Tunneling and the Spectrum of the Potts Model

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The three-dimensional, three-state Potts model is studied as a paradigm for high temperature quantum chromodynamics. In a high statistics numerical simulation using a Swendson-Wang algorithm, we study cubic lattices of dimension as large as $64^3$ and measure correlation functions on long lattices of dimension $20^2 \times 120$ and $30^2 \times 120$. These correlations are controlled by the spectrum of the transfer matrix. This spectrum is studied in the vicinity of the phase transition. The analysis classifies the spectral levels according to an underlying $S_3$ symmetry. Near the phase transition the spectrum agrees nicely with a simple four-component hamiltonian model. In the context of this model, we find that low temperature ordered-ordered interfaces nearly always involve a disordered phase intermediate. We present a new spectral method for determining the surface tension between phases.

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I. INTRODUCTION

The three-dimensional, three-state Potts model has long been studied as a paradigm for the phase structure of quantum chromodynamics (QCD) at high temperature in the heavy quark limit [1]. It has been found that at zero magnetic field, the Potts model has a weak first order phase transition, separating a low-temperature phase that breaks the $Z(3)$ symmetry and a high-temperature phase in which the symmetry is restored [2]. The underlying $Z(3)$ symmetry requires that at low temperature there be three ordered or broken symmetry phases with the same free energy. In a finite volume system the behavior of the theory in the vicinity of the phase transition is complicated by tunneling among four phases: the three ordered phases and the disordered (symmetry restored) phase.

The Potts model with no magnetic field corresponds to QCD with infinitely heavy quarks—in effect, without any dynamical quarks. A recent study of QCD without quarks by the APE group found that the correlation length of the system appears to grow as the physical volume is increased, suggesting an infinite correlation length in the infinite volume limit, a characteristic of a continuous phase transition [3]. Doubts were raised that the phase transition is first order. The APE study differed from other contemporary work [4] in measuring correlation lengths on lattices with one long dimension. Two more recent high statistics studies with the Potts model and with QCD, using different indicators of the order of the phase transition, have reconfirmed the first order character of the phase transition in both models [5,6]. These more recent studies used a finite-size scaling analysis of susceptibilities to demonstrate a first order transition. The now widely suspected explanation for the confusion over correlation lengths is that finite volume tunneling among the $Z(3)$-equivalent ordered phases introduces a correlation related to the typical domain size of those phases. This correlation length does indeed become infinite in an infinite volume system, as a natural consequence of the first order character of the phase transition.

To test this suspected explanation and to develop new insights into the effects of tunneling, we have carried out a new study of the three-state, three-dimensional Potts model.
on lattices with one long dimension \[3\]. Our study emphasizes the determination of the spectrum of the transfer matrix. We demonstrate explicitly how tunneling modifies the spectrum and, as a consequence, the correlation lengths in the vicinity of the phase transition. Our study parallels work done with the four-dimensional Ising model by Jansen et al \[5\]. Our work makes it possible to understand the results of the several references \[3–6\] in a common framework. In the next section we discuss the \( S_3 \) symmetry of the transfer matrix, develop a phenomenological four-component model for tunneling, and introduce the formulas needed for obtaining the spectrum. In Sec. \[III\] we present results of the simulation. We show that the spectrum and interface statistics agree well with predictions of the four-component model. We obtain the surface tension from the spectral splittings. In the final section we state our conclusions.

II. PHENOMENOLOGY OF THE POTTS MODEL

A. Transfer Matrix and Symmetries

The three-dimensional, three-state Potts model is a classical spin system with one spin \( s_i \) on each site \( i = (x, y, z) \) of a cubic lattice. Let the lattice dimension be \( L_x \times L_y \times L \). Spins take on the values \( s_i \in Z(3) = \{1, \exp(\pm 2\pi i/3)\} \). The partition function of the Potts model at zero magnetic field is given by

\[
Z(\beta) = \sum_{s_i} \exp \left( -\beta \sum_{(i\mu)} \text{Re} s_i^* s_{i+\hat{\mu}} \right),
\]

where \( i + \hat{\mu} \) is the nearest neighbor site in the positive \( \hat{\mu} \) direction and the sum \( s_i \) is over all configurations of spins. Let the spins on a plane of constant lattice coordinate \( z \) be denoted \( S_z = \{s_{x,y,z} | \ x \in 1, \ldots, L_x, \ y \in 1, \ldots, L_y \} \). Then, as is well known, the partition function can be written as the trace of the transfer matrix raised to the power \( L \):

\[
Z(\beta) = \text{Tr} T^L,
\]

where
\[ \langle S_z | T | S_{z+1} \rangle = \exp \left( -\beta \text{Re} s_{(x,y,z)}^* s_{(x,y,z+1)} - \beta \sum_{\mu=1,2} \text{Re} s_{(x,y,z)}^* s_{(x,y,z) + \hat{\mu}} \right). \]  

(3)

The transfer matrix can be regarded as a quantum mechanical operator acting on a Hilbert space of states described by configurations of spins arranged on the \((x, y)\) lattice plane. All operators of present interest are local, and can be expressed as a function of the spins. The expectation value of an operator \(O\) on this ensemble is expressed in terms of the transfer matrix as

\[ \langle O \rangle = \frac{\text{Tr}(T^L O)}{\text{Tr} T^L}. \]  

