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Logarithmic Corrections to Finite-Size Scaling in the Four-State Potts Model

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The leading corrections to finite-size scaling predictions for eigenvalues of the quantum Hamiltonian limit of the critical four-state Potts model are calculated analytically from the Bethe ansatz equations for equivalent eigenstates of a modified XXZ chain. Scaled gaps are found to behave for large chain length L as $x + d/\ln L + o[(\ln L)^{-1}]$, where x is the anomalous dimension of the associated primary scaling operator. For the gaps associated with the energy and magnetic operators, the values of the amplitudes d are in agreement with predictions of conformal invariance. The implications of these analytical results for the extrapolation of finite lattice data are discussed. Accurate estimates of x and d are found to be extremely difficult even with data available from large lattices, $L \sim 500$.

KEY WORDS: Finite-size scaling; Potts model; Bethe ansatz; conformal invariance.

1. INTRODUCTION

Despite considerable effort involving several techniques, numerical estimates of the critical exponents of the two-dimensional four-state Potts model have been poor. These failures are attributed to the onset of marginality effects in the q-state model at $q = q_c = 4$, resulting in logarithmic corrections to the critical behavior.[1,2] In the case of finite-size scaling, the leading logarithmic (in lattice size) corrections that occur in the eigenvalues of the transfer matrix at criticality have been calculated

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recently by Cardy[3] on the assumption of conformal invariance.[4] These results are of particular relevance to the extrapolation of finite lattice data by finite-size scaling.[5] To date, such data have been restricted to strips (chains) of width (length) $L_{\max} \leqslant 11$. Consequently, estimates of critical exponents have not been in close agreement with the expected values.[6-9]

If we write the transfer matrix as $T = e^{-aH}$, where a is the lattice spacing, then Cardy's results[3] for the energy levels E_α of H are, as $L \to \infty$,

$$E_\alpha - E_0 \sim \frac{2\pi\tau}{L}\left(x_\alpha + \frac{d_\alpha}{\ln L} + o[(\ln L)^{-1}]\right) \tag{1.1}$$

$$E_0 \sim e_\infty L - \frac{\pi\tau}{6L}\{c + O[(\ln L)^{-3}]\} \tag{1.2}$$

where e_∞ is the bulk ground state energy per site. Here $\{x_\alpha\}$ denote the dimensions of the primary scaling operators of the theory and c is the conformal anomaly. For the four-state Potts model, $c = 1$.[10] The amplitudes d_α can be expressed[3] in terms of operator expansion coefficients and should be universal. The inclusion of the factor τ allows these results to be extended[9] to $(1+1)$-dimensional quantum Hamiltonian formulations; τ ensures that the resulting equations of motion are conformally invariant. Similarly, in a transfer matrix formulation, τ can account for the effect of anisotropic interactions.[11]

Cardy[3] went on to show that the deviations observed in the (small) lattice data of Blöte and Nightingale[7] for the four-state Potts model were in qualitative agreement with (1.1) and (1.2). Recently, the available finite lattice data for the quantum Hamiltonian limit of the four-state Potts model have been extended considerably.[12,13] This extension was achieved by deriving an exact equivalence between eigenstates of the q-state quantum otts chain and those of a modified XXZ Heisenberg chain. The eigenvalues of this XXZ model on chains of up to 1024 sites could then be obtained by numerically solving Bethe-ansatz equations. Assuming a leading correction of the form (1.1), excellent agreement was obtained with the values $x_e = 1/2$ and $x_m = 1/8$ for the scaling dimensions of the energy density and magnetization operators. However, estimates of the amplitudes d_e and d_m were still only in rough agreement with Cardy's predictions of

$$d_e = 3/4, \qquad d_m = 1/16 \tag{1.3}$$

Since the equivalent XXZ model is solvable by the Bethe ansatz, it should be possible to compute *analytically* the leading finite-size corrections to the energy levels by the methods developed by de Vega,

[4] For a recent review of conformal invariance and its application to finite-size scaling, see ref. 4.

Woynarovich and Hamer.[14–16] Previously, this approach has led to exact calculations of the conformal anomaly, the surface energy, and several bulk and surface critical exponents of the *XXZ*, Potts, and Ashkin–Teller models.[15–20] In this paper, we continue this work and derive exact results for the amplitudes of the logarithmic corrections appearing in the four-state Potts model. These results are derived in Section 2 and gathered together in Section 3. Since Section 2 is rather technical, readers interested only in the results as they pertain to the Potts model may care to omit this section and turn directly to Section 3. To conclude the paper, we reexamine the large-lattice data of Alcaraz *et al.*[13] in Section 4.

2. ANALYTIC DERIVATION OF LOGARITHMIC CORRECTIONS TO FINITE-SIZE SCALING

2.1. General Formulas

We consider the Hamiltonian (case A of ref. 17)

$$H = -\frac{1}{2}\sum_{j=1}^{N} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z) \tag{2.1}$$

with $\Delta = -\cos\gamma$ and boundary conditions

$$\sigma_{N+1}^x \pm i\sigma_{N+1}^y = e^{i\Phi}(\sigma_1^x \pm i\sigma_1^y), \qquad \sigma_{N+1}^z = \sigma_1^z \tag{2.2}$$

in the limit $\gamma \to 0$. Since the total number m of down spins in the chain is conserved, it is convenient to label each spin sector by the number

$$n = \frac{1}{2}N - m \tag{2.3}$$

where we assume that N is even. The ground state lies in the sector $n = 0$, $m = N/2$.

The Bethe ansatz for the eigenstates of (2.1) has been discussed in detail elsewhere.[13,17] It involves[5] a momentum p_j for each down spin; but a convenient change of variables is

$$p = 2\tan^{-1}(2\lambda) \equiv \phi(\lambda), \qquad -\infty < \lambda < \infty \tag{2.4}$$

The boundary conditions (3.2) are satisfied if the λ_j obey the equations

$$N\phi(\lambda_j) = 2\pi I_j + \Phi + \sum_{l=1}^{m} \phi\left(\frac{\lambda_j - \lambda_l}{2}\right) \tag{2.5}$$

where the I_j are integers or half-integers.

[5] The results quoted here are obtained from those of ref. 17 by first rescaling variables and then taking the limit $\gamma \to 0$, as discussed in the Appendix.

Following de Vega and Woynarovich,[14] we define a function

$$z_N(\lambda)=\frac{1}{2\pi}\left[\phi(\lambda)-\frac{\Phi}{N}-\frac{1}{N}\sum_{j=1}^{m}\phi\left(\frac{\lambda-\lambda_j}{2}\right)\right] \tag{2.6}$$

and its derivative

$$\sigma_N(\lambda)=dz_N(\lambda)/d\lambda \tag{2.7}$$

so that

$$z_N(\lambda_j)=I_j/N \tag{2.8}$$

When N goes to infinity, the real roots λ_j of (2.5) tend to a continuous distribution with density $N\sigma_N(\lambda)$. The energy of the state specified by the set $\{\lambda_j\}$ of zeros is

$$E=\frac{1}{2}N-\sum_{j=1}^{m}\phi'(\lambda_j) \tag{2.9}$$

where the prime denotes differentiation with respect to λ.

The finite-size corrections to the root density are given by[14]

$$\begin{aligned}\sigma_N(\lambda)-\sigma_\infty(\lambda)= &-\frac{1}{\pi}\int_{-\infty}^{\infty}d\mu\ p(\lambda-\mu)\left[\frac{1}{N}\sum_{j=1}^{m}\delta(\mu-\lambda_j)-\sigma_N(\mu)\right]\\ &+\frac{1}{\pi N}\left[\sum_h p(\lambda-\lambda_h)-\sum_c p(\lambda-\lambda_c)\right]\end{aligned} \tag{2.10}$$

where the λ_c denote complex roots in the λ plane, the λ_h denote "holes" (i.e., unoccupied root positions on the real axis), and the λ_j run over *all* root positions on the real axis, including holes. The kernel $p(\lambda)$ is

$$p(\lambda)=\int_0^\infty dw\,\frac{\cos(\lambda w)}{1+e^w} \tag{2.11}$$

Finally, the finite-size corrections to the energy per site $e_N=E/N$ follow from

$$\begin{aligned}e_N-e_\infty= &-2\pi\int_{-\infty}^{\infty}d\lambda\,\sigma_\infty(\lambda)\left[\frac{1}{N}\sum_{j=1}^{m}\delta(\lambda-\lambda_j)-\sigma_N(\lambda)\right]\\ &-\frac{1}{N}\sum_c\left[\phi'(\lambda_c)-\frac{1}{\pi}\int_{-\infty}^{\infty}d\lambda\,\phi'(\lambda)\,p(\lambda-\lambda_c)\right]\\ &+\frac{2\pi}{N}\sum_h\sigma_\infty(\lambda_h)\end{aligned} \tag{2.12}$$

Applying the Euler–Maclaurin formula leads to[16,17]

$$\begin{aligned}
\sigma_N(\lambda)-\sigma_\infty(\lambda)=&\frac{1}{\pi}\int_{\Lambda_+}^{\infty} d\mu\,\sigma_N(\mu)\,p(\lambda-\mu)+\frac{1}{\pi}\int_{-\infty}^{-\Lambda_-} d\mu\,\sigma_N(\mu)\,p(\lambda-\mu)\\
&-\frac{p(\lambda-\Lambda_+)+p(\lambda+\Lambda_-)}{2N\pi}\\
&+\frac{1}{12N^2\pi}\left[\frac{p'(\lambda-\Lambda_+)}{\sigma_N(\Lambda_+)}-\frac{p'(\lambda+\Lambda_-)}{\sigma_N(-\Lambda_-)}\right]\\
&+\frac{1}{\pi N}\left[\sum_h p(\lambda-\lambda_h)-\sum_c p(\lambda-\lambda_c)\right]+O(N^{-4})
\end{aligned}\tag{2.13}$$

where Λ_+ $(-\Lambda_-)$ is the largest (smallest) root on the real axis. Similarly, the energy density is given by

$$\begin{aligned}
\frac{e_N-e_\infty}{2\pi}=&\int_{\Lambda_+}^{\infty} d\lambda\,\sigma_\infty(\lambda)\,\sigma_N(\lambda)+\int_{-\infty}^{-\Lambda} d\lambda\,\sigma_\infty(\lambda)\,\sigma_N(\lambda)\\
&-\frac{\sigma_\infty(-\Lambda_-)+\sigma_\infty(\Lambda_+)}{2N}+\frac{1}{12N^2}\left[\frac{\sigma'_\infty(-\Lambda_-)}{\sigma_N(-\Lambda_-)}-\frac{\sigma'_\infty(\Lambda_+)}{\sigma_N(\Lambda_+)}\right]\\
&-\frac{1}{2\pi N}\sum_c\left[\phi'(\lambda_c)-\frac{1}{\pi}\int_{-\infty}^{\infty} d\lambda\,\phi'(\lambda)\,p(\lambda-\lambda_c)\right]\\
&-\sum_h\sigma_\infty(\lambda_h)+O(N^{-4})
\end{aligned}\tag{2.14}$$

