Exponents and Logarithms of the Potts Model
Through a 1D Quantum Hamiltonian

H.J. Herrmann
Institut für Theoretische Physik der Universität zu Köln,
Köln, Federal Republic of Germany

Received May 11, 1981

Exact solution of the one-dimensional quantum q-state Potts model for finite chains and subsequent finite-size analysis yields values for the thermal critical exponent \( y = 1/\nu \) for \( q = 3 \) and \( q = 4 \). By taking into account the shift of the critical point due to the finite size we obtain \( y = 1.48 \pm 0.01 \) for \( q = 4 \) in good agreement with the \( y = \frac{3}{2} \) conjectured by den Nijs. Using the conjecture of den Nijs we find evidence for a logarithmic factor for \( q = 4 \) but not for \( q = 3 \).

1. Introduction

The two-dimensional \( q \)-state Potts model [1] has recently been of growing interest. It describes a system – in our case on a square lattice with periodic boundary conditions – with variables \( \sigma_i = 1, \ldots, q \) behaving according to the Hamiltonian

\[
-H = \sum_{\langle i,j \rangle} \delta_{\sigma_i \sigma_j}, \tag{1}
\]

Baxter [2] has shown exactly that for \( q \leq 4 \) the phase transition of this model is of second order while for \( 4 < q \) it is of first order. But except for the Ising case \( q = 2 \) and presumably the case \( q = 3 \) [3] no exact temperature exponent \( y = 1/\nu \) is known. Den Nijs [4] conjectured the relationship

\[
(y - 3)(y_{\delta v} - 2) = 3 \tag{2}
\]

between the exponent \( y \) of the Potts model for \( q \leq 4 \) and the exactly known exponent of the 8-vertex model \( y_{\delta v} = \frac{2}{\pi} \arccos \frac{\sqrt{q}}{2} \) [5].

This conjecture is in very good agreement with the numerical results for \( q \leq 3 \). But for \( q = 4 \) no numerical study on the pure Potts model has yet yielded the value \( y = 1.5 \) predicted by (2). The results for \( y \) of the numerical calculations for \( q = 4 \) are: series expansions \( 1.29 \pm 0.02 \) [6] and \( 1.33 \pm 0.05 \) [7], Kadanoff variational renormalization group (RG): 1.323 [8], quantum hamiltonian RG: 1.3219 [9], phenomenological RG: 1.365 [10], Monte Carlo RG: 1.34 [11] and cumulant and variational RG: 1.218 [12].

The failure to get the conjectured value by RG calculations is usually explained by marginality effects which can be seen in extensions of the Potts model [13, 14]. This marginal behaviour produces logarithmic factors in the singularity [15] which makes the evaluation of series expansions difficult. To conclusively test den Nijs’ conjecture for \( q = 4 \) it is thus of great interest to look for a numerical method which is not as sensitive to the above mentioned effects as the methods used.

Such a method may be the solution on finite chains of the one-dimensional quantum hamiltonian which can be obtained from the two-dimensional Potts model. Subsequently a careful finite-size analysis should be performed.

In Sect. 2 we present the quantum Potts hamiltonian and the method for solving it on chains of up to 10 sites for \( q = 3 \) and up to 8 sites for \( q = 4 \). In Sect. 3
we present the results and apply finite-size-scaling
taking into account the shift of the critical tempera-
ture in order to perform a well-founded extrapola-
tion to the thermodynamic limit. Using the values of
y conjectured by den Nijs, logarithmic factors and
corrections to scaling are obtained for $q = 4$.

