

# The 3-q Potts Model in 3 dimensions: An Interface Tension Study

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We study the behavior of the order–order interface tension of the 3- $q$  3D Potts model as a function of the interface area and the coupling constant by means of a Monte Carlo and the Capillary Wave Model (CWM). We check the validity of the CWM in the case of the 3D Potts model by comparing Monte Carlo data for the energy gap  $E$  with the CWM predictions. We verify that the zero-loop contribution to the CWM is an adequate way of describing rough interfaces only in the case of transversally symmetric lattices. We observe, also, that the 3D 3- $q$  Potts model order–order interface tension varies linearly with the coupling constant.

## I. Introduction

The interface tension  $\sigma$ , which is the free energy per unit of area of the interface, is a very important quantity for field theoreticians, as it has applications in the discussion of phase transitions in the early universe as well as in heavy-ion physics. If the high temperature phase transition of QCD is of the interface tension between hadronic matter and quark-gluon plasma is an important parameter for the formation of quark-gluon plasma in heavy-ion collisions and for the nucleation of hadronic matter in the early universe. To obtain an estimate of the interface tension of QCD we must neglect the quarks and concentrate on a pure SU(3) gauge theory. In this case, the phase transition is of first order and, at the critical temperature, the confined and deconfined phases coexist and the interface tension is non-zero.

In the last years many different methods have been introduced to compute numerically the SU(3) lattice theory interface tension. As the calculations are very hard and computationally very costly, the lattices involved are not very large. Because all of these problems, in the last few years particle physicists have begun to show a great interest in the study of spin models<sup>[1–4]</sup>. The reason for this interest lies in the fact that an effective theory for the order parameter of an  $(N + 1)$ -dimensional gauge theory has the same global symmetry as the  $N$ -dimensional  $Z(N)$  spin model. In this context, Svetitsky and Yaffe have predicted a first-order phase transition to the SU(3) gauge theory using results obtained for the  $Z(3)$  spin system<sup>[5]</sup>. In this context, also, the study of three-dimensional Potts models is very important. This model is computationally much more simple than lattice QCD, and, as a consequence, it

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is particularly suitable for testing the calculation methods.

The 3D-3q Potts model belongs to the same universality class of pure gauge QCD<sup>[6]</sup>. This means that both models have phase transitions that are characterized by spontaneous symmetry breaking of a global  $Z(3)$  symmetry. Thus, in contrast to what happens to full QCD, in the case of the pure gauge QCD and the 3q-3D Potts model there are three distinct ordered phases coexisting at temperatures above the critical one and a disordered phase below this temperature. At the critical temperature all four phases coexist with each other. Besides the order-disorder interfaces, there are also interfaces between the different oriented domains. Unlike the order-disorder interfaces, these order-order domain walls exist for all temperatures in the symmetry broken phase of the Potts model as well as the pure  $SU(3)$  gauge theory.

Interfaces separating coexisting phases at thermal equilibrium are present not only in the 3D-3q Potts model, but also in the 3D Ising model, among others. The behavior of these 3D finite volume interfaces are highly dependent of the temperature. At low temperatures, between the critical and roughening temperatures, these interfaces are often dominated by long-wavelength fluctuations, that is, they behave as fluid or rough interfaces<sup>[7,25]</sup> (all interface is said to be fluid when it may freely and continuously translated through space). These soft modes play an essential role in the description of finite-size effects in the free energy of the interfaces<sup>[7,27]</sup>.

While far below the roughening temperature interfaces are almost rigid and a theoretical approach can be taken<sup>[8]</sup>, above it one is forced to assume an effective model describing the collective degrees of freedom of the rough interfaces.

An effective model widely used to describe a rough interface is the Capillary Wave Model<sup>[9]</sup> where, in its simplest formula, the effective hamiltonian is proportional to the area of the interface. In a couple of papers<sup>[10,11]</sup>, it has been shown that a rough interface with a rather general shape ( $L_1 \neq L_2 \ll L_3$ ) can be efficiently described by the one-loop approximation to the CWM. In the case of the 3D Ising model, the CWM has successfully described many characteristics of its interfaces (like logarithmic growth of the interfa-

cial width<sup>[28]</sup> and FSE<sup>[11]</sup>), while for the 3D Potts model the CWM was applied for only one value of the coupling constant<sup>[12]</sup>. The one-loop approximation to the CWM (whose expression is also known as the gaussian form) differs from the zero-loop or classical description only when one deals with lattices that have different transverse sizes ( $L_1 \neq L_2$ ). When the transverse lattice sizes are equal ( $L_1 = L_2 = L$ ), it is observed that the expression for the one-loop approximation to the CWM is coincident with that of the classical description, that is, one obtains the usual expression for the interface free energy,

$$\frac{F}{\kappa T} = \sigma L^2 \quad (1)$$

where  $F$  is the interface free energy and  $\sigma$  is the reduced interface tension.

The calculation of higher-order corrections to the CWM is certainly needed in order to verify the validity of this model beyond the one-loop correction. While many different effective hamiltonians reduce to the gaussian form at one-loop level<sup>[24]</sup> they have different expressions for the two- and higher-loop corrections. The two-loop correction depends directly on the area of the interface and, as a consequence, the expression for the finite-size behavior of the energy splitting  $E$  occurring between two vacua on finite volumes does not coincide with the classical functional form,

$$E_{\text{class}}(L) \approx \exp(-\sigma L^2) , \quad (2)$$

even when one deals with symmetric transverse lattices.

