charge | Unitary | Comments |
|-------------|----------------|---------|----------|
| \((3, 2)\)  | 0              | Yes     | Trivial - not candidate |
| \((4, 3)\)  | 1/2            | Yes     | Standard critical point of Ising |
| \((5, 2)\)  | -22/5          | No      | \((A_4, A_1)\), Ising Yang-Lee singularity - candidate |
| \((3, 3)\)  | -3/5           | No      | \((A_4, A_2)\) - candidate |
| \((5, 4)\)  | 7/10           | Yes     | \((A_4, A_3)\) Standard critical point of tricritical Ising |
|             |                |         | First \((D_{1+p'/2}, A_{p-1})\) series, \(p'/2\) odd |
| \((6, 5)\)  | 4/5            | Yes     | Standard critical point of 3-state Potts |
| \((10, 3)\) | -44/5          | No      | \((D_6, A_2)\) - candidate |
| \((10, 7)\) | 8/35           | No      | \((D_6, A_0)\) - candidate |
| \((10, 9)\) | 14/15          | Yes     | Unitary - not a candidate |
|             |                |         | Second \((D_{1+p'/2}, A_{p-1})\) series, \(p'/2\) even |
| \((8, 3)\)  | -21/4          | No      | \((D_6, A_2)\) - candidate |
| \((8, 5)\)  | -7/20          | No      | \((D_6, A_4)\) - candidate |
| \((8, 7)\)  | 25/28          | Yes     | Unitary - not candidate |
|             | \((E_n, A_{p-1})\) series |

In Table 1, non-unitary models are candidates for the YLS of the 2D 3-state Potts model [13]. Among these models, we did not expect the complex \((E_n, A_p)\) models to describe the YLS of the simple 2D 3-state Potts model. Thus, we took as candidates the \((A_4, A_1)\), \((A_4, A_2)\), \((D_6, A_2)\), \((D_6, A_0)\), \((D_5, A_2)\), and \((D_5, A_4)\) conformal minimal models.

### 4. Finite-size Scaling at the YLS

The phenomenological renormalization group (PRG) and finite-size scaling enabled our numerical study of YLSs. In particular, we studied scaling in the length, \(N\), of the quantum
spin chain. In such scaling, the correlation length varies linearly with the length, $N$. The PRG fixes imposes such scaling via the energy gap and the equation [19, 10]:

$$(N - 1)m(B_{YL}(N), N - 1) =Nm(B_{YL}(N), N).$$ \hspace{1cm} (6)

The energy gap, $m(B, N)$, is defined by $m(B, N) = |E_1(B, N) - E_0(B, N)|$, where $E_0(B, N)$ and $E_1(B, N)$ are energies of the ground state and first excited state of the quantum spin chain.

The PRG equation relates energy gaps of quantum spin chains of lengths $N$ and $N - 1$ at a critical field, $B_{YL}(N)$. Thus, the PRG equation fixes the critical value of the magnetic field, $B_{YL}(N)$, for each chain length, $N$. The complex solutions for $B_{YL}(N)$ scale towards to YLS.

At these critical field values, CFT predicts how excitation energies of the quantum spin chain scale. For a state “i” of the quantum spin chain, CFT predicts [20] that $E_i(N) - E_0(N)$, will scale as:

$$E_i(N) - E_0(N) = \frac{\zeta 2\pi h_i + \bar{h}_i - (h + \bar{h})}{N}. \hspace{1cm} (7)$$

Above, $h_i$ and $\bar{h}_i$ are the dimensions of primary fields, and $h$ and $\bar{h}$ are the dimensions of the primary field of lowest dimension. The constant $\zeta$ is a non-universal and depends on a normalization.

For each candidate CFT, the low-lying excitation spectrum is from the associated partition function. For each low-lying state “i”, Table 2 lists the ratio of the excitation energy of state “i” over the excitation energy of the lowest excited state “1”. That is, excitation energies are normalized with respect to the lowest excitation. The excitation energies of Table 2 are directly measurable via finite-size scaling at the $B_{YL}(N)$’s, of Eq. (6).