2.2. An Example of Logarithmic Corrections

Consider the ground state of the Hamiltonian (2.1) in spin sector n for the case $\Phi=0$. For this state it is known[21] that the roots are all real and are distributed symmetrically on the real axis, so that $\Lambda_+=\Lambda_-\equiv\Lambda$. The jth root corresponds to

$$I_j=-\frac{m+1}{2}+j,\qquad j=1,\ldots,m\tag{2.15}$$

There are no complex roots or holes (gaps in the distribution of real roots). Thus (2.13) and (2.14) reduce to

$$\begin{aligned}
\sigma_N(\lambda)-\sigma_\infty(\lambda)=&\frac{1}{\pi}\int_{\Lambda}^{\infty} d\mu\,\sigma_N(\mu)\,p(\lambda-\mu)-\frac{p(\lambda-\Lambda)}{2N\pi}+\frac{p'(\lambda-\Lambda)}{12N^2\pi\sigma_N(\Lambda)}\\
&+\frac{1}{\pi}\left\{\int_{-\infty}^{-\Lambda} d\mu\,\sigma_N(\mu)\,p(\lambda-\mu)-\frac{p(\lambda+\Lambda)}{2N}-\frac{p'(\lambda+\Lambda)}{12N^2\sigma_N(\Lambda)}\right\}\\
&+O(N^{-4})
\end{aligned}\tag{2.16}$$

and

$$\frac{e_N - e_\infty}{4\pi} = \int_\Lambda^\infty d\lambda\, \sigma_\infty(\lambda)\, \sigma_N(\lambda) - \frac{\sigma_\infty(\Lambda)}{2N} - \frac{\sigma'_\infty(\Lambda)}{12N^2\sigma_N(\Lambda)} + O(N^{-4}) \tag{2.17}$$

respectively. From Yang and Yang,[21] we know that

$$\sigma_\infty(\lambda) = \frac{1}{2\cosh(\pi\lambda)} \sim e^{-\pi\lambda} \qquad \text{as} \quad \lambda \to \infty \tag{2.18}$$

Hence, using the fact that

$$\int_{-\infty}^\infty \phi'(\lambda)\, d\lambda = 2\pi \tag{2.19}$$

one finds the sum rules for the root density[20]

$$\int_{-\infty}^\infty \sigma_N(\lambda)\, d\lambda = \frac{1}{2} + \frac{n}{N} \tag{2.20}$$

$$\int_\Lambda^\infty \sigma_N(\lambda)\, d\lambda = \frac{1}{2N}\,[1 + \beta(n)], \qquad \beta(n) = 2n \tag{2.21}$$

Now for $\lambda \geqslant \Lambda$, the terms in curly brackets in (2.16) are small, and may be neglected in determining the leading-order finite-size corrections as $N \to \infty$. Then Eq. (2.16) takes the form of a Wiener–Hopf equation, which can be solved[16,17] for the root density $\sigma_N(\lambda)$, subject to the constraint (2.21). The results of this exercise are summarized in the Appendix. Substituting the resulting expression for $\sigma_N(\lambda)$ in (2.17) gives[20]

$$e_N - e_\infty \sim -\frac{\pi^2}{6N^2}\left[1 - \frac{3}{2}\beta^2(n)\right] = -\frac{\pi^2}{6N^2}(1 - 6n^2), \qquad N \to \infty \tag{2.22}$$

The next (logarithmic) corrections to this result arise[17] from the bracketed terms in (2.16), which were neglected in the leading-order calculation. We assume that these terms give rise to small perturbations $\Lambda \to \Lambda + \delta\Lambda$, $\sigma_N(\lambda) \to \sigma_N(\lambda) + \delta\sigma_N(\lambda)$. The resulting first-order perturbation to (2.16) is (for $\lambda \geqslant \Lambda$)

$$\begin{aligned}
\delta\sigma_N(\lambda) = {} & \frac{1}{\pi}\int_\Lambda^\infty d\mu\, \delta\sigma_N(\mu)\, p(\lambda - \mu) - \frac{p'(\lambda - \Lambda)\, \delta\sigma_N(\Lambda)}{12N^2\pi\sigma_0^2} \\
& - \frac{\delta\Lambda}{\pi}\left[\sigma_0\, p(\lambda - \Lambda) - \frac{p'(\lambda - \Lambda)}{2N} + \frac{p''(\lambda - \Lambda}{12N^2\sigma_0} + \frac{\sigma'_N(\Lambda)\, p'(\lambda - \Lambda)}{12N^2\sigma_0^2}\right] \\
& + \frac{1}{\pi}\left\{\int_{-\infty}^{-\Lambda} d\mu\, \sigma_N(\mu)\, p(\lambda - \mu) - \frac{p(\lambda + \Lambda)}{2N} - \frac{p'(\lambda + \Lambda)}{12N^2\sigma_0}\right\}
\end{aligned} \tag{2.23}$$

where

$$\sigma_0 = \sigma_N(\Lambda) \tag{2.24}$$

The analogous first-order perturbation to (2.17) is

$$\begin{aligned}\delta(e_N - e_\infty) = 4\pi \int_\Lambda^\infty d\lambda\, \sigma_\infty(\lambda)\, \delta\sigma_N(\lambda) + \frac{\pi\sigma'_\infty(\Lambda)\,\delta\sigma_N(\Lambda)}{3N^2\sigma_0^2} \\ - 4\pi\,\delta\Lambda\left[\sigma_0\sigma_\infty(\Lambda) + \frac{\sigma'_\infty(\Lambda)}{2N} + \frac{\sigma''_\infty(\Lambda)}{12N^2\sigma_0} - \frac{\sigma'_\infty(\Lambda)\,\sigma'_N(\Lambda)}{12N^2\sigma_0^2}\right]\end{aligned} \tag{2.25}$$

Now, from (A.19) of the Appendix,

$$\Lambda \sim \frac{1}{\pi}\ln N, \qquad N \to \infty \tag{2.26}$$

and hence

$$\sigma_\infty(\Lambda) = e^{-\pi\Lambda} + O(N^{-3}) \tag{2.27}$$

so that (2.25) can be rewritten

$$\begin{aligned}\delta(e_N - e_\infty) = 4\pi e^{-\pi\Lambda}\left\{\int_\Lambda^\infty d\Lambda\, e^{-\pi(\lambda-\Lambda)}\,\delta\sigma_N(\lambda) - \frac{\pi\,\delta\sigma_N(\Lambda)}{12N^2\sigma_0^2}\right. \\ \left. - \delta\Lambda\left[\sigma_0 - \frac{\pi}{2N} + \frac{\pi^2}{12N^2\sigma_0} + \frac{\pi\sigma'_N(\Lambda)}{12N^2\sigma_0^2}\right]\right\}\end{aligned} \tag{2.28}$$

The constraint (2.21) gives rise to the relation

$$\delta\Lambda = \frac{1}{\sigma_0}\int_\Lambda^\infty \delta\sigma_N(\lambda)\, d\lambda \tag{2.29}$$

Since

$$p(\lambda) \sim \frac{1}{4\lambda^2}, \qquad \lambda \to \infty \tag{2.30}$$

the driving terms in curly brackets in (2.23) can be approximated for $\lambda \geqslant \Lambda$ as

$$\begin{aligned}&\int_{-\infty}^{-\Lambda} d\mu\, \sigma_N(\mu)\, p(\lambda-\mu) - \frac{p(\lambda+\Lambda)}{2N} - \frac{p'(\lambda+\Lambda)}{12N^2\sigma_0} \\ &\quad \simeq \frac{1}{4(\lambda+\Lambda)^2}\int_\Lambda^\infty d\mu\, \sigma_N(\mu) - \frac{1}{8N(\lambda+\Lambda)^2} \\ &\quad = \frac{\beta(n)}{8N(\lambda+\Lambda)^2} \qquad \text{for} \quad n \neq 0\end{aligned} \tag{2.31}$$

where we have used (2.21). With this approximation, (2.23) again has the form of a Wiener–Hopf equation with the same kernel as (2.16) and can be treated using the same methods. This hierarchical of the Wiener–Hopf equations for the root density is similar to that discussed by Yang and Yang.[21]

2.3. The Wiener–Hopf Equation

Using (2.31), we may rewrite (2.23) as

$$\chi(t) - \int_0^\infty k(t-s)\,\chi(s)\,ds$$

$$= f(t) - c_2 k'(t) - c_1\left[\sigma_0 k(t) - \frac{k'(t)}{2N} + \frac{k''(t)}{12N^2\sigma_0} + \frac{\sigma_0' k'(t)}{12N^2\sigma_0^2}\right] \tag{2.32}$$

where $t = \lambda - \Lambda$, $\sigma_0' = \sigma_N'(\Lambda)$, and we define

$$k(\lambda) = p(\lambda)/\pi \tag{2.33}$$

$$f(\lambda) = c_3/(2\Lambda + \lambda)^2 \tag{2.34}$$

$$\chi(\lambda) = \delta\sigma_N(\lambda + \Lambda) \tag{2.35}$$

with

$$c_1 = \frac{1}{\sigma_0}\int_\Lambda^\infty \delta\sigma_N(\lambda)\,d\lambda \tag{2.36}$$

$$c_2 = \frac{\delta\sigma_N(\Lambda)}{12N^2\sigma_0^2} \tag{2.37}$$

$$c_3 = \frac{\beta(n)}{8N\pi} \tag{2.38}$$

Define Fourier transform pairs $\chi \leftrightarrow X$, $f \leftrightarrow F$, $k \leftrightarrow K$ by

$$X(w) = \int_{-\infty}^\infty e^{iwt}\chi(t)\,dt; \qquad \chi(t) = \frac{1}{2\pi}\int_{-\infty}^\infty e^{-iwt}X(w)\,dw \tag{2.39}$$

etc. The kernel function $K(w)$ can be "factorized" in the form[17]

$$[1 - K(w)]^{-1} = G_+(w)\,G_-(w) \tag{2.40}$$

where the functions $G_\pm(w)$ are holomorphic and continuous in the upper and lower halves $\pi_\pm$ of the complex w plane, respectively. The functions