In this paper we will study the finite-size behavior of rough order-order interfaces in the 3D-3q Potts model using Monte Carlo simulations with a Metropolis algorithm and the predictions of the CWM in its simplest formulation. To compare the predictions of the CWM with the numerical results obtained from the Monte Carlo simulations we are going to use 3D lattices with  $L_1 \times L_2 \times L_3$  sites, where  $L_3 \gg L_1, L_2$ , and periodic boundary conditions are imposed in all directions. With these lattice shapes we will practically eliminate all interfaces that are not orthogonal to the lattice longest size ( $L_3$ ).

The 3D Potts model, which is known to have a weak first order phase transition<sup>[13,3]</sup>, has been extensively studied in the last few years, mainly for its relation

to the finite-temperature SU(3) Yang–Mills theory. In most of these studies, the focus of attention lies in the properties of the order-order and order-disorder interface tensions<sup>[14,4,1]</sup>, which correspond to the interface tension between a hadronic and a quark-gluon phase in QCD. In all of these studies the interface tensions were obtained from the use of symmetric transverse lattices (in which  $L_1 = L_2$ ) and the classical formula eq.2.

We will follow the lines of [2] in order to obtain, by way of a numerical simulation, the values of the energy splitting  $E$  between two vacua on finite volumes. Afterwards, we will use the functional form of the fluid interface free energy on finite volumes, including higher-order capillary-wave contributions, in order to calculate the interface tension for a fixed value of the inverse of the temperature  $\beta$ . Finally, we obtain the behavior of the order-order interface tension as a function of the coupling constant  $\beta$ .

This paper is organized in the following way: In Section II, we describe the capillary wave model and we show the expressions for the zero-, one- and two-loop approximations for the partition function. In Section III, we define the Hamiltonian for the Potts model and we show how we can link the Capillary Wave model to the 3D 3-q Potts model. In Section IV we show the observables we are going to calculate, discuss how we are going to use these observables in order to check the

predictions of the CWM and to obtain the behavior of the order-order interface tension as a function of the coupling constant. We discuss, also, the particularities of the Monte Carlo simulations and we present our results. In the last section we present our conclusions.

## II. The capillary wave model

The basic hypothesis of the Capillary Wave Model (CWM) of rough interfaces is that one cannot neglect the long wavelength fluctuations in the position of the interfaces since they cost very little in energy. In this model, an effective hamiltonian describing the fluctuations of interfaces separating phases in equilibrium must be introduced. This hamiltonian is such that any distortion of an interface of tension  $\sigma$  will generate a change in the free energy that is proportional to the increment in area of the interface.

As our geometry forces the interface to be orthogonal to the longest lattice size, the interfaces will lie in a D-1 dimensional plane. The interface configurations are, thus, described by a function  $y(r, t)$  where  $r$  and  $t$  are transverse coordinates in orthogonal plane and  $y$  is the interface displacement from the equilibrium position. Making the hypothesis of single-valuedness of the function  $y(r, t)$  and, that, as a consequence we can neglect overhangs and bubbles from one phase in the other, we can write the effective hamiltonian as,

$$H_{CW} = \sigma \int_0^R dr \int_0^T dt \left( \sqrt{1 + \left(\frac{\partial y}{\partial r}\right)^2 + \left(\frac{\partial y}{\partial t}\right)^2} - 1 \right) = \sigma A(y) - RT \tag{3}$$

where  $\sigma$  is the order-order interface tension,  $R = L_1$  and  $T = L_2$  are the lattice sizes in the  $r$  and  $l$  directions and  $\sigma A(y)$  (where  $A(y)$  is the area of the interface) coincides with the Nambu-Goto string action in a special frame. The full hamiltonian is too complicated to be handled in an exact way, and, in order to apply the CWM we must expand the square root term in the hamiltonian in powers of the adimensional parameter  $(\sigma A)^{-1} = (\sigma RT)^{-1}$  where  $(\sigma A)^{-1} \rightarrow 0$ .

In the Capillary Wave Model the interface between two domains of different magnetization in the ordered phase of a 3D system is described by the partition function

$$Z_{CW} = \int [Dx] \exp\{-\sigma A(y)\} = C \exp(-\sigma RT) Z_q(\sigma, R, T) \tag{4}$$

where

$$Z_q = \int [Dy] \exp\{-H_{CW}(y)\} = Z_q^{1\text{loop}} \left(\frac{R}{T}\right) Z_q^{2\text{loop}} \left(\frac{R}{T}, \sigma RT\right) \dots \tag{5}$$

and  $C$  is all unknown constant.

Keeping only the leading order term in the expansion of  $H_{CW}$  we get the following expression for the effective hamiltonian,

$$H_G = \frac{\sigma}{2} \int_0^R dr \int_0^T dt \left( \left( \frac{\partial y}{\partial r} \right)^2 + \left( \frac{\partial y}{\partial t} \right)^2 \right) \tag{6}$$

which is the hamiltonian of a Gaussian model<sup>[29]</sup>.