(4)

Local operators can be regarded as depending on a specific lattice plane \(z\). The correlation between local operators \(A(z)\) and \(B(z')\) with \(z' > z\) is expressed as

\[ \langle A(z) B(z') \rangle = \frac{\text{Tr}(T^z A T^{z'-z} B T^{L-z'})}{\text{Tr} T^L}. \]  

(5)

A hamiltonian matrix \(H\) is defined in terms of the transfer matrix so that

\[ T = \exp(-H). \]  

(6)

Let us write the spectral decomposition of the transfer matrix in terms of the eigenvalues \(E_n\) of the hamiltonian \(H\) as

\[ T = \sum_n |n\rangle \exp(-E_n) \langle n|. \]  

(7)

Let \(n = 0\) denote the ground state. The correlation between two local operators \(A\) and \(B\) can be written in terms of the spectrum as follows:

\[ \langle A(z) B(z') \rangle = \frac{\sum_{mn} \langle m | A | n \rangle \langle n | B | m \rangle \exp[-(E_n - E_m)(z' - z)] \exp(-E_m L)}{\sum_m \exp(-E_m)}. \]  

(8)

In this way correlations between local operators give information about the spectrum of the transfer matrix. (Of course, only the energy level differences \((E_n - E_0)\) have physical significance.)

The Potts model is symmetric under global transformations of the three-fold permutation group \(S_3\). These transformations are generated by
\[ s_i \rightarrow e^{\pm 2\pi i/3}s_i ; \quad s_i \rightarrow s_i^* \quad \forall i. \quad (9) \]

Therefore each of the eigenstates of \( H \) and each of the operators of interest \( O \) can be classified according to the three irreducible representations \( S \) (symmetric), \( A \) (antisymmetric) and \( M \) (mixed, two-dimensional). For example, the spin operator, itself, belongs to \( M \), the operator \( |s|^2 \) belongs to \( S \), and the operator \( \text{Re} s_i \text{Im} s_j - \text{Im} s_i \text{Re} s_j \) belongs to \( A \).

**B. A Simple Model**

To begin with the classification of states, consider first the extreme case \( \beta \rightarrow \infty \). As is well known, the statistical ensemble reduces to three configurations of equal weight, with all spins aligned in either of the three \( Z(3) \) directions. In the Hamiltonian language the ground state of \( H \) at infinite \( \beta \) is three-fold degenerate, with all spins on the \((x, y)\) plane aligned in one of the three directions. Call these three states \(|1\rangle, |2\rangle, \text{ and } |3\rangle\). These states are related by a \( Z(3) \) transformation \( R \) as follows:

\[ |2\rangle = R |1\rangle \quad |3\rangle = R |2\rangle. \quad (10) \]

At the other extreme \( \beta = 0 \) the statistical ensemble contains all spin configurations with equal weight, and the ground state of the Hamiltonian is not degenerate. Call it \(|0\rangle\). These states have finite \( \beta \) counterparts.

Beginning from these extremes, we introduce a phenomenological model for the spectrum at intermediate \( \beta \) in a finite volume system. As \( \beta \) is decreased from infinity, mixing between the three degenerate states occurs. Because of the \( S_3 \) symmetry, the Hamiltonian matrix must be approximately of the form

\[
\begin{pmatrix}
0 & \epsilon & \epsilon \\
\epsilon & 0 & \epsilon \\
\epsilon & \epsilon & 0
\end{pmatrix}.
\]

As a result of mixing, the degeneracy of the three states is lifted, giving rise to a symmetric ground state \(|0s\rangle = |1\rangle + |2\rangle + |3\rangle\) and a twofold degenerate mixed-symmetry state \(|0m\rangle\).
of slightly higher energy. The mixing parameter $\epsilon$ depends on the transverse area $L_xL_y$. Since mixing between the degenerate vacuums requires a rearrangement of the spins over the entire $(x,y)$ plane, it is plausible that the dependence is

$$\epsilon = \exp(-\beta L_xL_y\alpha(\beta)),$$

where $\alpha(\beta)$ is the surface tension for the interface. Indeed at large $\beta$ it is easily shown that $\alpha(\beta) = 3/2$.

In the infinite volume system a phase transition takes place at $\beta = \beta_c$. In a finite volume, crossover occurs at $\beta_c$, where many observables change rapidly. For $\beta < \beta_c$ the ground state $|0s\rangle$ is then identified with the restored-symmetry-phase (disordered) vacuum $|0\rangle$, and the mixed symmetry state $|0m\rangle$ is identified as the lowest lying mixed-symmetry excitation of the symmetric vacuum.