The critical field values, $B_{YL}(N)$, approach a limit, $B_{YL}(\infty)$, as the length, $N$, of the quantum spin chain becomes large. At $B_{YL}(N)$, derivatives of the energy gap, $m(B, N)$, provide estimates, $\nu(N)$, of the exponent $\nu$ that defines the scaling behavior of the spin-spin correlation $\xi$ as [19, 10]:

$$1/\nu(N) = \frac{\log|m'(B, N)/m'(B, N - 1)||_{B=B_{YL}(N)}}{\log[N/(N - 1)]} + 1.$$ \hspace{1cm} (8)

Here, $m'(B, N) = \frac{dm(B, N)}{dB}$. The estimates, $\nu(N)$, converge to $\nu$ as $N \to \infty$.

5. Numerical methods

The measurements of the critical magnetic fields, $B_{YL}(N)$, were obtained by numerically solving PRG Eq.(6) for quantum spin chains of different lengths. For the numerical solutions, the Lanczos algorithm determined the energies of the quantum Ising and Potts chains [15]. Then, the critical field values $B_{YL}$’s were used to find the low-lying excitation spectra of Ising and 3-state Potts quantum spin chains of various lengths.

While Lanczos can provide the low-lying excitation spectra, it is inconvenient for determining the complete spectrum. In particular, an evaluation of the complete low-lying excitation
spectrum via the Lanczos algorithm would require finding a first Krylov space and then, finding other Krylov spaces orthogonal to the first space. To avoid such numerical complications, we used a commercial package of Maple\textsuperscript{TM} 9.5 to generate spectra based on previously determined values of the critical magnetic field. The measured excitation energies have been normalized by a division by the lowest excitation energy as already described to remove dependence on the non-universal constant $\zeta$ of Eq. (7).

6. Ising YLS
For the Ising quantum spin chain, we numerically evaluated the critical field, $B_{YL}(N)$, for $t = 0.1$ and various values of $N$ and then, numerically evaluated the complete low-lying excitation spectra as shown in Table 3 [17].

| State/| Degeneracy | $N = 6$ | $N = 7$ | $N = 8$ | $N = 9$ | $N = 10$ | $N = 11$ | $N = 12$ |
|-------|------------|--------|--------|--------|--------|--------|--------|--------|
| A/2   |            | 2.68432| 2.64386| 2.61415| 2.59207| 2.57540| 2.56260| 2.55253 |
| B/1   |            | 4.18193| 4.27896| 4.36713| 4.44474| 4.51197| 4.56977| 4.61912 |
| C/2   |            | 4.51738| 4.63236| 4.70368| 4.75182| 4.78652| 4.81281| 4.83329 |
| D/2   |            | 5.85889| 5.92080| 5.91240| 5.92644| 5.93703| 5.94544| 5.95210 |
| E/2   |            |        | 5.68559| 6.03104| 6.27270| 6.45018| 6.58573| 6.69223 |
| F/2   |            |        |        | 6.24252| 6.35798| 6.46344| 6.55966| 6.64694| 6.72535 |

We used a Bulirsch and Stoer (BST) algorithm[16] to extrapolate energies of state types A – F as $1/N \to 0$. The BST analysis indicated that the normalized energies of states of types A, B, C, D, E, and F scale to 2.4995(5), 5.005(1), 5.003(3), 5.99(1), 7.54(8), and 7.60(7), respectively.

| Normalized Energies | 0 | 1 | 2.5 | 5.0 | 6.0 | 7.5 |
|---------------------|---|---|-----|-----|-----|-----|
| Degeneracy          | 1 | 1 | 2   | 3   | 2   | 4   |

Table 3 shows the state sets A, B & C, D, and E & F, which have different normalized excitation energies as $1/N \to 0$ and their respective degeneracies of 2, 3, 2, and 4. Our numerical PRG measurements of excitation energies and associated degeneracies at the YLS of the Ising quantum spin chain are in excellent agreement with the normalized low-lying excitation spectrum of the $(A_4, A_1)$ CFT as shown in Table 4.

7. Potts YLS
For the three-state Potts quantum spin chain, we again numerically evaluated the critical field, $B_{YL}(N)$, for $t = 0.1$ and various values of $N$ and then, numerically evaluated the complete low-lying excitation spectra [18]. The low-lying excitation spectra is shown in Table 5.