Using eqs. 4 and 5 and the Gaussian hamiltonian eq.6 we obtain the expression for the one-loop approximation to the partition function,

$$\begin{aligned} Z_{CW}^{1\text{loop}}(R, T) &= C \exp(-\sigma RT) Z_q^{1\text{loop}} \left( \frac{R}{T} \right) = \\ &= \exp(-\sigma RT) C \sqrt{\frac{R}{q}} q^{-1/12} (1 + q + 2q^2 + 3q^3 + 5q^4 + 7q^5 + 11q^6 + \dots)^2, \end{aligned} \tag{7}$$

where  $q = \exp(2\pi i\tau)$  and  $C$  is a constant to be determined. It should be noted that the expression for  $Z_q^{1\text{loop}}$  coincides with that of the exact partition function of a 2D conformal invariant free boson in a torus of modular parameter  $\tau = i\frac{R}{T}$  [15]. From the above expression, it is evident that  $Z_{CW}^{1\text{loop}}(R, T)$  only depends on the ratio between  $R$  and  $T$  as a consequence, in the case of transversally symmetric lattices ( $R = T$ ),  $Z_{CW}^{1\text{loop}}$  will coincide with the expression for the zero-loop expansion to the CWM (or the classical formula).

The two-loop approximation for  $Z_{CW}$  can be obtained when one uses the first correction to the Gaussian hamiltonian eq.6 (or the next to the leading order term in the expansion of  $H_{CW}$ )<sup>[16]</sup>.

$$Z_{CW}^{2\text{loop}}(R, T) = C \exp(-\sigma RT) Z_q^{1\text{loop}} \left( \frac{R}{T} \right) Z_q^{2\text{loop}} \left( \frac{R}{T}, \sigma RT \right), \tag{8}$$

where

$$Z_q^{2\text{loop}} \left( \frac{R}{T}, \sigma RT \right) = 1 + \frac{1}{2\sigma RT} \left\{ \left[ \frac{\pi R}{6 T} E_2 \left( i\frac{R}{T} \right) \right]^2 - \frac{\pi R}{6 T} E_2 \left( i\frac{R}{T} \right) + \frac{3}{4} \right\} \tag{9}$$

and

$$E_2(\tau) = 1 - 24 \sum_{n=1}^{\infty} \frac{nq^n}{1 - q^n} \tag{10}$$

is the first Eisenstein series and  $C$  is a constant that, again, is to be determined. In contrast to what happens at the Gaussian level, the two-loop Capillary Wave contributions do not depend only on the ratio  $z = \frac{R}{T}$  but also on  $\sigma RT$ . Therefore, in the case of transversally symmetric lattices ( $R = T$ ),  $Z_{CW}^{2\text{loop}}$  does not coincide with the zero-loop expansion (or classical formula).

### III. The Potts model and the Capillary Wave Model

The three-state Potts model is defined by the partition function

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$$Z = \sum_{\{3/4\}} \exp \left\{ -\beta \sum_{i,n} [1 - Re(\sigma_i^* \sigma_{i+n})] \right\} \tag{11}$$

where the variables  $\sigma_i$  are defined on a three-dimensional cubic lattice and the values

$$\sigma_i = \exp \left( \frac{2\pi i n_i}{3} \right) \tag{12}$$

with  $n_i = 0, 1, 2$ .

One should note that the three-state Potts model is equivalent to the Z(3) spin model with spins  $s_j = \exp(2\pi i\sigma_j/3)$ . In the thermodynamic limit and in the region of ferromagnetic coupling, ( $\beta > 0$  where  $\beta = 1/k_B T$ ), the above model is known to undergo a phase

transition from a Z(3) symmetric phase for  $\beta < \beta_c$  to a spontaneously broken phase for  $\beta > \beta_c$  at a critical coupling  $\beta_c = 0.36708$  [17]. For  $\beta > \beta_c$ , three ordered phases coexist, while at  $\beta > \beta_c$  the disordered phase coexists with the previous ones. The most precise estimate for the roughening temperature is  $\beta_r \sim 0.93$  [18]. As we are considering finite lattices that can have a cylindric geometry, the degeneracy of the ground state is removed and the energy of the symmetric (Z(3)-invariant) ground state is separated by an energy splitting (or small gap)  $E$  from the two degenerate mixed-symmetry states. This energy splitting is due to the tunneling between the phases and is directly linked to the free energy of the interface<sup>[19]</sup>. In the dilute gas approximation, in which multi-interfaces are summed over but interface-interface interactions can be neglected, the energy splitting is directly proportional to the in-

terface partition function.

$$E = Z(\sigma, R, T) \tag{13}$$

It is at this point that we have a direct link between the CWM and the 3D3q Potts mode. If we know how to calculate, direct or indirectly, the energy gap  $E$  for the 3D Potts model, we have a way of checking the validity of the CWM in the description of rough interfaces as well as a way of obtaining the order-order interface tension for the 3D Potts model.

Therefore, according to the Capillary Wave Model, in the rough phase, that is, for  $\beta_r > \beta > \beta_c$  where  $\beta_r \sim 0.93$  [18] is the roughening temperature, we assume that<sup>[7,9,10]</sup>, up to the two-loop term in the expansion of the partition function, the energy gap is given by

$$E(R, T) = D \exp(-\sigma RT) Z_q^{1\text{loop}} \left( \frac{R}{T} \right) Z_q^{2\text{loop}} \left( \frac{R}{T}, \sigma RT \right), \tag{14}$$

where  $D = \delta/Z_q^1(1)$ ,  $\delta$  is a constant to be determined and  $R \geq T$ .

If we now consider only the one-loop term and take the limit where the transverse lattice is symmetric, that is, when  $R = T$  then, by eq. (7), we observe that

$$E(R, T) = Z_q^{1\text{loop}}(1) D \exp(-\sigma R^2) D \exp(-\sigma R^2), \tag{15}$$

which coincides with the classical formula<sup>[19]</sup>,

$$E_{\text{class}} = \vartheta \exp(-\sigma R^2). \tag{16}$$

On the other hand, since two-loop contributions depend both on the ratio  $z = R/T$  as well as on the interface area,  $A = RT$ , then, in the case of symmetric lattices ( $z = 1$ ,  $K = T$ ,  $A = R^2$ ), the only way of obtaining the classical formula for symmetric lattices is neglecting the two-loop contribution.