If the phase transition is first order, all four states coexist. Thus to model the rounding of the phase transition, we write the hamiltonian on the simplified basis of the four unmixed vacuum states, $|0\rangle$, $|1\rangle$, $|2\rangle$, and $|3\rangle$ as follows:

$$\begin{pmatrix}
\Delta & \lambda & \lambda & \lambda \\
\lambda & 0 & \epsilon & \epsilon \\
\lambda & \epsilon & 0 & \epsilon \\
\lambda & \epsilon & \epsilon & 0 \\
\end{pmatrix}.$$  

(13)

The row and column labels are in order 0, 1, 2, 3. The parameter $\Delta = \alpha(\beta-\beta_c)$ with $\alpha > 0$ is the energy difference between the disordered (symmetric) phase state $|0\rangle$ and the degenerate ordered phase (broken symmetry) states $|1\rangle$, $|2\rangle$, $|3\rangle$. This difference vanishes at crossover. The parameter $\lambda$ gives the mixing strength between the disordered phase vacuum $|0\rangle$ and the degenerate ordered phase vacuums, and the parameter $\epsilon$ gives the direct mixing strength between the ordered vacuums. The eigenenergies are

$$E_{0s} = \epsilon + \frac{1}{2}\Delta - \frac{1}{2}\sqrt{\Delta^2 - 4\epsilon\Delta + 4\epsilon^2 + 12\lambda^2}$$

$$E_{0m} = -\epsilon$$  

(14)
As expected, there are two states belonging to the symmetric representation of $S_3$: one, the ground state $|0s\rangle$ and the other, an excited state $|1s\rangle$; and there is one twofold degenerate mixed symmetry state $|0m\rangle$ as before. For large $\beta$ we expect the state $|1s\rangle$ to become degenerate with a new excited mixed symmetry state $|1m\rangle$ (not included in our four-component model), in the same pattern as the $|0s\rangle$ and $|0m\rangle$ states. With our criteria for assigning transverse planes to the four phases (see Sec. III B below), the numerical simulation indicates that $\epsilon \ll \lambda$. Thus in the region $\epsilon \ll |\Delta|$, we may approximate the energy levels with

$$E_{0s} = \frac{1}{2}\Delta - \frac{1}{2}\sqrt{\Delta^2 + 12\lambda^2} \quad (15)$$

$$E_{0m} = 0 \quad (16)$$

$$E_{1s} = \frac{1}{2}\Delta + \frac{1}{2}\sqrt{\Delta^2 + 12\lambda^2}. \quad (17)$$

Figure 1 summarizes the expected behavior of the excitation energies, as a function of $\alpha(\beta - \beta_c)/\lambda$, relative to the ground state energy, which has been renormalized to zero in this figure. The lowest two energy differences in this figure come from Eqs. (15-17) and the energy difference $E_{1m}$ is simply a sketch. We see that in a finite system the crossover results in a smooth connection between the energy levels on either side of $\beta_c$. In the infinite volume limit the crossover is much more rapid and the upper wings of the curves in Fig. 1 level off as a consequence of higher level crossings.

By introducing a four-level system we have assumed a first order phase transition. In a continuous phase transition the states $|0\rangle$ and $|0s\rangle$ should be equivalent, and a three-level system would suffice. Although the model focuses on the lowest few levels, it can, of course, be enlarged to incorporate other excited levels as well. Indeed, in order to incorporate the excited levels quantitatively, at least eight levels are needed: four for the states already considered, and four more for the corresponding excited states.

Let us be more explicit about the excitations of the ordered phase. In the infinite volume
limit these vacuums are not mixed. We postulate that the lowest excitation of the state $|1\rangle$ is a state $|1*\rangle$ of mixed symmetry, reachable by acting on the vacuum with the zero momentum spin operator

$$s(z) = \sum_{x,y} s_{(x,y,z)}.$$  \hfill (18)

We shall often refer to the corresponding Schrödinger-picture operator $s \equiv s(0)$. Without loss of generality we introduce only one new state as follows:

$$s |1\rangle = \gamma |1\rangle + \delta |1*\rangle.$$  \hfill (19)

The corresponding excitations in the other vacuums are reached by a $Z(3)$ transformation $R$ in analogy with Eq. (10) as follows

$$|2*\rangle = R |1*\rangle \quad |3*\rangle = R |2*\rangle.$$  \hfill (20)

Since $RsR^{-1} = \exp(-2\pi i/3)s$, the $Z(3)$ symmetry requires

$$s |2\rangle = e^{2\pi i/3(\gamma |2\rangle + \delta |2*\rangle)}$$
$$s |3\rangle = e^{-2\pi i/3(\gamma |3\rangle + \delta |3*\rangle)}.$$  \hfill (21)

Now just as mixing between the degenerate vacuums leads to a symmetric state $|0s\rangle$ and two mixed symmetry states $|0mk\rangle$ ($k = 1, 2$ labels the two degenerate components), we expect mixing among the excited state counterparts to result in a symmetric state $|1s\rangle$ and a mixed symmetry state $|1mk\rangle$. With this notation we are implicitly identifying these states with the levels of Fig. [I]. From the $S_3$ symmetry we then obtain explicit formulas for the matrix elements of the spin operator between these states:

$$\sum_{k=1,2} |\langle 1s | s |0mk\rangle|^2 = \delta^2$$
$$\sum_{k=1,2} |\langle 0s | s |0mk\rangle|^2 = \gamma^2$$
$$\sum_{k=1,2} |\langle 0s | s |1mk\rangle|^2 = \delta^2$$
$$\sum_{k=1,2} |\langle 1s | s |1mk\rangle|^2 = \gamma^2.$$  \hfill (23)
We note also that if mixing among the degenerate states is weak the symmetric operator $|s|^2$ satisfies

$$|\langle 1s | s^2 | 0s \rangle|^2 = \sum_{k=1,2} |\langle 1mk | s^2 | 0mk \rangle|^2.$$  \hspace{1cm} (24)

\section*{C. Correlations}

We now write working formulas for the correlations between the spin operators $s$ and $|s|^2$, based on the lowest lying levels discussed above.