$X(w)$ and $F(w)$ may be split into $\pm$ components (holomorphic and continuous in $\pi_{\pm}$, respectively) by

$$X(w) = X_+(w) + X_-(w) \tag{2.41}$$

where

$$X_{\pm}(w) = \int_{-\infty}^{\infty} e^{iwt} H(\pm t)\,\lambda(t)\,dt \tag{2.42}$$

with $H(t)$ the Heaviside step function:

$$H(t) = \begin{cases} 1, & \text{if } t > 0 \\ 0, & \text{if } t < 0 \end{cases} \tag{2.43}$$

Fourier transforming (2.32) yields

$$\frac{X_+(w) - C(w)}{G_+(w)} + G_-(w)[X_-(w) + C(w) - F_-(w)] = G_-(w)\,F_+(w) \tag{2.44}$$

where

$$C(w) = c_1 \left[\sigma_0 + \frac{iw}{2N} - \frac{w^2}{12N^2\sigma_0} - \frac{iw\sigma_0'}{12N^2\sigma_0^2} \right] - iwc_2 \tag{2.45}$$

is an entire function. To separate out terms which are analytic in the two half-planes $\pi_{\pm}$, we further split

$$G_-(w)\,F_+(w) = Q_+(w) + Q_-(w) \tag{2.46}$$

Now define a function

$$P(w) = Q_-(w) - G_-(w)[X_-(w) + C(w) - F_-(w)], \qquad w \in \pi_- \tag{2.47}$$

$$= \frac{X_+(w) - C(w)}{G_+(w)} - Q_+(w), \qquad w \in \pi_+ \tag{2.48}$$

Since the expression in (2.48) is analytic in π_+, while that in (2.47) is analytic in π_-, (2.47) is the analytic continuation of (2.48) into π_-. Consequently, $P(w)$ is *entire* and can be determined from the asymptotic behavior of one of its defining expressions. Hence we may solve for $X_+(w)$ or $X_-(w)$.

Since $H(t)\,\chi(t)$ must be integrable at the origin, $X_+(w) \to 0$ as $|w| \to \infty$ in π_+. Also, we have (see below) $Q_+(w) \to 0$ and

$$G_+(w) \sim 1 + \frac{g_1}{w} + \frac{g_2}{w^2} + \frac{g_3}{w^3} + O(w^{-4}) \qquad \text{as} \quad |w| \to \infty \tag{2.49}$$

where, from (A.8) and (A.9) of the Appendix, $g_1 = i\pi/12$ and $g_2 = \frac{1}{2}g_1^2$. Hence

$$P(w) = \frac{c_1 w^2}{12N^2\sigma_0} + iw\left[c_2 - c_1\left(\frac{1}{2N} - \frac{\sigma_0'}{12N^2\sigma_0^2} - \frac{ig_1}{12N^2\sigma_0}\right)\right] - \left[ic_2 g_1 + c_1\left(\sigma_0 - \frac{ig_1}{2N} + \frac{ig_1\sigma_0'}{12N^2\sigma_0^2} - \frac{g_1^2}{24N^2\sigma_0}\right)\right] \quad (2.50)$$

Now from (2.34),

$$F_+(w) = c_3 \int_0^\infty dt \frac{e^{iwt}}{(2\Lambda + t)^2} = c_3\left\{\frac{1}{2\Lambda} + iwE_1(-2iw\Lambda)e^{-2iw\Lambda}\right\} \quad (2.51)$$

where $E_1(-2iw\Lambda)$ is the exponential integral function, with a cut along the negative imaginary axis in the w plane. Taking a Cauchy integral of $G_-(w)F_+(w)$ around this branch cut, we obtain

$$Q_+(w) = ic_3 \int_0^\infty dy \frac{G_+(iy)\, ye^{-2y\Lambda}}{w + iy} \quad (2.52)$$

Finally, from (2.48) and (2.47), one obtains the solution

$$X_+(w) = \int_0^\infty e^{iwt}\chi(t)\, dt = C(w) + G_+(w)[P(w) + Q_+(w)] \quad (2.53)$$

where the functions on the right-hand side are now known.

There are two self-consistency conditions which must be applied to this solution. First, from (2.36),

$$c_1\sigma_0 = \int_\Lambda^\infty \delta\sigma_N(\lambda)\, d\lambda = X_+(0) = c_1\sigma_0 + G_+(0)[P(0) + Q_+(0)] \quad (2.54)$$

Hence one finds

$$c_2 = \frac{1}{ig_1}\left[c_3\frac{G_+(0)}{2\Lambda} - c_1\frac{A}{N}\right] \quad (2.55)$$

where we have used the approximation

$$Q_+(0) = c_3\int_0^\infty dy\, G_+(iy)e^{-2y\Lambda} \sim c_3\frac{G_+(0)}{2\Lambda} \qquad \text{as} \quad \Lambda \to \infty \quad (2.56)$$

and defined

$$\frac{A}{N} = \sigma_0 - \frac{ig_1}{2N} + \frac{ig_1\sigma_0'}{12N^2\sigma_0^2} - \frac{g_1^2}{24N^2\sigma_0} \quad (2.57)$$

Second, from (2.37),

$$12N^2\sigma_0^2 c_2 = \chi(0) = 2\chi_+(0) = \frac{1}{\pi}\int_{-\infty}^{\infty} dw\, X_+(w) \tag{2.58}$$

which may be evaluated by contour integration. Now for large w

$$Q_+(w) \sim \frac{ic_3}{w}\int_0^\infty dy\, G_+(iy)\, ye^{-2y\Lambda} \sim \frac{ic_3 G_+(0)}{4w\Lambda^2} \qquad \text{as} \quad \Lambda \to +\infty \tag{2.59}$$

Hence

$$12N^2\sigma_0^2 c_2 = -\frac{g_1^2}{2}c_2 + c_1\left(ig_1\sigma_0 + \frac{g_1^2}{4N} - \frac{ig_3}{12N^2\sigma_0} - \frac{g_1^2\sigma_0'}{24N^2\sigma_0^2}\right) + c_3\frac{G_+(0)}{4\Lambda^2} \tag{2.60}$$

which together with (2.55) gives

$$c_1\frac{B}{N} = c_3\frac{G_+(0)}{2\Lambda}\left(\frac{12N^2\sigma_0^2}{ig_1} - \frac{ig_1}{2} - \frac{1}{2\Lambda}\right) \tag{2.61}$$

where we have defined

$$\frac{B}{N} = \frac{12N^2\sigma_0^2}{ig_1}\frac{\Lambda}{N} + \frac{ig_1\sigma_0}{2} + i\frac{g_1^3 - 4g_3}{48N^2\sigma_0} \tag{2.62}$$

The constants c_1 and c_2 are now determined by (2.61) and (3.55).

2.4. The Energy Correction

The above results may now be fed back into the expression for the energy correction, (2.28). We need the quantities

$$\delta\Lambda = c_1 \tag{2.63}$$

$$\delta\sigma_N(\Lambda) = 12N^2\sigma_0^2 c_2 \tag{2.64}$$

and

$$\int_\Lambda^\infty d\lambda\, e^{-\pi(\lambda-\Lambda)}\,\delta\sigma_N(\lambda) = X_+(i\pi) \tag{2.65}$$

Using (2.55), (2.61), and (A.19) of the Appendix, one arrives after a little algebra at the result that as $N \to \infty$,

$$\delta(e_N - e_\infty) \sim \frac{2\pi c_3 G_+(0)}{\Lambda}\left(\frac{\pi}{2N} - \frac{ig_1\pi}{12N^2\sigma_0} + \frac{\pi\beta(n)}{2NG_+(0)}\right)\left\{\frac{N}{B}\left(\frac{12N^2\sigma_0^2}{ig_1} - \frac{ig_1}{2}\right)\right.$$
$$\left.\times\left(\frac{\pi\sigma_0}{ig_1} - \frac{\pi^2}{12N^2\sigma_0} - \frac{ig_1\pi}{24N^2\sigma_0}\right) - \frac{\pi + ig_1}{ig_1}\right\} \tag{2.66}$$

With the use of formulas (A.20)–(A.24) of the Appendix, the various factors appearing in this equation may be reexpressed as follows:

$$\frac{\pi}{2N}-\frac{ig_1\pi}{12N^2\sigma_0}+\frac{\pi\beta(n)}{2NG_+(0)}=\frac{3(a_n+D_n)(a_n-ig_1)-2ig_1\pi}{6N(a_n+D_n)} \tag{2.67}$$

$$\frac{4ig_1B}{D_n}=3(a_n+D_n)(a_n-ig_1)-2ig_1\pi \tag{2.68}$$

$$\frac{12N^2\sigma_0^2}{ig_1}-\frac{ig_1}{2}=\pi+\frac{3D_n(a_n+D_n)}{2ig_1} \tag{2.69}$$

$$\frac{\pi\sigma_0}{ig_1}-\frac{\pi^2}{12N^2\sigma_0}-\frac{ig_1\pi}{24N^2\sigma_0}=\frac{\pi D_n}{2Nig_1} \tag{2.70}$$

where, from (A.21) and (A.22),

$$D_n=(a_n^2+\bar{b})^{1/2} \tag{2.71}$$

with

$$a_n=\pi(11+12n\sqrt{2})/12 \tag{2.72}$$

$$\bar{b}=23\pi^2/216 \tag{2.73}$$

Hence (2.66) is reduced finally, for $n\neq 0$, to

$$\delta(e_N-e_\infty)\sim -\frac{\pi^2\beta^2(n)}{8N^2\ln N}=-\frac{n^2\pi^2}{2N^2\ln N} \quad \text{as} \quad N\to\infty \tag{2.74}$$

which is the desired result.

2.5. Other Excited States

The leading corrections for other excited states may be treated along very similar lines to those above. We merely indicate the important differences in each case.