#### IV. Monte Carlo simulations and observables

The measurements of the energy gap  $E$ , for different choices of lattice sizes will provide a first direct check on the functional form of the interface free energy and will allow us to estimate the interface tension  $\sigma$  in the case of the 3D Potts model.

In order to measure the energy gap  $E$  for the 3D Potts model we follow the procedure explained in Ref. [2]. We will consider a cylindrical lattice with  $L_3 \gg R, T$  where  $L_3$  is the height of the cylinder, and will impose periodic boundary conditions over all surfaces. We then define a time-slice magnetization as

$$S_k = \frac{1}{RT} \sum_{x_1=1}^R \sum_{x_2=2}^T \sigma(x_1, x_2, k), \tag{17}$$

where  $x_1$ ,  $x_2$  and  $k$  are coordinates in the  $R, T$  and  $L_3$  directions, respectively.

Using the transfer-matrix formalism we can express the correlation between two local operators as a function of the transfer matrix, that is, if we compute the two-point correlation function

$$G(k) = \langle S_0 S_k^* \rangle, \tag{18}$$

where  $k = 0, 1, \dots, L_3/2$ , we can extract the low-energy levels from the asymptotic dependence of  $G(k)$ , with  $k$ ,

$$G(k) \cdot Z = c_0 \{ \exp(-kE) + \exp(-(L_3 - k)E) \} +$$

$$+ c_1 \{ \exp(-E^\bullet k) + \exp(-(L_3 - k)E^\bullet) \} + \dots \quad (19)$$

$$Z = 1 + 2 \exp(-L_3 E) + \dots \quad (20)$$

where  $Z = \text{Tr} \exp(-L_3 H)$  is the partition function of the Potts model in the transfer matrix formalism. The second exponent in each bracket in the above expression is due to periodic boundary conditions in the  $L_3$  direction and  $E^\bullet$  is the next-to-leading energy.

The procedure we use to check the predictions of the CWM in the case of the 3D Potts model is the following: For a fixed value of the cylinder height and for each value of the coupling constant  $\beta$ , we calculate, for several sets of transverse lattice sizes  $R$  and  $T$ , the two point correlation function by means of a Monte Carlo numerical simulation. We then extract the value of the energy splitting  $E$  by fitting the Monte Carlo data for the two-point correlation function with eqs. 19 and 20.

The knowledge of the energy splitting  $E$ , for a fixed value of  $\beta$  and several sets of lattice sizes  $R$  and  $T$ , allow us to compute the order order interface tension and the constant  $\delta$  by fitting the Monte Carlo data for the energy splitting  $E$  with eq. 14.

We have performed our simulations with a Metropolis algorithm for different values of  $\beta$  ranging from  $\beta = 0.3678$  to  $\beta = 0.3685$ . The longest lattice size was kept fixed at  $L_3 = 120$  and the other sizes ranged from  $9 \leq T \leq 14$  to  $10 \leq R \leq 36$ . The range of values of  $\beta$  used are deep inside the ordered phase, which means that the existence of order-disorder interfaces is highly suppressed. On the other hand, for these values of  $\beta$  the correlation length is large enough to make lattice artifacts negligible and to allow us to consider domain walls as fluid (or rough) interfaces.