First, we observe that matrix elements must obey selection rules of the $S_3$ symmetry. For example, the spin operator $s$ is of mixed symmetry. The two components of the operator are just $(\text{Re } s, \text{Im } s)$. Thus matrix elements $\langle n | s | m \rangle$ vanish if $|m\rangle$ and $|n\rangle$ are both symmetric.

Since $|s|^2$ is a symmetric operator, matrix elements $\langle n | s^2 | m \rangle$ vanish if $|m\rangle$ and $|n\rangle$ are not in the same $S_3$ representation.

Therefore, the leading nonvanishing terms in the correlation for $|s|^2$ from Eq. (8) are

$$\langle |s(z)|^2 s(0)|^2 \rangle = |\langle 0s | s^2 | 0s \rangle|^2 + |\langle 1s | s^2 | 0s \rangle|^2 \left[e^{-E_{1s}z} + e^{-E_{1s}(L-z)}\right]$$

$$+ |\langle 1m | s^2 | 0m \rangle|^2 \left[e^{-(E_{1m}-E_{0m})z} + e^{-(E_{1m}-E_{0m})(L-z)}\right]e^{-E_{0m}L},$$  \hspace{1cm} (25)

and for $s$ it is

$$\langle s(z)s^*(0) \rangle = |\langle 0m | s | 0s \rangle|^2 \left[e^{-E_{0m}z} + e^{-E_{0m}(L-z)}\right] + |\langle 1m | s | 0s \rangle|^2 \left[e^{-E_{1m}z} + e^{-E_{1m}(L-z)}\right]$$

$$+ |\langle 1s | s | 0m \rangle|^2 \left[e^{-(E_{1s}-E_{0m})z} + e^{-(E_{1s}-E_{0m})(L-z)}\right]e^{-E_{0m}L}$$

$$+ |\langle 1m | s | 0m \rangle|^2 \left[e^{-(E_{1m}-E_{0m})z} + e^{-(E_{1m}-E_{0m})(L-z)}\right]e^{-E_{0m}L},$$  \hspace{1cm} (26)

The six transitions taken into account in these expressions are indicated in Fig. 1.

Clearly, in order for the several transitions for be discernible in the fits to correlation functions, it is necessary that the spectral components be both strong and well-separated.

With our data we are able to distinguish two spectral components for the mixed operator and find only one significant spectral component for the symmetric operator. These
transitions correspond to dropping all terms with the factor \(\exp(-E_{0m}L)\). For the mixed operator, this approximation can be justified as follows: (1) Over the range \(\beta < \beta_c\), the factor \(\exp(-E_{0m}L)\) is small (at the largest, of order 1/10). This factor multiplies the third term on the rhs in both expressions and the fourth term in the second expression. Appealing to our phenomenological model and Eqs. (23) and (24), which makes it possible to compare the second and third terms, we see that we may drop terms in \(\exp(-E_{0m}L)\) from the summation, thereby eliminating all transitions leading to the level \(E_{0m}\). (2) Over the range \(\beta > \beta_c\), the spectral lines for all transitions from the levels \(1s\) and \(1m\) to \(0s\) and \(0m\) are too close to be resolvable with our statistics. Thus the second spectral component in the mixed operator is presumably a composite of all three transitions permitted by the selection rules. For the symmetric operator our failure to locate the second spectral component presumably reflects an insufficiently strong coupling to this operator.

We are left, finally, with a three-parameter expression for the symmetric operator and a four-parameter expression for the mixed operator:

\[
\begin{align*}
\langle |s(z)|^2 |s(0)|^2 \rangle & = A_1 + A_2 [e^{-E_{1sz}} + e^{-E_{1s(L-z)}}] \\
\langle s(z)s^*(0) \rangle & = C_1 [e^{-E_{0mz}} + e^{-E_{0m(L-z)}}] + C_2 [e^{-E_{1mz}} + e^{-E_{1m(L-z)}}].
\end{align*}
\]

\(28\)

**III. NUMERICAL SIMULATION**

Since the simulation of tunneling effects requires an algorithm that gives efficient and rapid sampling of the phase space, particularly in the crossover region, we used the Swendson-Wang (SW) algorithm [9]. The code was checked by comparing measured observables in selected extensive runs with results from simulations using a heat bath algorithm.

Simulations were carried out on cubic lattices of size \(N^3\), for \(N = 16, 20, 24, 30, 48,\) and \(64\) in order to confirm the first order nature of the phase transition through the use of finite-size scaling analysis. For this purpose we measured the specific heat and the fourth-order cumulant. Table I summarizes the extent of this data sample. The majority of the
simulations were carried out on “cylindrical” lattices to obtain the spectrum of the transfer matrix. These lattices were of size $120 \times 20^2$ for 18 values of $\beta$ and with size $120 \times 30^2$ for 17 values of $\beta$, as summarized in Table II. Runs of as many as two million sweeps made it possible to gain control of the correlated data and to obtain good estimates of the parameter errors.