2.5.1. Ground State in Spin Sector n for $\Phi\neq 0$. If the phase angle Φ is nonzero, the root density $\sigma_N(\lambda)$ is no longer symmetric in λ, and it is no longer true that $\Lambda_+=\Lambda_-$, so that one must consider separately the perturbations to $\sigma_N(\lambda)$ in the regions $\lambda\geqslant\Lambda_+$ and $\lambda\leqslant-\Lambda_-$. The constraints equivalent to (2.21) are

$$\int_{\Lambda_+}^{\infty}\sigma_N(\lambda)\,d\lambda=\frac{1}{2N}[1+\beta_+(n)] \tag{2.75}$$

$$\int_{-\infty}^{-\Lambda_-}\sigma_N(\lambda)\,d\lambda=\frac{1}{2N}[1+\beta_-(n)] \tag{2.76}$$

where

$$\beta_{\pm}(n) = 2n \mp \Phi/\pi \tag{2.77}$$

The leading-order finite-size correction is given by[20]

$$e_N - e_\infty \sim -\frac{\pi^2}{6N^2}\left\{1 - \frac{3}{4}\left[\beta_+^2(n) + \beta_-^2(n)\right]\right\}, \qquad N \to \infty \tag{2.78}$$

For the next correction, we find, as $N \to \infty$,

$$\delta(e_N - e_\infty) \sim -\frac{\pi^2 \beta_+(n)\, \beta_-(n)}{8N^2 \ln N} = -\frac{1}{8N^2 \ln N}(4n^2\pi^2 - \Phi^2) \tag{2.79}$$

2.5.2. Lowest Lying "Zero-String" State in Sector n, $\Phi = 0$. This state is the "1-type" of Alcaraz *et al.*[13] In the sector $n = 0$, it is the first excited state above the ground state. At $\gamma = 0$, this state is degenerate with the lowest energy state in the sector $n = 1$.

The Bethe-ansatz solution has a single complex root at $\lambda = i\infty$ with the remaining $m - 1$ roots distributed symmetrically on the real λ axis without any "holes" (i.e., gaps in the distribution). To leading order, the finite-size correction is given by

$$e_N - e_\infty \sim -\frac{\pi^2}{6N^2}\left[1 - 6(n+1)^2\right] \tag{2.80}$$

The contribution of the complex root to $e_N - e_\infty$, namely the term

$$\phi'(\lambda_c) - \frac{1}{\pi}\int_{-\infty}^{\infty} d\lambda\, \phi'(\lambda)\, p(\lambda - \lambda_c) \tag{2.81}$$

in (2.14), is identically zero,[14] while the contribution of the complex root in (2.13), namely $-p(\lambda - \lambda_c)/\pi N$, also vanishes. The sum rule corresponding to (2.21) is

$$\int_A^{\infty} \phi_N(\lambda)\, d\lambda = \frac{1}{2N}\left[1 + \beta_1(n)\right], \qquad \beta_1(n) = 2(n+1) \tag{2.82}$$

Otherwise, the treatment is identical to that for the ground state, leading to a result, as $N \to \infty$, for the next-to-leading correction of

$$\delta(e_N - e_\infty) \sim -\frac{\pi \beta_1^2(n)}{8N^2 \ln N} = -\frac{(n+1)^2\, \pi^2}{2N^2 \ln N} \tag{2.83}$$

2.5.3. Lowest Lying "2-String" State in Sector n, $\Phi = 0$. The Bethe-ansatz solution for this state has two complex roots lying exactly at $\lambda = \pm i/2$ with the remaining $m-2$ roots distributed symmetrically on the real λ axis, again without any "holes."[13,18] To leading order, the finite-size correction is that given by (2.80). The contribution of the complex roots to $e_N - e_\infty$ is again identically zero and the sum rule corresponding to (2.21) is again (2.82). However, in addition to the driving terms in curly brackets in (2.16), there is an extra contribution from the complex roots:

$$-\frac{1}{\pi N}\left[p\left(\lambda-\frac{i}{2}\right)+p\left(\lambda+\frac{i}{2}\right)\right] \sim -\frac{1}{2\pi N\lambda^2} \quad \text{as} \quad \lambda \to \infty \tag{2.84}$$

Hence one arrives at the asymptotic result, as $N \to \infty$,

$$\delta(e_N - e_\infty) \sim -\frac{\pi^2\beta_1(n)[\beta_1(n)-8]}{8N^2 \ln N} = -\frac{\pi^2(n+1)(n-3)}{2N^2 \ln N} \tag{2.85}$$

for the next-to-leading correction.

We turn now to the interpretation of these results and, in particular, their application to the spectrum of the quantum Hamiltonian limit of the four-state Potts model.

3. LOGARITHMIC AMPLITUDES IN THE POTTS MODEL

The $(1+1)$-dimensional Hamiltonian field theory of the q-state Potts model was first discussed by Sólyom and Pfeuty[22] from a τ-continuum limit of the transfer matrix rerived by Mittag and Stephen.[23] On a chain of L sites with periodic boundary conditions the Hamiltonian can be written as

$$H^0_{\text{Potts}} = -\sum_{m=1}^{L}\sum_{k=1}^{q-1}\Omega^k_m - \lambda\sum_{m=1}^{L}\sum_{k=1}^{q-1}R^k_m R^{q-k}_{m+1} \tag{3.1}$$

where the operators Ω_m and R_m at site m obey a $Z(q)$-algebra:

$$\Omega_m R_m = \omega^{-1} R_m \Omega_m, \qquad \Omega_m R^\dagger_m = \omega R^\dagger_m \Omega_m, \qquad \Omega^q_m = R^q_m = 1 \tag{3.2}$$

with $\omega = e^{2\pi i/q}$. Criticality corresponds to $\lambda = \lambda_c = 1$.

The periodic boundary conditions imply

$$R_{L+1} = R_1 \tag{3.3}$$

More generally,[9] we can apply a "twisted" boundary condition, replacing (3.3) by

$$R_{L+1} = \omega^{\tilde{q}} R_1, \qquad \tilde{q} = 0, 1, 2, \ldots, q-1 \tag{3.4}$$

We denote the resulting Hamiltonian by $H^{\tilde{q}}_{\text{Potts}}$. In a basis that diagonalizes the Ω_m's, these Hamiltonians can be block-diagonalized into sectors labeled by the eigenvalues of

$$\prod_{m=1}^{L} \Omega_m = \omega^{\hat{q}}, \qquad \hat{q} = 0, 1,..., q-1 \tag{3.5}$$

We denote $H^{\tilde{q}}_{\text{Potts}}$ acting in the sector $\hat{q}$ by $H^{\tilde{q},\hat{q}}_{\text{Potts}}$.

Our interest in this paper is in the spectrum of (3.1) for $q=4$ and, in particular, in $E_0^{0,0}$, the ground state energy of $H^{0,0}$, which is also the actual ground state energy of (3.1) with periodic boundary conditions; $E_1^{0,0}$, the energy of the first excited state of $H^{0,0}$, for which

$$E_1^{0,0} - E_0^{0,0} = \frac{2\pi\tau_p x_e}{L} + o(L^{-1}) \tag{3.6}$$

where x_e is the anomalous dimension of the energy operator; $E_0^{0,1}$, the lowest energy of $H^{0,1}$, for which

$$E_0^{0,1} - E_0^{0,0} = \frac{2\pi\tau_p x_m}{L} + o(L^{-1}) \tag{3.7}$$

with x_m the anomalous dimension of the magnetic operator, and $E_0^{1,\tilde{q}}$, the lowest energy of $H^{1,\tilde{q}}$ with $\tilde{q} \neq 0$, for which

$$E_0^{1,\tilde{q}} - E_0^{0,0} = \frac{2\pi\tau_p x_{\text{pf}}(\tilde{q})}{L} + o(L^{-1}) \tag{3.8}$$

where x_{pf} is the anomalous dimension of the spin-$\tilde{q}/4$ parafermion.[24,25]

For the XXZ Hamiltonian (2.1), the scale factor τ appearing in (1.1) and (1.2) is known to be $\tau = \pi$ at $\gamma = 0$.[15] Hence, the corresponding factor τ_p that enters (3.6)–(3.8) also takes the value $\tau_p = \pi$.[12,13]

As a function of L, $E_0^{0,0}$ should behave as in (1.2). [See also (3.14) and (3.15) below.] The leading correction terms in (3.6)–(3.8) should be of the form (1.1), i.e., of order $1/(L \ln L)$. We will derive the amplitudes d_e, d_m, and d_{pf} from the results of Section 2. To do so, we make use of earlier work[6,13] and relate the relevant Potts eigenstates to eigenstates of the XXZ chain.

In the thermodynamic limit, Hamer[6] showed that the Potts Hamiltonian (3.1) is equivalent to the XXZ chain (2.1) on $N=2L$ sites with

$$\Delta = -\frac{1}{2}\sqrt{q} \tag{3.9}$$

These arguments were extended to *finite* L by Alcaraz *et al.*[13], who took explicit account of the effect of boundary conditions. Specifically, they established that the ground state energy $E_0^{0,0}$ of (3.1) with periodic boundary conditions is given by

$$E_0^{0,0}(L, q) = \left(2 - \frac{1}{2} q\right) L + q^{1/2} E_0(\Delta, \Phi; 2L) \tag{3.10}$$

where $E_0(\Delta, \Phi; M)$ is the ground state of (2.1) with Δ given by (3.9) and

$$\Phi = 2 \cos^{-1}\left(\frac{1}{2}\sqrt{q}\right) \tag{3.11}$$

Hence, for $q = 4$, we have $\Delta = -1$ and $\Phi = 0$.