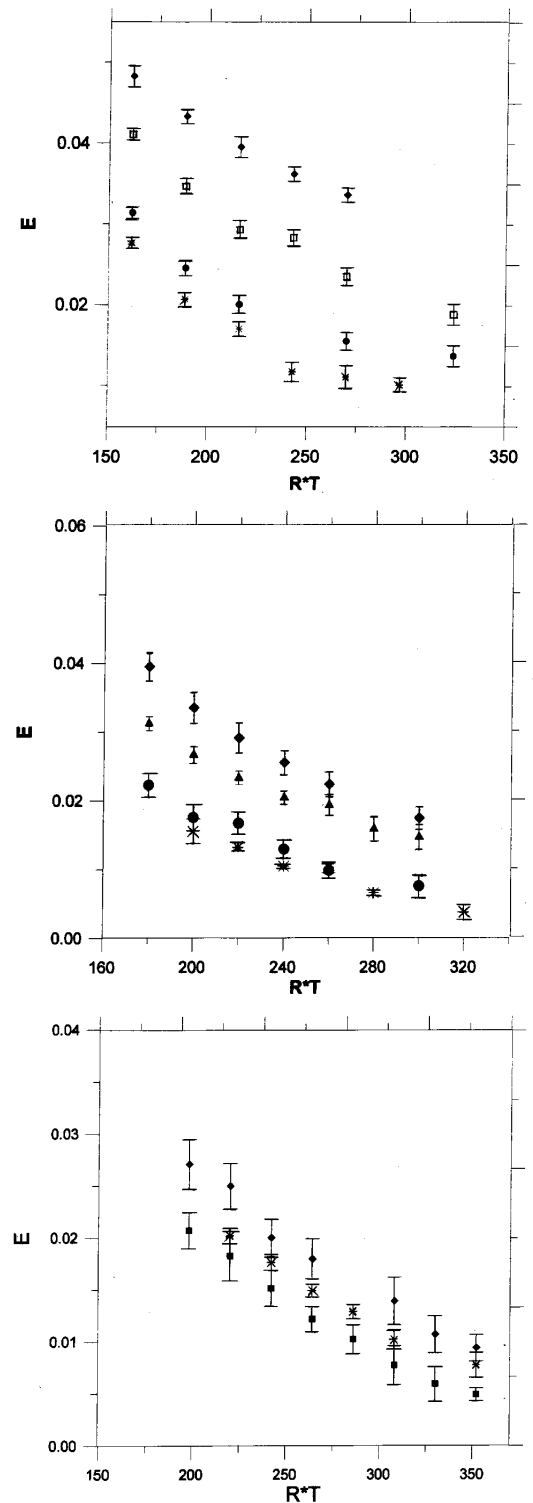


Figure 1. Behavior of the energy gap  $E$  as a function of the interface area  $RT$  ( $R \neq T$ ) for different values of  $\beta$ . From up to down the correspond to  $\beta = 0.3678$ ,  $\beta = 0.3680$ ,  $\beta = 0.3682$  and  $\beta = 0.3685$ . In figure 1c they correspond to  $\beta = 0.3678$ ,  $\beta = 0.3680$  and  $\beta = 0.3682$ . In Fig. 1a,  $K = 9$ , in Fig. 1b,  $K = 10$  and in Fig. 1c,  $R = 11$ .

Data can be affected by Monte Carlo time correlations as well as by time-slice correlations. In order

to have control over these correlations we have made a careful study of our measurements. We have only picked observables that are situated far apart in the Monte Carlo time in order to ensure that the covariance matrix is almost diagonal and that our data is not correlated. The same kind of care was observed when we dealt with time-slice correlations.

We have performed approximately from 600,000 to 1,400,000 sweeps in each run and, in each run we have verified that all the data taken for posterior analysis was already thermalized. We have also made, for each set of fixed parameters, a large number of runs modifying only the seed of the random-number generator. We use these results to evaluate the errors.

In Fig. 1, we show the behavior of the energy gap  $E$  as a function of the interface area  $RT$  ( $R \neq T$ ) for different values of  $\beta$ . From up to down they correspond to  $\beta = 0.3678$ ,  $\beta = 0.3680$  [12],  $\beta = 0.3682$  and  $\beta = 0.3685$  [20], except in figure 1c where they correspond to  $\beta = 0.3678$ ,  $\beta = 0.3680$  and  $\beta = 0.3682$ . In Fig. 1a,  $R = 9$ ; in Fig. 1b,  $R = 10$  and in Fig. 1c,  $R = 11$ . From these figures we observe that the effect of raising the value of  $\beta$  consists lowering the energy gap  $E$  for a fixed  $RT$ . We observe, also, that the values of the energy gap  $E$  for different values of the coupling constant and same values of  $R$  and  $T$  interpolate smoothly as  $\beta$  grows.

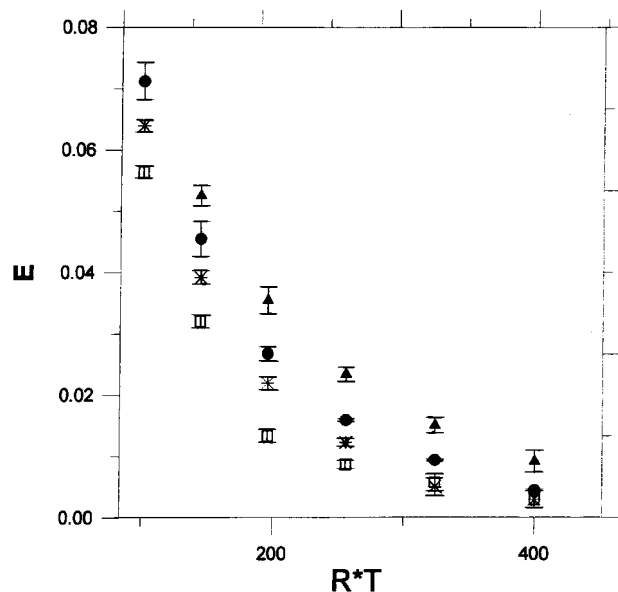


Figure 2. Behavior of the energy gap  $E$  as a function of the interface area  $RT(R = T)$  for different values of  $\beta$ . From up to down they correspond to  $\beta = 0.3678$ ,  $\beta = 0.3680$ ,  $\beta = 0.3682$  and  $\beta = 0.3685$ .

In Fig. 2, we show the behavior of the energy gap  $E$  as a function of the interface area  $RT(R = T)$  for different values of  $\beta$ . From up to down the points correspond to  $\beta = 0.3678$ , ( $\beta = 0.3680$  [12],  $\beta = 0.3682$  and  $\beta = 0.3685$  [20]). Here, again, we observe that as  $\beta$  is raised, the energy gap  $E$  lowers, for fixed  $RT$ , and that  $E$  interpolates smoothly as the coupling constant grows.

In Fig. 3, we present the behavior of the energy gap  $E$  as a function of  $RT$  for different lattice sized and for  $\beta$  fixed at  $\beta = 0.3678$ . The line here represents the best-fit data to  $R = T$  (symmetric) lattices, while  $\blacklozenge$ ,  $*$ ,  $\square$  and  $\diamond$  represent  $R = 9$ ,  $R = 10$ ,  $R = 11$  and  $R = T$  respectively.