A. Simulations on cubic lattices

In Fig. 2 is shown a histogram in the average energy for the $64^3$ lattice near $\beta_c$. A clean separation of the phases is apparent. The importance of finite size scaling for determining the order of a phase transition has been repeatedly emphasized [5,6]. Although these references already provide excellent confirmation of the first order character of the phase transition, our high statistics results make an even stronger case. Indeed, with such a clean separation of phases in the $64^3$ lattice, it is scarcely necessary to belabor the point. Nevertheless, we present the finite size scaling results for the sake of completeness. The fourth order cumulant [10],

$$V_L(\beta, V) = 1 - \frac{\langle E^4 \rangle}{3 \langle E^2 \rangle^2},$$  

(29)

is minimum near the crossover $\beta_c$. At a continuous phase transition, the minimum value $V_L(\beta_c, V)$ tends to $\frac{2}{3}$ in the infinite volume limit. At a first order phase transition, however, the limit is not so constrained, but obeys a scaling law,

$$V_L(V)_{\text{min}} \to 1 - \frac{(E_+^2 + E_-^2)^2}{12(E_+ E_-)^2} + O(1/V),$$  

(30)

where $E_+$ and $E_-$ are the most probable energies in the two coexisting phases.

The minimum value of the cumulant was found by combining measurements at a range of $\beta$ values near $\beta_c$, using a Ferrenberg-Swendson “scanning” or “histogram” technique [11]. The resulting minimum values are plotted in Fig. 3. A linear fit yields the asymptotic value $0.647(3)$, clearly distinct from $\frac{2}{3}$.
We turn now to the specific heat. At finite volume the specific heat $C_v$ peaks at the crossover. The maximum value $C_{v,max}$ increases with increasing volume. If the phase transition is first order, the peak scales as

$$C_{v,max} = a + bV.$$  \hspace{1cm} (31)

The maximum is again determined using the Ferrenberg-Swendson technique. These values are plotted in Fig. 4. A linear increase is apparent.

A value of $\beta_c$ can be fixed, either from the peak in the specific heat, or from the minimum of the cumulant $V_L$. The two values do not necessarily agree at finite volume, but should agree in the infinite volume limit. In the infinite volume limit we find $\beta_c,\infty = 0.36704(2)$ in agreement with Gavai, Karsch and Petersson [5].

### B. Simulations on cylindrical lattices

Measurements on the asymmetrical lattices were taken every 250 SW sweeps. Observables recorded were these: the spin averages $s(z)$ as a function of $z$ [Eq. (18)], the average energy,

$$E = \beta \sum_{(\mu)} \text{Re} s_i^* s_{i+\mu}/V,$$  \hspace{1cm} (32)

and the number of clusters $N_c$. Subsequent analysis produced the symmetric and mixed operator correlations and spectrum, the mean spins, and the projected-spin order parameter

$$s_{\text{proj}} = \max \text{Re}(\bar{s}, e^{2\pi i/3} \bar{s}, e^{-2\pi i/3} \bar{s}),$$  \hspace{1cm} (33)

where $\bar{s} = \sum s_i/V$. Also constructed were interface statistics. They are described below. For observables not discussed here, see Ref. [6].

#### a. Spectrum of the Transfer Matrix

Correlations in the operators $|s(z)|^2$ and $s(z)$ were measured and fit to the formulas (28) for both transverse sizes $20^2$ and $30^2$. As usual, fluctuations in the measurements were strongly correlated in $z$, so it was necessary to determine
these correlations and incorporate them in the $\chi^2$ analysis. Because of the large size of the data sample, it was possible to use all principal factors in the analysis of covariance. The spectrum was determined from a global fit to the data. The fitting range began at a minimum distance $z_{\text{min}}$ and extended to the full length of the lattice. The minimum distance was varied until a semblance of a plateau in the spectrum was reached, within the determined statistical errors. The values quoted are based on the minimum distance that gave the highest confidence level for the fit. The minimum distance thus determined varied smoothly from 2 for the mixed operator at the smallest $\beta$ where the correlation length is shortest to 8 at the largest $\beta$ where the correlation length is longest. For the symmetric operator $z_{\text{min}}$ was 5 for the smallest and largest $\beta$’s, ranging gradually to 15 – 20 for the intermediate values where the correlation length is longest. The resulting spectrum is summarized in Figs. 5, 6, 7, and 8 and in Tables III and IV. There is obviously a strong resemblance with features of the simple model of Sec. II B. From Fig. 7 and 8, we see that the correlation length tends to infinity as $\beta$ increases above $\beta_c$, just as with lattices of similar geometry in SU(3) Yang-Mills theory [3]. As we have seen in the simple model, this feature is an expected consequence of finite volume tunneling between the degenerate ordered phases.