2. Solution of the Quantum Potts Hamiltonian
on Finite Chains

Let us consider the anisotropic Potts model

$$
-\beta H = \sum_{\langle \sigma, \tau \rangle} (J_\| \delta_{\sigma, \tau} + J_\perp \delta_{\sigma, \tau})
$$

with the coupling constants $J_\|$ on horizontal bonds
and $J_\perp$ on vertical bonds. Mitig and Stephen [16]
have shown for the transfer matrix $T$ that:

$$
T \propto e^{J_{\|} \sum_{n=1}^{N} \lambda_{n} + J_{\perp} \sum_{i=1}^{4} t_{i}^{n}}
$$

$K_{\perp}$ being the dual coupling constant

$$
e^{K_{\perp}} = \frac{1 + (q-1) e^{-J_{\perp}}}{1 - e^{-J_{\perp}}}
$$

and

$$
t_{n} = \begin{pmatrix}
0 & 1 & \ldots & 0 \\
0 & 1 & \ldots & 1 \\
1 & 0 & \ldots & 0
\end{pmatrix}
$$

a $q \times q$ matrix at site $n$. The phase transition takes
place at $\lambda = \lambda_c = 1$ with $\lambda = K_{\perp} J_{\perp}$.

It can be seen that for a 1D quantum hamiltonian
$\beta \mathcal{H}$ fulfilling $T \propto \exp(-\beta \mathcal{H})$ the
groundstate energy density is proportional to the free energy density $f$ of
(3) and that its energy gap is proportional to the
reciprocal $v_{c}^{-1}$ of the correlation length of (3) (see
e.g. [17]). If we take the limit $J_{\|} \to 0$ and $J_{\perp} \to \infty$ with
$\lambda$ fixed the commutators vanish when we apply
the Baker-Hausdorff formula to (4) and we obtain

$$
\beta \mathcal{H} = -J_{\|} \left[ \sum_{n=1}^{N} \delta_{\sigma, \tau_{n+1}} + \sum_{n=1}^{q-1} \sum_{i=1}^{4} \lambda_{n}^{i} \right].
$$

With the unitary transformation of states [18]

$$
|k\rangle = \frac{1}{\sqrt{q}} \sum_{l=1}^{q} e^{2\pi i (l-1) k} |l\rangle, \quad k = 1, \ldots, q
$$

one obtains the more convenient form

$$
\beta \mathcal{H} = \frac{1}{q} \hat{H} - \frac{1}{q} \sum_{n=1}^{N} \mathbf{1}
$$

with

$$
\hat{H} = -\sum_{n=1}^{N} \sum_{k=1}^{q-1} t_{n}^{k} e^{2\pi i k} - \lambda \sum_{n=1}^{q-1} u_{n}
$$

and the $q \times q$ matrix at site $n$

$$
u_{n} = \begin{pmatrix}
q & 1 & \ldots & 0 \\
1 & 1 & \ldots & 0 \\
0 & 0 & \ldots & 1
\end{pmatrix}
$$

As the second term in (8) is only a constant ($\mathbf{1}$ is the
unity operator), we shall in the following consider
only $\hat{H}$. As we are going to calculate critical
exponents by suitable plots it is sometimes important
to take a physical coupling constant. Therefore we
will often consider $J$ defined through

$$
\lambda = \frac{1}{J} \ln \left( \frac{1 + (q-1) e^{-J}}{1 - e^{-J}} \right)
$$

instead of $\lambda$.

The next step is to solve $\hat{H}$ on finite chains. As we
are only interested in the groundstate energy and the
energy gap it suffices to calculate the two lowest
lying energy levels of $\hat{H}$. For a chain of length $N$
the $q^{N} \times q^{N}$ matrix of $\hat{H}$ separates into $q$
blocks because of the suitable choice of representation (7).
All off-diagonal elements are equal to $-1$. A further separation
into smaller blocks could be possible by taking into account the translational and reflexion symmetries of the (closed) chain. But in that case off-diagonal elements with different values would arise and then the algorithm we will actually use would not work. Thus we shall not take into account those symmetries.