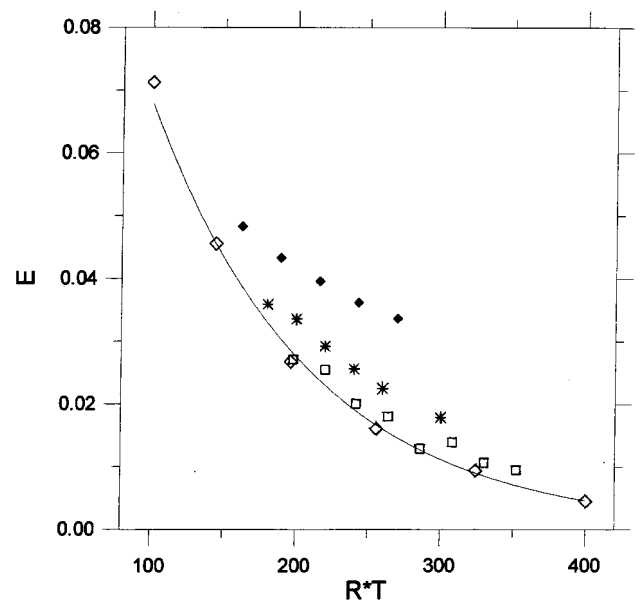


Figure 3. Behavior of the energy gap  $E$  as a function of  $RT$  for different lattice sizes and for  $\beta$  fixed at  $\beta = 0.3678$ . The line here represents the best-fit data to  $K = T$  (symmetric) lattices, while  $\blacklozenge$ ,  $*$ ,  $\square$  and  $\diamond$  represent  $R = 9$ ,  $R = 10$ ,  $R = 11$  and  $R = T$  respectively.

Practically all of the existing results for the interface tension of the 3D three state Potts Model are obtained using only transversally symmetric (or  $R = T$ ) lattices. Since we want to test the validity of the one- and two-loop approximation to the CWM in the description of the interface tension not only for symmetric lattices, our Monte Carlo data for the energy gap  $E$  will be taken from both  $R = T$  and  $R \neq T$  lattices. In order to test the classical formula, which is the one that all the authors use, we have, first of all, fitted the Monte

Carlo data for the energy gap  $E$  taken from symmetric lattices with eq. 16 for each value of  $\beta$ , obtaining the following values for the interface tension and the constant  $\delta$  for  $\beta = 0.3678$ .

$$\sigma = 0.00918 \quad \delta = 0.1749 \quad (21)$$

with a  $\chi^2$  per degree of freedom given by

$$\chi^2 = 0.3082 . \quad (22)$$

In our next test of the classical formula we fit our Monte Carlo data for  $E$  taken from  $R = T$  and  $R \neq T$  lattices to eq. 16 and, in this way, we obtain the following values for the quantities shown in the previous equation, for the same value of  $\beta$ ,

$$\sigma = 0.002015 \quad \delta = 0.002698 \quad \chi^2 = 60.5879 . \quad (23)$$

From these results we observe that while the classical formula is perfectly adequate to be used with symmetric lattices, it is not the most suitable one to be used when one consider asymmetric lattices ( $R \neq T$ ).

In order to test the validity of the CWM as a correct and powerful way of calculating the interface tension for the 3D Potts Model we are going to fit our Monte Carlo data for  $E$ , take from both  $R = T$  and  $R \neq T$  lattices with eq. 14. Neglecting, initially, the two-loop contributions in equation 14, we obtain the following results for the same quantities described above and for the same value of  $\beta$ .

$$\sigma = 0.009133 \quad \delta = 0.17449 \quad \chi^2 = 2.3289 \quad (21)$$

If we, instead, take into account corrections up to two-loop in equation 14, the quantities above will assume the following values,

$$\sigma = 0.009079 \quad \delta = 0.13825 \quad \chi^2 = 2.8659 \quad (25)$$

One should now compare the above results (for both one- and two-loop corrections) to those obtained in eq. 23, since in those three cases Monte Carlo data taken from both  $R = T$  and  $R \neq T$  lattices were used in the fittings while in the case of eq. 21 only the  $R = T$  data were taken into account. Comparing the results given

in eqs. 23, 24 and 25 we readily verify that the one- and two-loop approximations to the CWM allow us to have a reliable way of calculating the interface tension in the case of generic ( $R = T$  and  $R \neq T$ ) lattices, while the classical equation, eq. 16, is more adequate to be used in the case of for symmetric lattices.

As we have stated before, the  $R = T$  limit of the CWM two-loop approximation does not coincide with the classical formula, in contrast to what happens to the  $R = T$  limit of the one-loop approximation. In this sense, we can understand the reason why the values of eq. 24, obtained by fitting  $R = T$  and  $R \neq T$  data to the one-loop approximation, seem to be closer to those of eq. 21.

Table I. Monte Carlo and CWM predicted values for the energy gap  $E$  for some sets of lattice sizes.

$R \times T$	E(MC)	E(1loop)	E(2loop)
<b>9 × 24</b>	<b>0.03953</b>	<b>0.03543</b>	<b>0.03383</b>
<b>9 × 18</b>	<b>0.048285</b>	<b>0.047257</b>	<b>0.047402</b>
<b>10 × 20</b>	<b>0.033563</b>	<b>0.03340</b>	<b>0.03227</b>
<b>10 × 24</b>	<b>0.025577</b>	<b>0.02609</b>	<b>0.024599</b>
<b>10 × 30</b>	<b>0.017840</b>	<b>0.018469</b>	<b>0.016990</b>
<b>11 × 20</b>	<b>0.025419</b>	<b>0.02654</b>	<b>0.02527</b>
<b>11 × 24</b>	<b>0.017990</b>	<b>0.01960</b>	<b>0.018200</b>
<b>12 × 12</b>	<b>0.045537</b>	<b>0.046839</b>	<b>0.043248</b>
<b>18 × 18</b>	<b>0.00880</b>	<b>0.00945</b>	<b>0.00905</b>