b. Tunneling Statistics

In Fig. 9 we plot the slice spin averages $s(z)$ for a representative configuration at $\beta > \beta_c$, showing tunneling between the ordered phases. We devised two statistics: $N_{\text{do}}$, to give a measure of the number of phase boundaries between the disordered and one of the ordered domains, and a statistic $N_{\text{oo}}$, for phase boundaries between two ordered domains. A portion of the lattice was considered to be in the disordered phase on the plane $z$, if $|s(z)| < 0.23$ for at least three consecutive values of $z$. If $|s(z)| > 0.23$ for at least three consecutive values of $z$, the lattice plane was considered to be in one of the three ordered phases, according to the value of $\arg s(z)$. The value 0.23 was chosen to correspond to the minimum of the histogram of occurrences of values of $|s|$ at the crossover, and so corresponds to a value intermediate between the disordered and ordered phases. The requirement of three consecutive planes was adopted to permit occasional excursions from the ideal value of 0.23 within a single phase. We encountered no configurations that did not
have at least three consecutive planes. Indeed the phase coherence was extremely high with many lattices consisting of a single phase.

Obviously our classification criteria are arbitrary. Our approach differs from that of Karsch and Patkó [12] who classified all boundaries as type oo for $\beta > \beta_c$. The ambiguity all methods must deal with is distinguishing a broad interface between two ordered phases from a transition to an intermediate disordered phase. Any definition must recognize, however, that in perturbation theory, finite volume mixing necessarily produces a disordered phase intermediate for $\beta$ slightly above $\beta_c$.

Shown in Figs. 10, 11, and 12 are results for the measure of the mean numbers $N_{oo}$ and $N_{do}$. It is apparent that with our definitions of these boundaries, a transition between two ordered phases is unlikely to take place directly, but proceeds through what we identify as a disordered phase intermediate. (Figure 11 shows the number of oo phase boundaries for the $120 \times 20^2$ lattices. The corresponding number for $120 \times 30^2$ is negligible.) Thus if we interpret these results in terms of the model of Sec. II B, we find that $\epsilon << \lambda$. Thus the approximation, Eqs. (15-17) applies. Inverting these expressions, the parameters $\Delta$ and $\lambda$ of the simple model can then be derived from the observed spectrum:

$$\Delta = E_{1s} - 2E_{0m}$$

$$\lambda = \sqrt{E_{0m}(E_{1s} - E_{0m})/3}$$

Let us estimate the number of “do” (ordered/disordered) phase boundaries expected in our four-component model. Since $\lambda$ in the four-component hamiltonian mixes the disordered and ordered states, we can introduce a chemical potential for do boundaries by replacing $\lambda$ with $\lambda e^\mu$. Thus the number of do boundaries is just

$$\langle N_{do} \rangle = \lambda \frac{\partial}{\partial \lambda} \ln Z,$$

but from Eqs. (2), (6), and (15) we have $\ln Z \approx -LE_{0s}(\lambda)$, so

$$\langle N_{do} \rangle \approx 6L\lambda^2 / \sqrt{\Delta^2 + 12\lambda^2}.$$
This predicted value (for $\beta > \beta_c$) is plotted together with the observed number in Fig. 11. The agreement is quite satisfactory.

c. Surface Tension The surface tension between two ordered phases can be estimated in perturbation theory (dilute interface approximation) through

$$\lambda^2/\Delta = e^{-\beta\alpha_{ord}}.$$ (38)

The quantity on the left is the transition probability between two ordered phases via a disordered phase intermediate in second order perturbation theory, based on the four-component hamiltonian, and the quantity on the right is the Boltzmann weight for the interface. Thus estimated, it is plotted in Fig. 13. There is a strong dependence on the transverse size, suggesting a significant finite size correction. Karsch and Patkós [12] measured the surface tension in the Potts model and also find a strong dependence on transverse size. They follow a statistical approach based on the frequency of oo interfaces, using a different definition from ours, which excludes all do interfaces. For example the configuration of Fig. 9 yields nine “bare domain walls” in their language, but all presumably classified in their scheme as “defects” and not genuine interfaces. Perhaps it is not surprising, therefore, that our surface tension is two to three times lower than theirs (after making allowances for different conventions in the hamiltonian). Clearly the determination of surface tension is model dependent.

IV. SUMMARY AND DISCUSSION

Our high statistics study of the three-state three-dimensional Potts model using the Swendson-Wang updating scheme once again confirms the first order character of the phase transition. At volumes as large as $64^3$ the separation of coexisting phases is so clear that a sophisticated finite size scaling analysis is scarcely necessary.

Exploiting an $S_3$ symmetry in lattices with one long dimension, we have obtained the lowest spectral levels of the transfer matrix in this model and find excellent agreement with
the spectrum of a simple four-component model, featuring a first order phase transition. This analysis provides a clear explanation of the mechanism that gives rise to an infinite correlation length in the low temperature phase.

The statistics of phase boundaries at low temperature are consistent with a perturbative treatment of tunneling in the four-component model. With our assignment of planes to phases, we find that ordered-ordered phase boundaries almost always involve an intermediate disordered phase. We introduced a spectral method for estimating the surface tension, based on the four-component model.