The smallest eigenvalues of the matrix were calculated
by a method due to Lanczos [19]: Let $\lambda_{1}$ and $e_{1}$
be the eigenvalues and eigenvectors of the matrix $A$
with $|\lambda_{1}| > |\lambda_{2}| > \ldots$ and $u$ an arbitrary vector – a
good choice for $u$ is the normalized vector of the
diagonal elements $d_{1}$ of $A$. With

$$
\lambda_{1}^{(n)} = \frac{|A^{n} u|}{|A^{n-1} u|} \quad \text{and} \quad e_{1}^{(n)} = \frac{A^{n} u}{|A^{n} u|}
$$

we have $\lambda = \lim_{n \to \infty} \lambda_{1}^{(n)}$ and therefore $\lambda_{1}^{(n)}$ is an approximation for $\lambda_{1}$ for large $n$. $|e_{1}^{(n)} - e_{1}^{(n-1)}|$ is a measure for the accuracy of this approximation. $\lambda_{2}$ could now be calculated by making the same procedure in the vectorspace orthogonal to $e_{1}^{(n)}$. (We found that the smallest eigenvalues of our matrix have the largest absolute values and the smallest and second smallest eigenvalues are in different blocks, so that it suffices to perform only the calculation of $\lambda_{1}$.)
To obtain the product
\[ y = A x \]  
(11)
we use the following method saving computation time and memory space: Considering the distribution of the off-diagonal elements of \( A \) a listing vector \( l_i \) for the \( i \)-th row can be generated by a quick algorithm. This listing vector contains the indices of the \( 2N \) columns of \( A \) for which the off-diagonal elements are not zero, i.e. \(-1\). Thus the \( i \)-th component of (11) is
\[ y_i = d_i x_i - \sum_{j=1}^{2N} x_{ij}. \]  
(12)
With this method we can calculate the smallest eigenvalue of a 20,000 \times 20,000 matrix to a precision of \(10^{-6}\) in 200 s on a CDC Cyber 76 computer. For such a precision 60 to 120 iterations are necessary.

### 3. Results and Finite-Size Scaling

For the infinite system the energy gap
\[ \Delta = \hat{E}_0 - \hat{E}_1 \]  
(13)
of \( \hat{H} \) is expected to behave as
\[ \Delta \propto \xi^{-1} \propto (\lambda - 1)^v \]  
(14)
close to \( \lambda_c = 1 \) with \( v = y^{-1} \).
For a finite system (14) is smeared out at \( \lambda_c \) as is shown in Fig. 1 for \( q = 4 \). If we determine \( v \) by a log-log plot this smearing out produces a deviation from the linear behaviour near the critical point. This can be seen in Fig. 2 where the ‘physical’ energy gap
\[ \Delta = \frac{J}{q} \]  
(15)
(see (8)) is plotted versus \( J_c - J \) from (10) over three decades for \( q = 3 \) and \( q = 4 \). Far away from \( J_c \) the relation (14) is not valid anymore and at \( J = 0, \Delta \) goes to infinity. To estimate this deviation at small \( J, \Delta \) divided through its high-temperature limit \( q \lambda \) is also plotted in Fig. 2. We see that the regions where the finite size becomes important and where the high-temperature effects dominate nearly overlap and thus the linear region is so small that \( v \) cannot be extracted reliably. The conjecture of den Nijs (2), i.e. \( v = \frac{3}{2} \) for \( q = 3 \) and \( v = \frac{4}{2} \) for \( q = 4 \), is also plotted in Fig. 2 and is seen to be consistent with our slopes.

To obtain accurate values for \( v \) in spite of the strong finite-size effects seen in Fig. 2 we use a scaling hypothesis due to Fisher and Barber [20] (see also [21]): If for the infinite system a thermodynamic function \( \Psi \) obeys the law
\[ \Psi(J) \propto (J - J_c)^v \]  
(16)
at \( J_c \), finite-size scaling asserts that for a system of length \( N \) the function should behave like
\[ \Psi_N(J) \propto N^{-\frac{2}{v}} g_\Psi(N^{\frac{1}{v}}(J - J_c)) \]  
(17)
with a scaling function \( g_\Psi \). Particularly we have
\[ \Psi_N(J_c) \propto N^{-\frac{2}{v}} \]  
(18)
and

$$\frac{\partial \psi_N}{\partial J} \bigg|_{J=J_c} \propto N^{\frac{1-\zeta}{\nu}}. \quad (19)$$