From the spectra of Table 5, we determined how excitation energies of low-lying eigenstates scale with the chain length $N$. This determination requires identifying corresponding eigenstates in chains of different length, $N$. Our identification of eigenstate correspondences was based on two rules. The first rule was that the energies of corresponding eigenstates vary smoothly and monotonically with $N$. The second rule was that the correspondences of eigenstates for different $N$ should properly account for eigenstate degeneracies. In particular, old eigenstates do not disappear as $N$ increases. That is, degeneracies remain constant or increase with $N$. These rules identifying corresponding low-lying energy eigenstates for different chain length, $N$. 


Applying the above rules enables separating the low-lying eigenstates of Table 5 into sets A – F. Different ones of the sets A – F first appeared at different chain lengths, \(N\), as expected. For example, the set D first appeared in chains of length 4 whereas the set E first appeared in the chain of length 5.

The states of sets A – E are plotted as a function of \(1/N\) in Figures 1 – 4.  

CFT describes the excitation spectra near criticality or as \(1/N \to 0\). Thus, we extrapolated the excitation energies of the eigenstates in Figures 1 – 4 to \(1/N = 0\) to determine the low-lying excitation energies at the Yang-Lee edge singularity of the 2D 3-state Potts model. Referring to Figure 1, the doubly degenerate A eigenstates have energies that extrapolate towards about 2.5 as \(1/N \to 0\). Referring to Figure 2, both the doubly degenerate B eigenstates and single C eigenstate have energies that extrapolate to about 5.1 as \(1/N \to 0\). Referring to Figure 3, the doubly degenerate D eigenstates have energies that extrapolate to about 6.2 as \(1/N \to 0\). Finally, referring to Figure 4, the E eigenstates have energies that extrapolate to about 7.8 as \(1/N \to 0\). Thus, Figures 1 – 4 provide an observed low-lying excitation spectra of \(\{1, 2.5, 5, 6, 7.5\}\). These results are in very good agreement with the values \(\{1, 2.5, 5.1, 6.2, 7.8\}\) as predicted for the excitation spectrum of the \((A_4, A_1)\) minimal CFT of Table 4. Also, Figures 1 – 4 show

\[\begin{array}{cccccccccc}
N = 4 & g & s & N = 5 & g & s & N = 6 & g & s & N = 7 & g & s & N = 8 & g & s \\
2.26083 & 2 & A & 2.32641 & 2 & A & 2.36741 & 2 & A & 2.39452 & 2 & A & 2.41354 & 2 & A \\
3.06697 & 1 & B & 3.56700 & 2 & B & 3.88032 & 2 & B & 4.09253 & 2 & B & 4.24476 & 2 & B \\
4.56147 & 1 & C & 4.68089 & 1 & C & 4.8630 & 1 & F & 4.81263 & 1 & C & 4.84954 & 1 & C \\
5.03441 & 1 & D & 5.47927 & 2 & D & 4.75981 & 1 & C & 4.94654 & 2 & F & 5.35160 & 2 & F \\
5.94491 & 1 & 6.30921 & 2 & E & 5.66128 & 2 & D & 5.76468 & 2 & D & 5.72334 & 1 \\
5.94494 & 2 & 7.20262 & 2 & 6.59225 & 2 & E & 6.78325 & 2 & E & 5.82923 & 2 & D \\
\end{array}\]

Figure 1. Measured energies of type A states as a function of number of sites, \(N\).
that degeneracies of these same excitation states are (1, 2, 3, 2, ?),\(^3\) which also agrees with the degeneracies of the \((A_4, A_1)\) minimal CFT.

Thus, both degeneracies and energies of the low-lying excitation spectrum at the Yang-Lee edge singularity of the 3-state Potts model agree with those of the \((A_4, A_1)\) minimal CFT. No other candidate minimal CFTs of Table 2 has a low-lying excitation spectra that agrees with the finite-size scaling spectrum that we measured at the YLS of the 2D 3-state Potts model.

Finally, we also found the exponent, \(\nu\), at the YLS of 3-state Potts model by solving Eq. (8). For \(N = 5, 6,\) and 7, our estimates of \(\nu(N)\) are 0.4105, 0.4123, and 0.4134, respectively. These estimates vary due to finite-size corrections to Eq. (8). An extrapolation of the measured\(^3\) The observed degeneracy of the states of energy 7.5 is indicated as unknown, because our measurements were not to high enough chain lengths and energies to determine this degeneracy.