One important goal of finite size spectral analysis is to remove tunneling-related finite-size effects from the spectrum, with the hope of extracting the infinite volume values of the excitation spectrum. Would this be feasible using our methods? Unfortunately, to remove significant finite size effects apparently requires introducing more parameters into the four-component model and into our fitting functions than data of the quality of ours warrants. The four component model would have to be augmented by at least four more components. Thus we must rely upon alternate, empirical methods. For example, Fukugita et al [6] calculate in a cubic volume. In the vicinity of the phase transition, they classify configurations into two groups: disordered and ordered, according to the value of the global order parameter. They then measure “pure-phase” correlation lengths in each subset. For small volumes there is a region of overlap in which this classification risks misidentification of the phase. The contamination of incorrectly classified configurations decreases as the volume is increased and the overlap decreases. Thus one may hope for an empirically determined extrapolation to the infinite volume limit.

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FIGURES

FIG. 1. Phenomenological model of the lowest three energy levels at crossover. The ground state energy has been adjusted to zero at all $\beta$. The level $E_{1m}$ does not come from the model; it is based merely on a guess. The others come from the four-component model Eq. (15-17). Transitions induced by a mixed operator are indicated with “M” and a symmetric operator with “S”.

FIG. 2. Histogram in the average energy at $\beta = 0.36705$ (near the critical value) on a $64^3$ lattice, showing cleanly separated coexisting phases.

FIG. 3. Finite size scaling of the minimum in the fourth order cumulant.

FIG. 4. Finite size scaling of the peak in the specific heat.

FIG. 5. Energy level $E_{1s}$ of symmetry $S$ for the $20^2 \times 120$ lattice, as a function of $\beta$.

FIG. 6. The same, but for the $30^2 \times 120$ lattice

FIG. 7. Energy levels $E_{0m}$ and $E_{1m}$ of symmetry $M$ for the $20^2 \times 120$ lattice, as a function of $\beta$.

FIG. 8. The same, but for the $30^2 \times 120$ lattice
FIG. 9. Plot of the complex modulus and argument of the spin vector $s(z)$ vs $z$ (averaged over the transverse plane) for a typical configuration selected from the data sample at $\beta = 0.3672$ (near the phase transition) on a $20^2 \times 120$ lattice. The plot symbol indicates the phase to which the lattice plane is assigned, based on modulus and argument. The vertical bars indicate an assigned phase boundary, based on our arbitrary rule that at least three consecutive planes must be classified in that phase. The horizontal line in the modulus plot indicates our division between ordered and disordered phases. Two ordered-ordered phase boundaries appear in this configuration, each with a disordered phase intermediate.

FIG. 10. Average number of phase boundaries separating ordered symmetry phases for $120 \times 20^2$.

FIG. 11. Average number of phase boundaries separating a disordered phase from an ordered phase for $120 \times 20^2$. Crosses are measured directly. Octagons are calculated from the spectrum in the four-component model.

FIG. 12. Same, but for $120 \times 20^3$.

FIG. 13. Ordered-ordered interface surface tension determined by spectral methods in the four-component model. Octagons are for $20^2$; crosses are for $30^2$. 
### TABLE I. Data sample for cubic lattices

| $V$   | $\beta$     | sweeps ($10^6$) |
|-------|-------------|-----------------|
| $16^3$| 0.3663      | 0.6             |
| $20^3$| 0.3665      | 0.5             |
| $24^3$| 0.3667      | 0.7             |
| $30^3$| 0.3669      | 0.7             |
| $48^3$| 0.3670      | 0.5             |
| $64^3$| 0.36705     | 0.5             |
| $\beta$  | $120 \times 20^2$ | $120 \times 30^2$ |
|--------|-----------------|-----------------|
| .3650  | 1.0             | 1.0             |
| .3655  | —               | 1.0             |
| .3660  | 1.0             | 1.0             |
| .3665  | 1.0             | 1.0             |
| .3668  | 2.0             | 1.0             |
| .3669  | 2.0             | 2.0             |
| .36695 | 2.0             | 2.0             |
| .3670  | 2.0             | 2.0             |
| .36705 | 2.0             | 2.0             |
| .3671  | 2.0             | 2.0             |
| .36715 | 2.0             | 2.0             |
| .3672  | 3.0             | 2.0             |
| .36725 | 2.0             | 2.0             |
| .3673  | 1.0             | 1.0             |
| .3674  | 1.0             | 1.0             |
| .3675  | 1.0             | 1.0             |
| .3678  | 1.0             | —               |
| .3680  | 1.0             | 1.0             |
| .3685  | 1.0             | —               |
TABLE III. Effective masses and couplings for the $120 \times 20^2$ lattice