Application of (18) to the groundstate energy density $\varepsilon_0$ and the energy gap $\Delta$ yields

$$\varepsilon_0(J_c) \propto f(J_c) \propto N^{-2} \quad \text{and} \quad \Delta(J_c) \propto N^{-1}. \quad (20)$$

In Fig. 3 $\varepsilon_0(J_c)$ and $\Delta(J_c)$ are plotted for $q=3$ and $q=4$. One sees that the relationships (20) are fulfilled very well for $N \geq 5$. Therefore we conclude that finite-size scaling is valid for these $N$. As expected the energy gap vanishes in the extrapolation to the infinite system.

To get $\nu$ we combine (15) and (19) and obtain with (10) and the chain rule:

$$\Delta - 2 \left. \frac{d\Delta}{d\lambda} \right|_{\lambda=1} \propto N^{\frac{1-\zeta}{\nu}} = N^{\nu-1}. \quad (21)$$

The same expression is used by Roo many et al. [21] who were not able to explain where it comes from. We see that the deeper reason for the validity of (21) is the use of a 'physical' energy gap $\Delta$ and a 'physical' coupling constant $J$. Considering pairs of different lattice sizes we determine an effective $\nu$ from (21) with our data. The result is plotted in Fig. 4 for $q=3$ and $q=4$. The values are compared with those obtained by Nightingale et al. [22] with the phenomenological renormalization method. As this method also uses the transfer matrices for finite strips - although not in the anisotropic limit - similarities to our result are to be expected. From Fig. 4 we see that den Nijs' conjecture is confirmed quite well for $q=3$. But for $q=4$ an approximation to the conjectured value $\nu=1.5$ is not at all obvious. This fact could probably be explained with logarithmic corrections to the singularity because in that case (17) and (21) would be changed. But even without considering a logarithmic behaviour the situation for $q=4$ can be understood. This will be presented next.

It was somewhat arbitrary to plot $\psi_N$ linearly versus $N$ in Fig. 4 and it is not obvious how this plot should extrapolate to the large $N$ limit. We now want to present a phenomenological argument for a natural extrapolation to the infinite system. From Fig. 3 we concluded that finite-size-scaling is valid for $N \geq 5$. Nevertheless the exponent varies for these $N$. We assume that this variation comes from the shift of the critical point in a finite system:

Let $z_N$ be the effective exponent which one obtains for a function $\Psi$ in the system of length $N$:

$$\psi_N \propto (T - T_N)^{z_N}. \quad (22)$$
The function $\Psi_N$ is centered around $T_c$, which deviates from $T_c$ in most cases [23] as:

$$T_N - T_c = c N^{-1/\nu_N}$$  \hspace{1cm} (23)

$c$ being a constant. In the limit $N \to \infty$ (23) becomes

$$\Psi \propto (T - T_c)\nu.$$  \hspace{1cm} (24)

Let $T_0$ be the point where the curves of $\Psi_N$ and $\Psi$ cross (or, alternatively, take $T_1$ where the curves have a ratio of 1:2). Then according to finite-size scaling $T_0$ should go to $T_c$ as

$$T_0 - T_c = d N^{-1/\nu_N}$$  \hspace{1cm} (25)

with a constant $d$. Inserting this in (22) and (24) one obtains

$$((d - c) N^{-1/\nu_N})^\nu = (d N^{-1/\nu_N})^\nu$$

and therefore

$$az_N + b = \frac{z - z_N}{N} \ln N,$$  \hspace{1cm} (26)

$a$ and $b$ being constants. For the temperature exponent, (26) becomes

$$a y_N + b = y_N(y - y_N) \ln N.$$  \hspace{1cm} (27)

For $N \to \infty$ this is a series expansion of $y_N - y$ in powers of $\frac{1}{\ln N}$ which in first order gives the formula of Reynolds et al. [24] and in second order the parabola of Eschbach et al. [11].