For $\Delta = -1$, the ground state energy of the periodic XXZ chain approaches its bulk limit as[15,16]

$$E_0 \sim N e_\infty - \frac{\pi^2}{6N}\left[1 + \frac{A}{(\ln N)^3}\right], \qquad N \to \infty \tag{3.12}$$

where $e_\infty = \frac{1}{2} - 2 \ln 2$, as first obtained by Hulthén.[26] With the definitions (2.71)–(2.73), the amplitude of the logarithmic correction term is given exactly by

$$A = \frac{1}{12}\left(\frac{a_0 + 3D_0}{a_0 + D_0}\right)^2 = \frac{1}{12}\left(\frac{11\sqrt{3} + 3\sqrt{409}}{11\sqrt{3} + \sqrt{409}}\right)^2 = 0.343347... \tag{3.13}$$

in accord with the calculation of Woynarovich and Eckle.[16]

Combining (3.12) with (3.10) implies that

$$E_0^{0,0}(L, q = 4) = L e'_\infty - \frac{\pi^2}{6L} c(L) \tag{3.14}$$

where $e'_\infty = 4 e_\infty = 2 - 8 \ln 2$ and $c(L)$ is an "effective anomaly" that varies as

$$c(L) \sim 1 + \frac{A}{(\ln 2L)^3} \qquad \text{as} \quad L \to \infty \tag{3.15}$$

Hence, we recover the expected value $c = 1$ for the conformal anomaly of the four-state Potts model. However, the amplitude (3.13) of the leading correction term differs from that predicted by Cardy[3] for the usual (Euclidean) version of the Potts model. This is due presumably to a different normalization of the marginal field in the Hamiltonian formulation; we discuss this point further in Section 4.

On the other hand, the amplitudes d_α appearing in (1.1) should be universal and hence the same for the Hamiltonian and Euclidean formulations. To compare with Cardy's results, we write (1.1) and (1.2) in the form

$$e_L^\alpha - e_\infty \sim -\frac{\pi^2}{6L^2}(1-12x_\alpha) + \frac{2\pi^2 d_\alpha}{L^2 \ln L} \tag{3.16}$$

For the modified XXZ chain on $L = N$ sites, comparison with (2.79) yields

$$d(n, \Phi) = -n^2/4 + \Phi^2/16\pi^2 \tag{3.17}$$

which for $\Phi = 0$ reduces to the result found by Woynarovich and Eckle.[16]

The calculation of the amplitudes d_α for the Potts states defined in (3.6)–(3.8) proceeds in two steps. We first identify the XXZ equivalences of the Potts energies $E_1^{0,0}$, $E_0^{0,1}$, and $E_0^{1,\tilde{q}}$. This has been done by Alcaraz *et al.*[13] In all three cases, the Potts eigenvalue on an L-site chain can be expressed exactly in terms of an eigenvalue of an XXZ chain on $N = 2L$ sites with $\Delta = -1$ by the equivalence

$$E_{\text{Potts}} \Leftrightarrow 2E_{XXZ} \tag{3.18}$$

The specific XXZ states are[13]:

$E_1^{0,0}$: The lowest lying two-string eigenstate in the sector $n = 0$ with $\Phi = 0$.

$E_0^{0,1}$: The lowest energy state in the sector $n = 0$ with $\Phi = \pi$.

$E_0^{1,\tilde{q}}$: The lowest energy state in the sector $n = 1$ with $\Phi = 2\pi\tilde{q}/q$.

With these identifications we can now compute the relevant dimensions x_α and amplitudes d_α from the results of Section 2. For the energy operator, the required results are contained in (2.80) and (2.85). Comparison with (3.3) gives[6]

$$x_e = 1/2 \qquad \text{and} \qquad d_e = 3/4 \tag{3.19}$$

Similarly, for the magnetic operator we find from (2.78) and (2.79)

$$x_m = 1/8 \qquad \text{and} \qquad d_m = 1/16 \tag{3.20}$$

[6] We note in passing the generalization of this result for the anomalous dimension to $\gamma \neq 0$. The general result corresponding to either the 0-string or 2-string mass gap in sector n is $x = x_{n,1} + n$, where $x_{n,m} \equiv n^2 x_p + m^2/4x_p$ with $x_p = (\pi - \gamma)/2\pi$.[12]

thereby confirming precisely Cardy's predictions. Finally, for the parafermions, the amplitudes follow directly from (3.17), with $\Phi = 2\pi p/4$, $p = 1, 2, 3, 4$. We find

$$d_{\mathrm{pf}}(p) = -1/4 + p^2/64 \tag{3.21}$$

which appears to be a new result.

4. NUMERICAL RESULTS

In the preceding sections, we have computed analytically the amplitudes of the dominant logarithmic corrections to finite-size scaling for several energy levels of the quantum Hamiltonian version (3.1) of the four-state Potts model. For the levels associated with the energy and magnetic operators precise agreement was obtained with the predictions of Cardy[3] based on conformal invariance.

As mentioned in the Introduction, numerical estimates of the critical exponents of the four-state Potts model have been difficult. Direct estimates of d_e and d_m have proved even more difficult.[3,13] We conclude this paper by reconsidering the large-lattice data of Alcaraz *et al.*[13] in the light of the results of Section 3. We restrict attention to the energy and magnetic operators.

Define estimators

$$x_e(L) = \left(\frac{L}{2\pi^2}\right)(E_1^{0,0} - E_0^{0,0}) \tag{4.1}$$

$$x_m(L) = \left(\frac{L}{2\pi^2}\right)(E_0^{1,0} - E_0^{0,0}) \tag{4.2}$$

From the results of Section 3, these estimators should behave for large L as

$$x_\alpha(L) = x_\alpha + \frac{d_\alpha}{\ln 2L} + R_\alpha(L) \tag{4.3}$$

where $R_\alpha(L) = o(1/\ln L)$; see also (4.8) below.

Using the data of Alcaraz *et al.*,[13] we have computed $x_e(L)$ and $x_m(L)$ for $L \leqslant 512$ and $L \leqslant 256$, respectively. The calculation of the relevant eigenvalues involved solving the Bethe-ansatz equations of the *XXZ* Hamiltonian on chains of up to 1024 sites; we refer to refs. 13 and 27 for details of this computation. These estimators are plotted versus $1/\ln 2L$ in Figs. 1 and 2. A trend toward the limiting values of $x_e = 1/2$ and $x_m = 1/8$ is apparent. Moreover, the estimates appear to vary linearly with $1/\ln 2L$

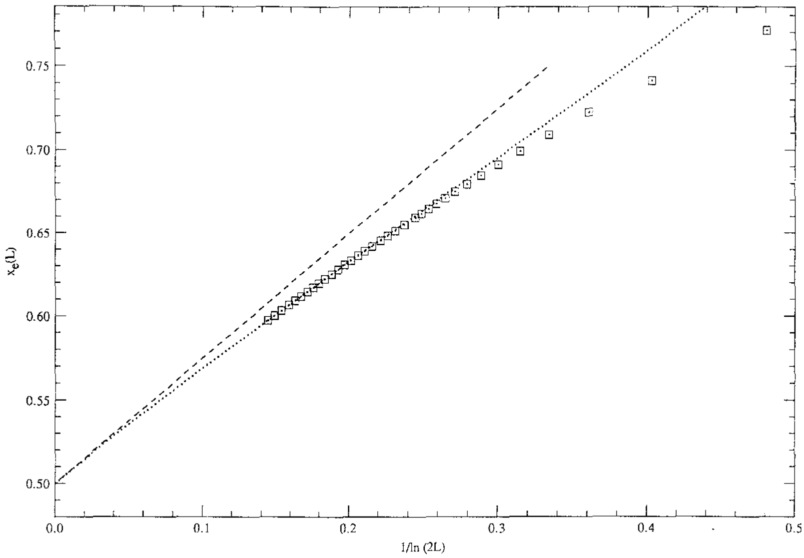

Fig. 1. Estimator $x_e(L)$ for the energy operator of the four-state Potts model plotted against $1/\ln 2L$. Symbols denote exact finite lattice estimates for $L \leqslant 512$. The dashed line is the exact asymptotic behavior derived in Section 3, while the dotted line depicts the empirical fit discussed in the text.

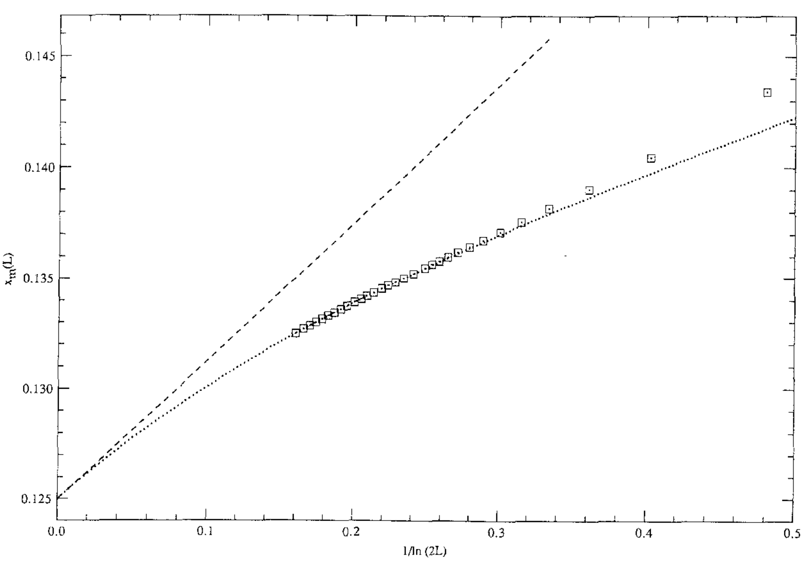

Fig. 2. Estimator $x_m(L)$ for the magnetic operator of the four-state Potts model plotted against $1/\ln 2L$. Symbols and lines have the same meanings as in Fig. 1.

for L greater than 100–130. A straight line fit to the data for $x_e(L)$ for $L > 130$ ($1/\ln 2L < 0.18$) yields the estimates:

$$x_e = 0.506, \qquad d_e = 0.634 \tag{4.4}$$

Similarly, using data for $L > 100$ ($1/\ln 2L < 0.2$) gives

$$x_m = 0.127, \qquad d_m = 0.036 \tag{4.5}$$

While these estimates of x_e and x_m are reasonable, those of d_e and d_m are significantly lower than the exact values.

One can attempt a more direct estimate of the limiting value x_α of the sequences $\{x_\alpha(L)\}$ and the asymptotic slope d_α by constructing *two-point* fits to the form $x + d/\ln 2L$ using data from two lattices. This procedure yields the modified estimators

$$\hat{x}_\alpha(L) = \frac{\ln(2L)\, x_\alpha(L) - \ln(2L')\, x_\alpha(L')}{\ln(2L) - \ln(2L')} \tag{4.6}$$

$$\hat{d}_\alpha(L) = \frac{\ln(2L)\ln(2L')[x_\alpha(L) - x_\alpha(L')]}{\ln(2L') - \ln(2L)} \tag{4.7}$$

where in our calculations $L' = L - 2$. The behavior of these estimators is illustrated in Tables I and II. The new estimates are comparable with the values quoted in (4.4) and (4.5).