| $\beta$   | $A_1$  | $A_2$  | $E_{1s}$ | $C_1$   | $E_{0m}$ | $C_2$   | $E_{1m}$ |
|----------|-------|-------|----------|---------|----------|---------|----------|
| .3650    | 2.38(1)| 0.5(1)| .231(27) | 2.9(1)  | .167(5)  | 0.18(11)| .54(28)  |
| .3660    | 3.20(3)| 0.94(7)| .168(10)| 3.3(9)  | .10(2)   | 1.0(9)  | .20(7)   |
| .3665    | 4.36(4)| 1.6(2)| .118(9)  | 5.8(1)  | .072(1)  | 0.31(4)| .54(11)  |
| .3668    | 6.11(6)| 2.6(3)| .109(8)  | 8.0(1)  | .048(1)  | 0.30(5)| .34(11)  |
| .3669    | 7.17(7)| 2.5(2)| .088(6)  | 9.3(1)  | .0397(6)| 0.34(9)| .41(12)  |
| .36695   | 7.8(1) | 2.9(4)| .095(11)| 10.1(2)| .037(1)  | 0.34(1)| .41(18)  |
| .3670    | 8.51(8)| 2.7(4)| .088(10)| 10.8(1)| .0346(6)| 0.24(6)| .31(16)  |
| .36705   | 9.59(9)| 2.8(4)| .084(9)  | 11.8(1)| .0302(4)| 0.26(8)| .38(17)  |
| .3671    | 10.5(1)| 3.0(4)| .084(9)  | 12.4(1)| .0272(4)| 0.35(5)| .28(8)   |
| .36715   | 11.8(1)| 2.8(4)| .082(9)  | 13.2(3)| .0233(6)| 0.6(3) | .12(5)   |
| .3672    | 13.2(1)| 2.8(1)| .082(3)  | 14.1(4)| .0207(6)| 0.5(3) | .11(7)   |
| .36725   | 14.4(1)| 2.6(2)| .081(5)  | 14.5(6)| .0180(7)| 0.8(4)| .10(5)   |
| .3673    | 15.8(2)| 2.8(4)| .085(11)| 15.4(4)| .0159(7)| 0.8(2)| .14(9)   |
| .3674    | 18.6(2)| 1.8(2)| .068(12)| 16.2(3)| .0122(5)| 1.8(8)| .21(7)   |
| .3675    | 20.7(2)| 1.5(3)| .076(14)| 16.9(3)| .0102(5)| 0.9(3)| .18(8)   |
| .3678    | 25.5(1)| 1.3(1)| .142(11)| 15.6(5)| .0039(6)| 1.3(1)| .14(3)   |
| .3680    | 27.2(1)| 1.12(5)| .175(9) | 15.9(4)| .0029(4)| 1.2(2)| .23(4)   |
| .3685    | 30.4(1)| 1.03(6)| .256(13)| 15.7(3)| .0007(3)| 1.2(1)| .28(3)   |
TABLE IV. Effective masses and couplings for the $120 \times 30^2$ lattice

| $\beta$ | $A_1$  | $A_2$  | $E_{1s}$ | $C_1$  | $E_{0m}$ | $C_2$  | $E_{1m}$ |
|---------|--------|--------|----------|--------|----------|--------|----------|
| .3650   | 1.02(1)| 0.2(1) | .30(5)   | 1.2(1) | .182(8)  | .1(1)  | .39(16)  |
| .3655   | 1.11(1)| 0.23(6)| .25(3)   | 1.29(8)| .157(6)  | .15(7) | .45(14)  |
| .3660   | 1.23(1)| 0.38(8)| .25(3)   | 1.56(2)| .143(3)  | —      | —        |
| .3665   | 1.48(1)| 0.44(9)| .15(2)   | 1.74(9)| .101(4)  | .24(9) | .30(6)   |
| .3668   | 2.03(3)| 0.74(6)| .065(7)  | 2.3(2) | .052(3)  | .59(18)| .16(3)   |
| .3669   | 3.21(6)| 1.28(5)| .061(4)  | 3.7(1) | .031(1)  | .72(12)| .13(1)   |
| .36695  | 4.09(9)| 1.61(4)| .044(4)  | 5.2(1) | .0262(6)| .39(4) | .19(2)   |
| .3670   | 6.3(2) | 2.02(7)| .038(5)  | 7.3(1) | .0185(3)| .41(3) | .20(2)   |
| .36705  | 9.9(3) | 2.1(1) | .033(6)  | 9.9(1) | .0133(2)| .38(3) | .21(3)   |
| .3671   | 14.4(2)| 1.6(1) | .039(6)  | 11.8(1)| .0092(2)| .55(4) | .14(1)   |
| .36715  | 17.4(3)| 1.3(2) | .030(9)  | 12.6(1)| .0664(2)| .65(3) | .16(1)   |
| .3672   | 19.6(1)| 0.98(3)| .066(4)  | 12.5(2)| .0044(2)| .75(4) | .12(1)   |
| .36725  | 20.9(1)| 0.85(8)| .085(7)  | 12.2(2)| .0028(2)| .86(3) | .12(1)   |
| .3673   | 21.6(1)| 0.7(1) | .09(1)   | 12.6(2)| .0027(3)| .73(4) | .13(1)   |
| .3674   | 23.1(1)| 0.5(2) | .11(2)   | 12.3(3)| .0011(4)| .69(4) | .15(2)   |
| .3675   | 24.1(1)| 0.5(1) | .13(1)   | 12.7(2)| .0010(3)| .8(1)  | .19(2)   |
| .3680   | 27.8(1)| 0.50(7)| .22(2)   | 14.0(3)| .0001(3)| .50(5) | .22(1)   |