The best way of checking the validity and usefulness of the CWM predictions is comparing Monte Carlo data for some values of the energy gap  $E$  with the predicted values obtained from the fitting of equations 14 and 15. In table I we present the values of  $E$  obtained from Monte Carlo data and the predicted values obtained from the fit of all data to the one- and two-loop expansions of the CWM for  $\beta = 0.3678$ . As it can be easily verified from the results of Table I, the CWM predicted values of the energy gap  $E$  are in a very good agreement with those obtained in the Monte Carlo simulations but the two-loop expansion predictions are, in



general, slightly better than those of the one-loop expansion. The same kind of behavior observed in the previous tests for  $\beta = 0.3678$  is also obtained for all other values of studied.

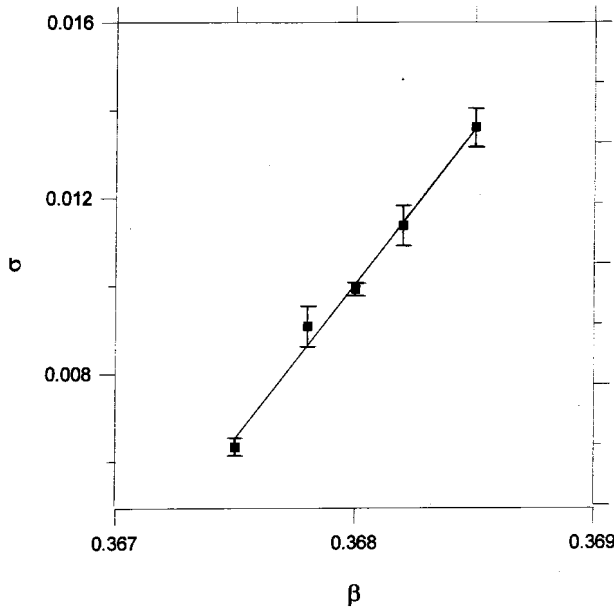


Figure 4. Behavior of  $\sigma_{2\text{-loop}}$  as a function of  $\beta$  [21].

In Fig. 4, we plot the interface tension  $\sigma_{2\text{-loop}}$  obtained from the best fit of all data to formula 14 as a function of  $\beta$  for the range of temperatures studied. From this figure we observe that the two-loop interface tension rises linearly as a function of  $\beta$  for  $\beta > \beta_c$ . Using the data obtained for  $\sigma_{2\text{-loop}}$  as a function of  $\beta$  we can get a straight-line fit for the interface tension in the ordered region, that is, in the region where  $\beta \geq \beta_c$ . From a least-square fit we obtain:

$$\sigma_{\text{ord}} = 0.00347 + 6.9905 \cdot (\beta - \beta_c) \quad (26)$$

in the case of the expansion of the CWM up to two loops. A linear behavior for the interface tension was also observed in a mean field calculation<sup>[22]</sup> and in a Monte Carlo simulation<sup>[1]</sup> using  $R = T$  lattices and the classical formula eq. 2. We should stress here that all the interface tension values used in the straight line fit equation 26 were obtained when one uses the CWM two-loop expansion expression 14 and Monte Carlo data for the energy gap  $E$  taken from both symmetric and asymmetric lattices.

A linear behavior for the interface tension is very welcome since it allows us to extrapolate the interface tension to its value when  $\beta \cong \beta_c$ . As it is well known there is a weak first order phase transition at  $\beta = \beta_c$  and, as a consequence, three ordered phases co-exist with a disordered phases requires the fulfillment of the following inequality<sup>[23]</sup>

$$\sigma_{\text{ord}} \leq 2\sigma_{\text{dis}} \quad (\beta = \beta_c) \quad (27)$$

where  $\sigma_{\text{dis}}$  is the order-disorder interface tension. Frei and Patkos<sup>[22]</sup> have suggested that when the equality in the above equation holds we can speak of complete wetting, while when the strict inequality holds at co-existence we have the phenomenon of incomplete wetting. The verification of the hypothesis of complete or incomplete wetting is of great importance in the study of finite temperature QCD and the physics of the early universe.

## V. Conclusions

In this paper we have studied, by means of a canonical Monte Carlo simulation, the question of the validity of the one- and two-loop approximations of the Capillary Wave Model in the description of order-order interfaces in the 3D three state Potts Model for all kinds of lattice sizes and for several values of the coupling constant  $\beta$ . Up to now all the works in which the interface tension was calculated used the classical formula eq. 16 independently of the interface symmetries, the only exception being Ref. [12] where the authors have studied the interface tension of the 3D Potts Model using a Swendsen-Wang cluster simulation for only one value of  $\beta$  and for asymmetric lattice sizes.

We have varied the values of the coupling constant  $\beta$  and have observed the following results;

i) We have calculated, for each value of  $\beta$  and for several values of the interface sizes, the energy gap  $E$  and have verified that these values interpolate smoothly for all values of  $\beta$  as this quantity grows.

ii) We have verified that, for all the values of  $\beta$  studied, the classical free energy formula is more adequate to be used in the study of symmetric (or square) interfaces than in the study of asymmetric ones.

iii) We have verified that, for all the values of  $\beta$  studied, the one- and two-loop approximations of the

Capillary Wave Model are an useful and reliable way of describing all kinds of interface sizes.

iv) We have compared our Monte Carlo data for the energy gap (in the case of  $R = T$  and  $R \neq T$  lattices)  $E$  with the predicted values for  $E$  obtained using the one- and two-loop CWM approximations and we have verified that the CWM predictions are in very good agreement with the measured Monte Carlo data and that the two-loop predictions are slightly better than the one-loop predictions.