Taking the correct value $y$ for the infinite system a plot of $y_N(y_N - y) \ln N$ versus $y_N$ should give a straight line according to (27). This was e.g. confirmed for the Monte Carlo data of [11] in the percolation case. In Fig. 5 this plot is shown for $q = 4$ for different $y_N$. One can see that the values for $5 \leq N \leq 8$ the conjectured $y = 1.5$ gives the best straight line. It should be noted that the accuracy of the points is $10^{-6}$.

Equation (27) can also be evaluated exactly by minimizing the squared deviation of the straight line with respect to $a$, $b$, and $y$. One then obtains for the best $y$:

$$y = \frac{\alpha^2 (c_{1,1} c_{2,1} - 4 c_{3,2})}{4 \alpha^2 + \alpha^2 (c_{1,1}^2 + 4 c_{2,2})}$$  \hspace{1cm} (28)

with $\alpha = c_{2,0} - \frac{c_{1,0}^2}{4}$, $\gamma = c_{2,1} - \frac{c_{1,1} c_{1,0}}{4}$ and $c_{ij} = \sum_{N} y_N^i \ln^j N$.

For $5 \leq N \leq 8$ this yields:

$$y = 1.48.$$  \hspace{1cm} (29)

As very similar numbers are subtracted several times from each other in (28), much precision is lost and in (29) a rounding error of 0.01 arises.

Now we will analyse our data for logarithmic corrections. A logarithmic factor of the form

$$\xi \propto (T - T_c)^{-\nu} \ln^\nu(T - T_c)$$  \hspace{1cm} (30)

as proposed by Nauenberg and Scalapino [15] for $q = 4$ changes (21) in

$$\Delta = -2 \frac{d \Delta}{d \lambda} \bigg|_{\lambda = 1} \propto N^{\nu - 1} \ln^{\nu - 1} N.$$  \hspace{1cm} (31)

Considering three values with different $N$ the exponents $y$ and $x/\nu$ are calculated with (31) and shown in Table 1 for $q = 3$ and $q = 4$. For $q = 3$ we see no approach to the conjectured $y = 1.2$ similar to that of Fig. 4. Thus if $y = 1.2$ is the correct value no logarithmic corrections are suggested by our data for $q = 3$. On the other hand for $q = 4$ the values for $y$ are improved very much towards the conjectured $y = 1.5$, suggesting the existence of a logarithmic factor. Although $x/\nu$ increases with $N$ for $q = 4$ it is still

<table>
<thead>
<tr>
<th>$N$</th>
<th>$q = 3$</th>
<th>$q = 4$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$y$</td>
<td>$x/\nu$</td>
</tr>
<tr>
<td>3, 4, 5</td>
<td>1.19958</td>
<td>0.04493</td>
</tr>
<tr>
<td>4, 5, 6</td>
<td>1.20511</td>
<td>0.05320</td>
</tr>
<tr>
<td>5, 6, 7</td>
<td>1.20829</td>
<td>0.05860</td>
</tr>
<tr>
<td>6, 7, 8</td>
<td>1.21022</td>
<td>0.06221</td>
</tr>
<tr>
<td>7, 8, 9</td>
<td>1.21144</td>
<td>0.06466</td>
</tr>
<tr>
<td>8, 9, 10</td>
<td>1.21213</td>
<td>0.06613</td>
</tr>
</tbody>
</table>
Table 2. Values of the exponent \( x/y \) for \( q = 3 \) and \( q = 4 \) and fixed \( y \)