While we have not analytically explored the nature of the correction term $R_\alpha(L)$ in (4.1) and (4.2), we expect on the basis of the analysis of

Table I. Numerical Estimates of x_e and d_e for the Four-State Potts Model

Raw data		Two-point fits		Extrapolates	
L	$x_e(L)$	$\hat{x}_e(L)$	$\hat{d}_e(L)$	$\hat{x}'_e(L)$	$\hat{d}'_e(L)$
8	0.722621	0.558055	0.456272	—	—
16	0.684992	0.525623	0.552330	—	—
32	0.657247	0.514612	0.593200	0.533194	0.176705
64	0.636473	0.509946	0.613913	0.515719	0.413351
128	0.620490	0.507572	0.626150	0.508215	0.541012
256	0.607858	0.506164	0.634398	0.504555	0.614867
512	0.597639	0.505226	0.640551	0.502685	0.658165
Exact	0.5	0.5	0.75	0.5	0.75

Table II. Numerical Estimates of x_m and d_m for the Four-State Potts Model

Raw data		Two-point fits		Extrapolates	
L	$x_m(L)$	$\hat{x}_m(L)$	$\hat{d}_m(L)$	$\hat{x}'_m(L)$	$\hat{d}'_m(L)$
8	0.139056	0.126799	0.033982	—	—
16	0.136454	0.127699	0.031374	—	—
32	0.135233	0.127530	0.032034	0.122810	0.099589
64	0.134106	0.127176	0.036240	0.123800	0.086033
128	0.133217	0.126843	0.035346	0.124439	0.074816
256	0.132493	0.126570	0.036953	0.124778	0.067814
Exact	0.125	0.125	0.0625	0.125	0.0625

Woynarovich and Eckle[16] and an extension (see below) of Cardy's renormalization group argument that

$$R_\alpha(L) = \frac{p_\alpha \ln(\ln 2L) + q_\alpha + o(1)}{(\ln 2L)^2}, \qquad L \to \infty \tag{4.8}$$

This form for the dominant correction term is substantiated in Fig. 3, where we plot

$$r_e(L) \equiv (\ln 2L)^2 R_e(L) = (\ln 2L)^2 \left[x_e(L) - \frac{1}{2} - \frac{3}{4 \ln 2L} \right] \tag{4.9}$$

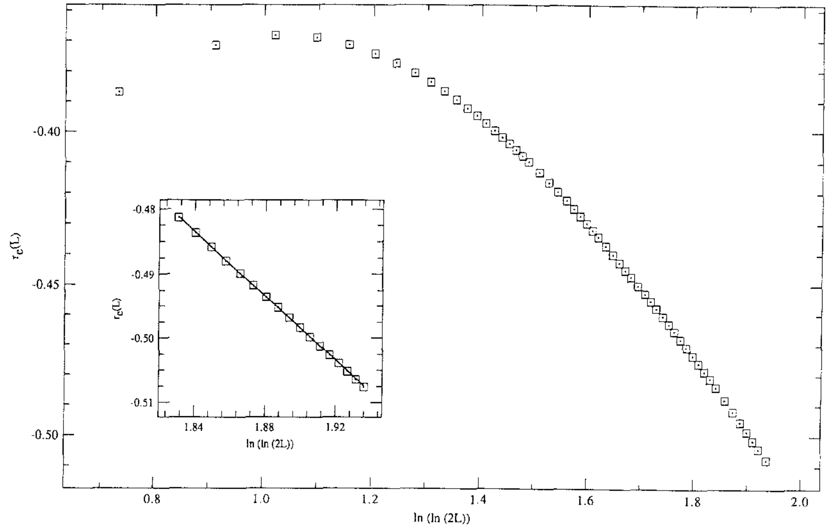

Fig. 3. The reduced correction term $r_e(L)$ defined by (4.9) as a function of $\ln(\ln 2L)$. Symbols denote exact finite lattice estimates for $L \leqslant 512$. The insert depicts the linear fit to data for $256 \leqslant L \leqslant 512$ used to construct the empirical expression for $r_e(L)$ discussed in the text.

versus $\ln(\ln 2L)$. As shown in the insert in this figure, data for $256 < L < 512$ are well represented by a straight line, although in terms of $\ln(\ln 2L)$ this is a rather small range! A least-square fit to the data in this range gives

$$p_e \approx -0.25, \qquad q_e \approx -0.024 \tag{4.10}$$

If we accept these values and omit all higher order terms, a reasonably satisfactory fit can be obtained (see Fig. 1) for $L > 25$. A similar analysis of the data for $x_m(L)$ results in a similar fit (see Fig. 2) with

$$p_m \approx -0.030, \qquad q_m \approx -0.037 \tag{4.11}$$

Assuming that the leading correction term is of the form (4.8) also allows the estimates in Tables I and II to be refined by a simple strategy. Define $\hat{x}_l = \hat{x}(L = 2^{l-1})$ and similarly for $\hat{d}_l$. From (4.8), we find that both $\hat{x}_l$ and $\hat{d}_l$ should approach their limits as $(p' \ln l + q')/l^k$ with $k = 2$ for $\hat{x}_l$ and $k = 1$ for $\hat{d}_l$. It is now easy to use three successive values of x_l and d_l to improve the estimate of the limits. These improved estimates, denoted $\hat{x}'$ and $\hat{d}'$, are listed in the last two columns of Tables I and II. A definite and significant improvement in the estimates of x_e and x_m is evident. In addition, it is now clear that, in fact, the estimates of the amplitudes d_e and d_m *have not stabilized* and that a definite trend in the direction of the exact values is evident.

We do not know of any *a priori* predictions of the coefficients in the correction term $R_\alpha(L)$. However, the values found by our fitting procedures are physically reasonable. Consequently, such corrections are the most likely explanation of the extremely slow convergence to the exact asymptotic behavior that is so evident in Figs. 1 and 2. Rather soberingly, our empirical fits of $R_e(L)$ and $R_m(L)$ suggest that the leading correction term would become directly visible in finite lattice data only for $L \sim 10^{10}$!

The possibility that the logarithmic amplitudes might be visible only in data from extremely long chains or extremely wide strips was recognized by Cardy in his original discussion.[3] He suggested that it might be more appropriate to analyze the finite lattice data in terms of an effective coupling constant $g(\ln L)$ conjugate to the marginally irrelevant operator $\mathcal{O}_{\rm cor}(\mathbf{r})$ that is responsible for the appearance of the logarithmic terms in the first place.

Since, for the four-state Potts model, the dimension of $\mathcal{O}_{\rm cor}(\mathbf{r})$ is $x_{\rm cor} = 2$, $g(l)$ renormalizes under a change of length scale as

$$dg/dl = -\pi b g^2 + O(g^3) \tag{4.12}$$

where b is a constant which is universal[3] if the operator $\mathcal{O}_{\text{cor}}$ is normalized so that its two-point function decays as $1/r^{2x_{\text{cor}}}$. Integrating (4.12) gives

$$g(\ln L) = \frac{g_0}{1 + \pi b g_0 \ln L} \tag{4.13}$$

Here g_0 is the bare physical coupling that measures the deviation of the physical critical Hamiltonian H_c from the conformally invariant fixed point Hamiltonian H^*; namely

$$H_c = H^* + g_0 \sum_{\mathbf{r}} \mathcal{O}_{\text{cor}}(\mathbf{r}) \tag{4.14}$$

The effect of this term on the eigenspectrum of H^* can be studied perturbatively provided the renormalized coupling (4.13) is used as the expansion parameter. This was the analysis carried out by Cardy,[3] who showed that the ground state energy varies as g^3, while gaps vary linearly with g. Specifically, in the notation of (3.14), (3.15), (4.1), and (4.2),

$$c(L) = 1 + 8\pi^3 b[g(\ln L)]^3 + O(g^4) \tag{4.15}$$

$$x_\alpha(L) = x_\alpha + 2\pi b_\alpha g(\ln L) + O(g^2) \tag{4.16}$$

where the numbers b_α are related to operator product expansion coefficients.[3] Substituting (4.13), we recover (1.1) and (3.15) with

$$d_\alpha = 2b_\alpha/b \tag{4.17}$$

and

$$A = 8/b^2 \tag{4.18}$$

Cardy's alternative method[7] for analyzing finite lattice data for logarithmic amplitudes can now be stated as follows:

1. Calculate $c(L)$ from data for the ground state energy and then use (4.15) to compute $g(\ln L)$ ignoring higher order terms.
2. Use (4.16) to estimate x_α and b_α by plotting $x_\alpha(L)$ against $g(\ln L)$.

The advantage of this method over a direct extrapolation in L arises from the fact that corrections should be simple powers of $g(\ln L)$ instead of complicated combinations of logarithms of $\ln L$. Indeed, if we explicitly

[7] This procedure was tried by Cardy[3] for the Euclidean Potts model using the transfer matrix data of Blöte and Nightingale.[7] More recently, it has been used by Wills[28] in a finite lattice study of the restricted solid-on-solid (RSOS) models.[29]

include a term $+\pi b\beta g^3$ in (4.12), we find on integration that (4.13) is replaced by

$$\pi b \ln L = \frac{1}{g} - \frac{1}{g_0} - \beta(\ln g - \ln g_0) + \beta \ln\left(\frac{1-\beta g}{1-\beta g_0}\right) \tag{4.19}$$

Hence, for large L, we obtain

$$g(\ln L) = \frac{1}{\pi b \ln L}\left\{1 - \frac{\beta \ln(\ln L)}{\pi b \ln L} + O\left(\frac{1}{\ln L}\right)\right\} \tag{4.20}$$

which on substitution in (4.16) reproduces a correction term $R_\alpha(L)$ of precisely the form (4.8).

Unfortunately, there is an implicit problem concerning the value of the number b that enters (4.12) and (4.15). If, as discussed above, $\mathcal{O}_{\rm cor}$ is appropriately normalized, then $b = 4/\sqrt{3}$, as assumed by Cardy in his analysis of the Euclidean Potts model. However, there seems to be no reason to assume *a priori* that this normalization is valid. Indeed, comparing (4.18) with (3.13) yields

$$b = 4\sqrt{6}\left(\frac{11\sqrt{3}+\sqrt{409}}{11\sqrt{3}+3\sqrt{409}}\right) = 4.827011... \tag{4.21}$$

Consequently, it seems necessary to regard b as a further parameter to be determined, at least in principle, from the behavior of $c(L)$ for large L.