From the above descriptions, it is clear to us that the CWM in the one- and two-loop approximations provides an excellent description of order-order interfaces for the 3D 3q Potts model. This conclusion was also obtained in Refs. [10] and [11] for the 3D Ising model. This result is a strong indication of the universality of this description of interface physics in 3D statistical models.

Using the expressions for the one- and two-loop expansions to the Capillary Wave Model and data from different kinds of lattice sizes we have studied the behavior of the order-order interface tension as a function of the coupling constant  $\beta$ . We have verified that the one- and two-loop interface tensions rise linearly when the coupling constant  $\beta$  grows, for  $\beta \geq \beta_c$ . Using the two-loop interface tension data as a function of  $\beta$  we have obtained a straight-line fit for the interface tension in the ordered region. Since our results come from the use of both symmetric and asymmetric lattices and also from the two-loop approximation to the CWM, instead of the classical approximation, we cannot compare directly our results to those of Ref. [1] which are obtained using only symmetric lattices and the classical approximation. Anyway, the fact that a straight-line fit results from both works allows us to infer that the effect of using all kinds of lattice sizes and corrections to the classical equation do not change qualitatively the behavior of the order-order interface tension as a function of the coupling constant.

It is worth stressing that the CWM corrections to the finite-size behavior of the interface free energy do not introduce any new free parameters with respect to the "classical" picture.

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#### References

1. F. Karsch and A. Patkós, Nucl. Phys. **B350**, 563 (1991); R. Gavaí and L. Polley, Phys. Lett. **B324**, 78 (1994).
2. S. Klessinger and G. Münster, Nucl. Phys. **B386**, 701 (1992).
3. R. Gavaí and F. Karsch, Nucl. Phys. **B322**, 738 (1989).
4. Jing-Dong Wang and C. DeTar, Phys. Rev. **D47**, 4091 (1993).
5. L.G. Yaffe and B. Svetitsky, Phys. Rev. **D26**, 963 (1982); Nucl. Phys. **210** [FS6], 423 (1982)
6. M. Fukugita, A. Yukawa and M. Okawa, Nucl. Phys. **B337**, 181 (1990).
7. M. P. Gelfand and M. E. Fischer, Physica **A166**, 1 (1990).
8. C. Borgs, Int. Journ. Mod. Phys. **C3**, 897 (1992).
9. F.P. Buff, R.A. Lovett and F.H. Stillinger Jr., Phys. Rev. Lett. **15**, 621 (1965).
10. M. Caselle, F. Gliozzi, and S. Vinti, Phys. Lett. **B302**, 74 (1993).
11. M. Caselle, R. Fiore, F. Gliozzi, M. Hasenbusch, K. Pinn and S. Vinti, CERN-TH 7291/94-DFTT 22/94.
12. P. Provero and S. Vinti, Physica **A211**, 436 (1994).
13. H.W. Blöte and R.H. Swendsen, Phys. Rev. Lett. **43**, 799 (1979); S.J. Knack Jensen and O.J. Mouritsen, Phys. Rev. Lett. **43**, 1736 (1979); F. Y. Wu, Rev. Mod. Phys. **54**, 235 (1982).
14. B. Grossmann, M. L. Laursen, T. Trappenberg and U. J. Wiese, Nucl. Phys. **B39a**, 584 (1993).
15. C. Itzykson and J. B. Zuber, Nucl. Phys. **B275** [FS17], 580 (1986); B. Bunk, Int. Journ. Mod. Phys. **C3**, 889 (1992).

16. K. Dietz and T. Filk, Phys. Rev. **D27**, 2944 (1983).
17. R. Gavai, F. Karsch and B. Peterson, Nucl. Phys. **B322**, 738 (1989).
18. J. M. Drouffe and J. B. Zuber, Phys. Rep. **C102**, 1 (1983).
19. M. E. Fischer, J. Phys. Soc. Japan Suppl. **26**, 87 (1969); M. E. Fischer and V. Privman, J. Stat. Phys. **33**, 385 (1983); E. Brézin and Z. Zinn-Justin, Nucl. Phys. **B257** [FS14], 367 (1985); G. Münster, Nucl. Phys. **B340**, 559 (1990); T. Trappenberg and U. J. Wiese, Nucl. Phys. **B372**, 703 (1992).
20. Besides our Monte Carlo data, we have used also, for this value of  $\beta$ , some Swendsen-Wang data by S. Vinti (private communication).
21. The  $\beta = 0.3675$  data was graciously given to us by S. Vinti (Private communication).
22. Z. Frei and A. Patkós, Phys. Lett. **B229**, 102 (1989).
23. B. Widom, J. Chem. Phys. **62**, 1332 (1975).
24. M. Luscher, Nucl. Phys. **B180** [FS2], 317 (1981).
25. V. Privman, Int. Journ. Mod. Phys. **C3**, 857 (1992).
26. J. M. Drouffe and J. B. Zuber, Phys. Rep. **C102**, 1 (1983).
27. J. Briemont, A. El Mellouki and J. Frölich, J. Stat. Phys. **42**, 743 (1986).
28. M. Hasenbusch and K. Pinn, Physica **A192**, 342 (1993).
29. T. H. Berlin and M. Kac, Phys. Rev. **86**, 821 (1952).