<table>
<thead>
<tr>
<th>( N )</th>
<th>( q = 3, \ y = 1.2 )</th>
<th>( q = 4, \ y = 1.5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>3, 4</td>
<td>0.04545</td>
<td>0.26229</td>
</tr>
<tr>
<td>4, 5</td>
<td>0.04556</td>
<td>0.29654</td>
</tr>
<tr>
<td>5, 6</td>
<td>0.04452</td>
<td>0.32020</td>
</tr>
<tr>
<td>6, 7</td>
<td>0.04312</td>
<td>0.33785</td>
</tr>
<tr>
<td>7, 8</td>
<td>0.04165</td>
<td>0.35173</td>
</tr>
<tr>
<td>8, 9</td>
<td>0.04021</td>
<td></td>
</tr>
<tr>
<td>9, 10</td>
<td>0.03885</td>
<td></td>
</tr>
</tbody>
</table>

Table 3. Values of the exponents \( x/y \) and \( \omega \) for \( q = 4 \) and fixed \( y \).
Different lengths \( N \) of chains are taken into account for the fit

<table>
<thead>
<tr>
<th>( N )</th>
<th>( x/y )</th>
<th>( \omega )</th>
</tr>
</thead>
<tbody>
<tr>
<td>3, ..., 8</td>
<td>0.426</td>
<td>1.63</td>
</tr>
<tr>
<td>3, ..., 7</td>
<td>0.421</td>
<td>1.67</td>
</tr>
<tr>
<td>3, ..., 6</td>
<td>0.414</td>
<td>1.72</td>
</tr>
</tbody>
</table>

far away from the conjectured \( x/y = 3/2 \) [15]. As shown in Table 2 this can be improved if \( y \) is fixed at the value conjectured by den Nijs. We also see from Table 2 that \( x/y \) decreases for \( q = 3 \) and is smaller than in Table 1 suggesting it might be zero in the infinite system.

Finally we try to include corrections to scaling:

\[
\Delta - 2 \frac{dA}{dk} \bigg|_{k=1} \propto N^{-1}(1 + rN^{-\omega}) \tag{32}
\]

\( r \) being a constant and \( \omega \) the corrections to the scaling exponent. By fitting

\[
\ln \left( \frac{\Delta - 2 \frac{dA}{dk} \bigg|_{k=1}}{(y-1) \ln N + \frac{x}{y} \ln \ln N} \right) = (y-1) \ln N + \frac{x}{y} \ln \ln N \tag{33}
\]

as a linear function of \( N^{-\omega} \) [25] and assuming \( y = 1.5 \) we obtain for \( q = 4 \) the exponents shown in Table 3. (In order to estimate finite size effects to the fit we have included our data up to \( N = 8, 7 \) and 6, respectively.) We see that the exponents \( x/y \) obtained this way are larger than those of Table 2 and that they increase with \( N \). This gives more support to the conjecture of [15], as extrapolation to \( N \to \infty \) in Table 3 could give much larger values. The results for \( \omega \) decrease with \( N \) and a value around one as is usually expected is possible. For \( q = 3 \) the fit (33) gives no physically reasonable values for the exponents confirming our previous conclusion that a logarithmic factor should not be present for \( q = 3 \).

Summarizing we find that our calculation confirms the conjecture of den Nijs for \( q = 3 \) and \( q = 4 \) if in the latter case we take into account the shift of \( T_c \) for finite systems. Taking den Nijs’ conjecture for granted we find evidence that for \( q = 4 \) there is a logarithmic factor as postulated by Nauenberg and Scalapino while for \( q = 3 \) there is none. Taking corrections to scaling into account we feel that our present data do not exclude the postulated exponent \( x/y = 3/2 \) for \( q = 4 \). Larger systems need to be investigated to arrive at reliable conclusions about this detail.

I am grateful to Profs. E. Müller-Hartmann, D. Stauffer, and J. Zittartz for many useful discussions.

References


H.J. Herrmann
Institut für Theoretische Physik
Universität zu Köln
Zülpicher Strasse 77
D-5000 Köln 41
Federal Republic of Germany