The practicality of this approach is tested in Fig. 4, where we plot $[c(L)-1]^{-1/3}$ versus $\ln 2L$. From (4.13) and (4.15) this graph should asymptote to a straight line with slope $\frac{1}{2}b^{2/3} = 1.428....$ While Fig. 4 is qualitatively in agreement with this prediction, the apparent asymptotic slope yields a value for $b \approx 5.23$, which is rather larger than the exact value given by (4.21) and, as in our earlier analysis, suggests that the true asymptotic regime has not been reached.

In view of this difficulty in estimating b reliably, we consider $x_e(L)$ and $x_m(L)$ as functions of

$$u(L) \equiv [c(L)-1]^{1/3} \approx 2\pi b^{1/3} g(\ln L) \tag{4.22}$$

instead of simply g. This functional dependence is shown in Figs. 5 and 6. For small u, we expect from (4.16) that

$$x_\alpha(L) = x_\alpha + \tilde{d}_\alpha u + O(u^2) \tag{4.23}$$

where

$$\tilde{d}_\alpha = b_\alpha b^{-1/3} = \frac{1}{2} b^{2/3} d_\alpha \tag{4.24}$$

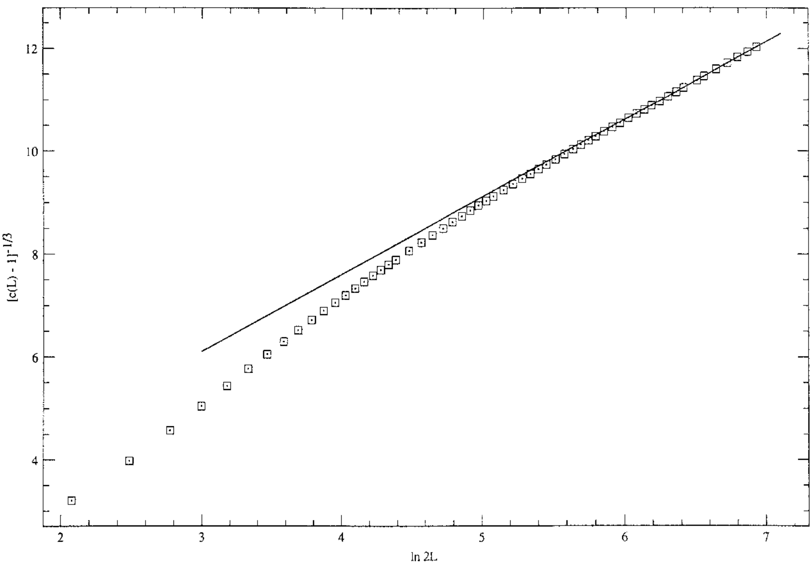

Fig. 4. Plot of $[c(L)-1]^{-1/3}$ versus $\ln 2L$. Symbols denote exact finite lattice values for $L \leqslant 512$. The straight line is obtained from a linear fit to data for $L > 350$.

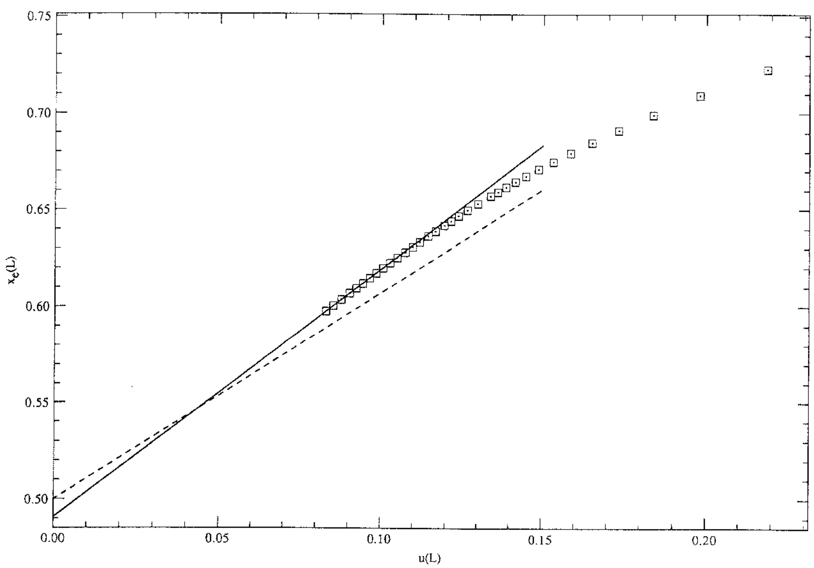

Fig. 5. Estimator $x_e(L)$ as a function of the "effective coupling" $u(L)$. Symbols denote actual finite lattice values. The solid line is the exact asymptotic behavior predicted from the results of Section 3 [see (4.23) and (4.25)], whereas the dashed line is a obtained from a linear fit to the finite lattice data for $u(L) < 0.1$, i.e., $L > 120$.

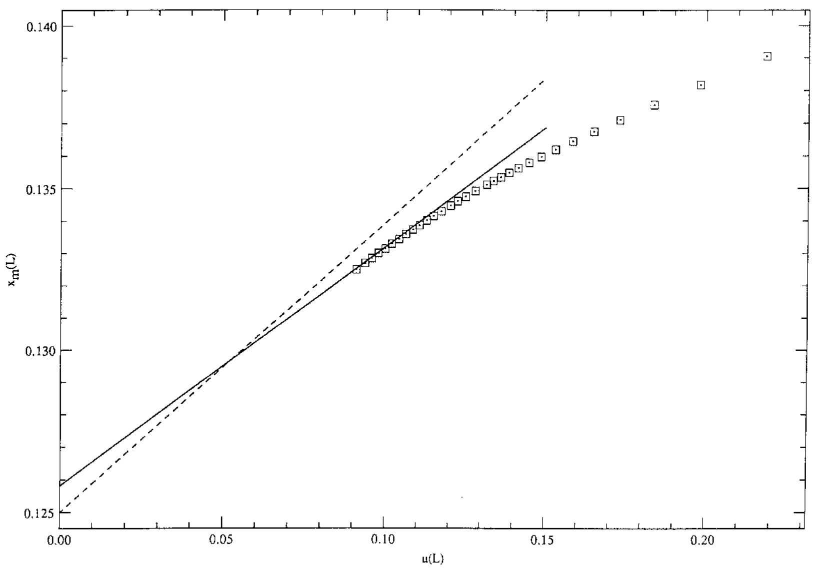

Fig. 6. Estimator $x_m(L)$ as a function of $u(L)$. Symbols and lines have the same meaning as in Fig. 5.

In particular,

$$\tilde{d}_e = \frac{3}{8} b^{2/3} = 1.071067..., \qquad \tilde{d}_m = \frac{1}{32} b^{2/3} = 0.089256... \qquad (4.25)$$

Comparison of Figs. 5 and 6 with Figs. 1 and 2 suggests that (4.23) affords a somewhat better approximation to the available finite lattice data than does (4.16) omitting the correction term. The two approximations are compared more quantitatively in Fig. 7, where we plot the respective percentage deviations from the exact finite lattice values. Use of $u(L)$ rather than $1/\ln 2L$ does result in an improvement in the case of $x_m(L)$, but for $x_e(L)$ the improvement is only slight. Interestingly, in this case the two approximations have errors of opposite sign.

Overall the improvement does not appear to be substantial. This is reflected in direct estimates of x_e, $\tilde{d}_e$, x_m, and $\tilde{d}_m$ from linear fits of $x_e(L)$ and $x_m(L)$ as functions of u. As indicated in Figs. 5 and 6, such fits still deviate significantly from the exact asymptotic behavior and lead to the esimates

$$x_e \approx 0.491, \qquad \tilde{d}_e \approx 1.29 \qquad (4.26)$$

and

$$x_m \approx 0.126, \qquad \tilde{d}_m = 0.074 \qquad (4.27)$$

If we use the exact value (2.73) for b, we then obtain $d_e \approx 0.90$ and $d_m \approx 0.05$, both of which are a considerable distance from the exact values.

We can obtain better estimates of $\tilde{d}_e$ and $\tilde{d}_m$ if we *assume* the exact values of x_e and x_m. To do so, define

$$r_\alpha(u) \equiv \frac{x_\alpha(L) - x_\alpha}{u(L)}, \qquad \alpha = e, m \tag{4.28}$$

$$= \tilde{d}_\alpha + O(u), \qquad u \to 0 \tag{4.29}$$

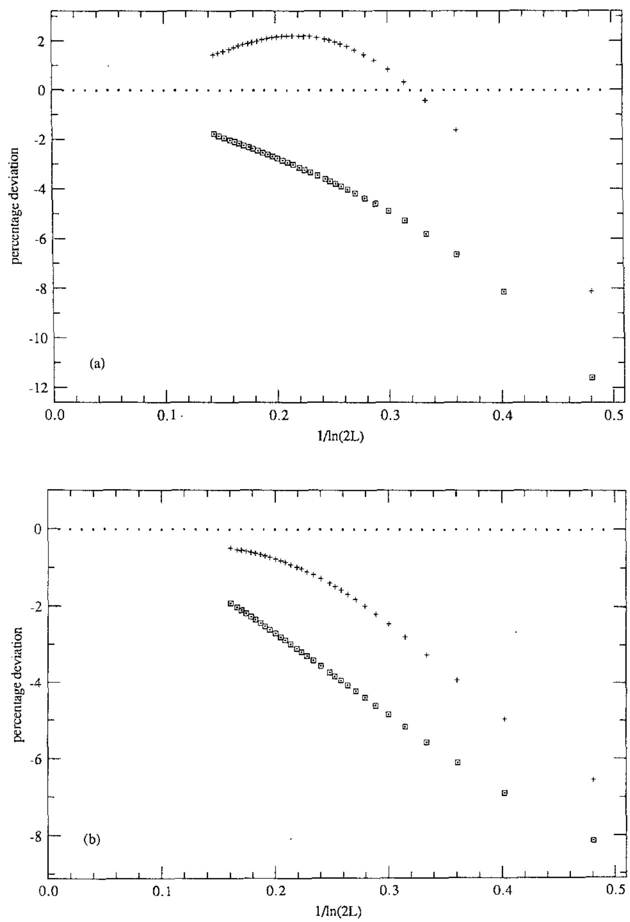

Fig. 7. Percentage deviations of the two approximations (□) $x_\alpha + d_\alpha/\ln 2L$ and (+) $x_\alpha + \tilde{d}_\alpha u(L)$ from the exact finite lattice value of $x_\alpha(L)$ for (a) the energy operator ($\alpha = e$) and (b) the magnetic operator ($\alpha = m$).