---

\(^3\) The observed degeneracy of the states of energy 7.5 is indicated as unknown, because our measurements were not to high enough chain lengths and energies to determine this degeneracy.
Figure 4. Measured energies of type E states as a function of number of sites, $N$.

$\nu(N)$’s to $1/N = 0$ provides the best estimate of the measured value for $\nu$. We used a BST algorithm to perform the extrapolation. The BST algorithm predicted that the $\nu(N)$’s converge to a value in the interval [0.417, 0.418] as $1/N \rightarrow 0$. This result also agrees very well with the $\nu$ of 5/16, i.e., 0.4167, in the $(A_4, A_1)$ minimal CFT.

8. Conclusions

Our finite-size scaling measurements of the low-lying excitation spectra and the exponent $\nu$ show that the YLS of the 2D 3-state Potts and Ising models are described by the $(A_4, A_1)$ conformal minimal model. In particular, both 2D discrete spin models have Yang-Lee singularities in the same universality class.

References

[1] Yang C N and Lee T D 1952 Phys. Rev. 87 404
[2] Yang C N and Lee T D 1952 Phys. Rev. 87 410
[3] Fisher M E 1978 Phys. Rev. Lett. 40 1610
[4] Ch. Binek 1998 Phys. Rev. Lett. 81 5644; Ch. Binek, W. Kleemann, and H. A. Katori 2001 J. Phys. B13 L811
[5] Cardy J L 1985 Phys. Rev. Lett. 54 1354
[6] Belavin AA, Polyakov AM, and Zamolodchikov AB 1984 Nucl. Phys. B 241 333
[7] Friedan D, Qiu Z and Shenker S 1984 Phys. Rev. Lett. 52 1575; 1986 Comm. Math. Phys. 107 535; 1985 Phys. Lett. B 151 37
[8] Cappelli A, Itzykson C, Zuber J-B 1987 Nucl. Phys. B 280 445; 1987 Comm. Math. Phys. 113 1; Kato A 1987 Mod. Phys. Lett. A 2 585; for a review see e.g., Itzykson C and Drouffe J-M 1989 Statistical Field Theory (Cambridge University ) chapter IX, table II
[9] Uzelac K and Jullien R 1981 J. Phys. A 14 L151
[10] Itzykson C, Saleur H, and Zuber J-B 1986 Europhys. Lett. 2 91
[11] Fisher M E and Barber M N 1972 Phys. Rev. Lett. 28 1516; for a brief review see, e.g., Henkel M 1999 Conformal Invariance and Critical Phenomena(Springer-Verlag) chapter 3
[12] Fradkin E and Susskind L 1978 Phys. Rev. D 17 2637; Suzuki M 1971 Prog. Theor. Phys. 46 1337; for a review see e.g., Henkel M 1999 Conformal Invariance and Critical Phenomena (Springer-Verlag ) chapters 8-10
[13] McCabe J and Wydro T 2003 in Proc. of the 7th Int. School on Theoretical Physics : Symmetry and Structural Properties of Condensed Matter (World Scientific) p 9
[14] von Gehlen G, Rittenberg V, and Vescan T 1987 J. Phys. A 20 2577
[15] For a review see e.g.: Parlett P N, *The Symmetric Eigenvalue Problem* (Prentice-Hall 1998) 261-321; Jennings A, *Matrix Computation for Engineers and Scientists* (Wiley 1977) 316-319; Kerner W 1989 *J. Comp. Phys.* **85** 1

[16] Burlisch M N and Stoer J 1964 *Numer. Math.* **6** 413

[17] J. McCabe and T. Wydro 2005 Preprint cond-mat/0510201 (submitted to *Int. Journ. of Mod. Physics B*)

[18] T. Wydro and J. McCabe 2005 *Int. Journ. of Mod. Physics B* **B 19** 3021

[19] Nightingale M P 1976 *Physica* **83A** 561; Derrida B and de Seze L 1982 *J. Physique* **43** 475; see, e.g., Nightingale M P 1990 *Finite Size Scaling and Numerical Simulation of Statistical Systems* (World Scientific) chapter VII

[20] Cardy J L 1984 *J. Phys. A* **17** L385