These functions are illustrated in Figs. 8 and 9. In the case of r_e, we observe a dramatic nonmonotonic behavior. Clearly, this behavior will significantly affect any attempt to estimate $r_e(0)$ unless data for sufficiently small u (sufficiently large L) are available. Given our data, we can make a reasonable extrapolation (see Figs. 5 and 6), from which we conclude that

$$r_e(0) \approx 1.07, \qquad r_m(0) \approx 0.091 \tag{4.30}$$

which are in much better agreement with the exact values. In particular, the ratio $\tilde{d}_e/\tilde{d}_m$, which should be independent of b, has the value 11.8, in good agreement with the exact value of 12. In contrast, our earlier estimates yield 17.4 for this ratio.

While this final analysis has led to a partial numerical confirmation of our analytic results, it is obvious that, in the absence of the analytical results, an accurate confirmation of the predictions of conformal invariance would have been impossible even given the extensive finite lattice data that we had available. Consequently, conventional finite lattice studies (usually restricted to $L < 20$) of systems exhibiting a marginally irrelevant operator should be interpreted with considerable trepidation.

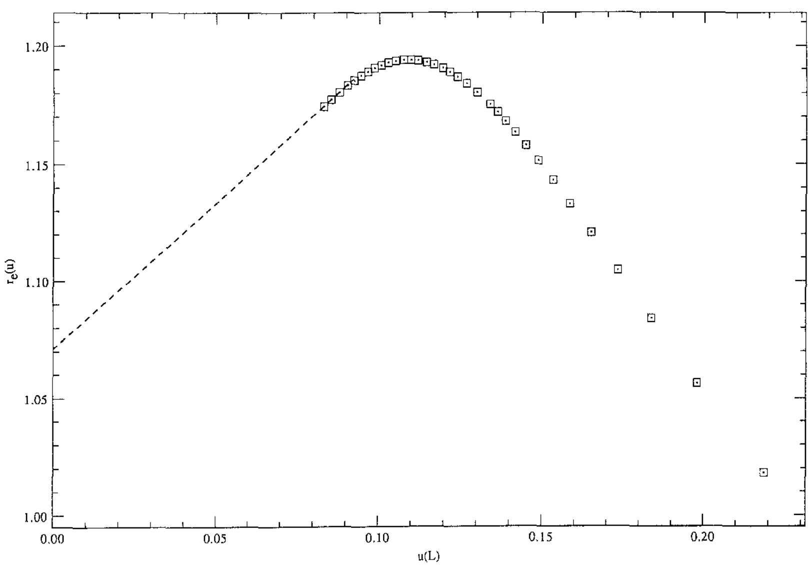

Fig. 8. The reduced deviation $r_e(u) = [x_e(L) - x_e]/u(L)$ as a function of $u(L)$. Symbols denote exact finite lattice values, while the dashed line is an extrapolation based on a linear fit to the data for $u < 0.09$.

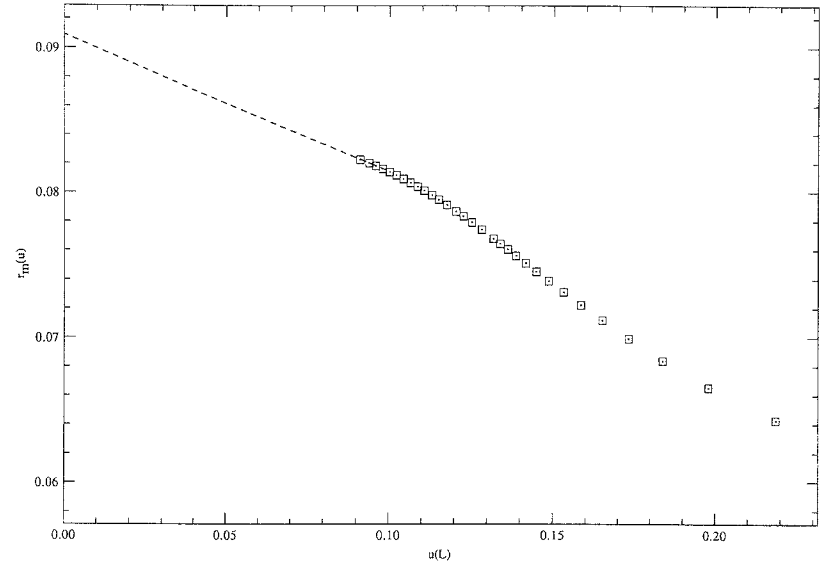

Fig. 9. The reduced deviation $r_m(u) = [x_m(L) - x_m]/u(L)$ as a function of $u(L)$. Symbols and line have the same meaning as in Fig. 8.

APPENDIX

We recall here some relevant results from refs. 17 and 20 concerning the solution of the Wiener–Hopf equation (2.16) for the leading-order finite-size corrections to the root density. We are here interested in the special case $\gamma = 0$, obtained from earlier results[17,20] by first rescaling variables as follows: $\lambda \to \gamma\lambda$, $w \to w/\gamma$, $\sigma \to \sigma/\gamma$, $p \to p/\gamma$, and then taking the limit $\gamma \to 0$.

Neglecting the terms in curly brackets, one may rewrite (2.16) in the form

$$\chi(t) - \int_0^\infty k(t-s)\,\chi(s)\,ds = f(t) - \frac{1}{2N}k(t) + \frac{k'(t)}{12N^2\sigma_0} \tag{A.1}$$

where

$$k(\lambda) = p(\lambda)/\pi \tag{A.2}$$

$$f(\lambda) = \sigma_\infty(\lambda + \Lambda) \tag{A.3}$$

$$\chi(\lambda) = \sigma_N(\lambda + \Lambda) \tag{A.4}$$

$$t = \lambda - \Lambda \tag{A.5}$$

Define Fourier transform pairs $\chi \leftrightarrow X$, $f \leftrightarrow F$, $k \leftrightarrow K$ as in (2.39) and factorize[17] the kernel function $K(w)$ as

$$[1 - K(w)]^{-1} = G_+(w)\, G_-(w) \tag{A.6}$$

where the functions $G_\pm(w)$ are holomorphic and continuous in the half-planes $\pi_\pm$ respectively, and are given by

$$G_+(w) = G_-(-w) = \frac{(2\pi)^{1/2}}{\Gamma(1/2 + z)} z^z e^{-z}, \qquad z = -\frac{iw}{2\pi} \tag{A.7}$$

As $|w| \to \infty$ in π_+, one finds

$$G_+(w) \sim 1 + \frac{g_1}{w} + \frac{g_2}{w^2} + \frac{g_3}{w^3} + O(w^{-4}) \tag{A.8}$$

where

$$g_1 = i\pi/12, \qquad g_2 = 1/2\, g_1^2 \tag{A.9}$$

At $w = 0$,

$$G_+(0) = \sqrt{2} \tag{A.10}$$

The Wiener–Hopf equation (A.1) can be solved[17] by standard techniques, much as in Section 3. Splitting $X(w)$ as

$$X(w) = X_+(w) + X_-(w) \tag{A.11}$$

where

$$X_+(w) = \int_0^\infty e^{iwt} \chi(t)\, dt \tag{A.12}$$

$$X_-(w) = \int_{-\infty}^0 e^{iwt} \chi(t)\, dt \tag{A.13}$$

are holomorphic and continuous in $\pi_\pm$, respectively, one obtains a solution

$$X_+(w) = C(w) + G_+(w)[P(w) + Q_+(w)] \tag{A.14}$$

where $C(w)$ and $P(w)$ are entire functions:

$$C(w) = \frac{1}{2N} + \frac{iw}{12N^2\sigma_0} \tag{A.15}$$

$$P(w) = \frac{ig_1}{12N^2\sigma_0} - \frac{1}{2N} - \frac{iw}{12N^2\sigma_0} \tag{A.16}$$

$$Q_+(w) = \frac{G_+(i\pi)\, e^{-\pi\Lambda}}{(\pi - iw)} \tag{A.17}$$

The constraint (2.21)

$$X_+(0) = \int_\Lambda^\infty \sigma_N(\lambda)\, d\lambda = \frac{1}{2N}[1 + \beta(n)] \tag{A.18}$$

gives rise to the relation

$$\frac{G_+(i\pi)e^{-\pi\Lambda}}{\pi} = \frac{1}{2N} - \frac{ig_1}{12N^2\sigma_0} + \frac{\beta(n)}{2NG_+(0)} \tag{A.19}$$

and using this one finds

$$\sigma_0 \equiv \sigma_N(\Lambda) = \chi(0) = \frac{1}{4N}[a_n + (a_n^2 + \bar{b})^{1/2}] \tag{A.20}$$

where

$$a_n = \pi + ig_1 + \frac{\pi\beta(n)}{G_+(0)} = \frac{\pi}{12}(11 + 12n\sqrt{2}) \tag{A.21}$$

and

$$\bar{b} = \frac{2}{3}(g_1^2 - 2ig_1\pi) = \frac{23\pi^2}{216} \tag{A.22}$$

In the present work, we also need an expression for

$$\sigma'_N(\Lambda) = \lambda'(0) = \frac{-i}{2\pi}\int_{-\infty}^{\infty} dw\, wX(w) \tag{A.23}$$

which may be evaluated by splitting $X(w)$ into components $X_+(w)$ and $X_-(w)$ and performing contour integrations. The result is

$$\sigma'_N(\Lambda) \equiv \sigma'_0 = \frac{ig_1\pi^2 - \pi g_1^2 + ig_3 - ig_1^3/2}{12N^2\sigma_0} + \frac{g_1^2/2 - ig_1\pi - \pi^2 - (\pi + ig_1)\pi\beta(n)/G_+(0)}{2N} \tag{A.24}$$

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