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Monte Carlo calculation of the surface free energy for the two-dimensional 7-state Potts model, and an estimate for four-dimensional SU(3) gauge theory *

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Using the recently proposed multicanonical ensemble, we perform Monte Carlo simulations for the two-dimensional 7-state Potts model and calculate its surface free energy density (surface tension) to be $2f^s = 0.0241 \pm 0.0010$. This is an order of magnitude smaller than other estimates in the recent literature. Relying on existing Monte Carlo data, we also give a preliminary estimate for the surface tension of four-dimensional SU(3) lattice gauge theory with $L_t = 2$.

1. Introduction

First-order phase transitions play a major role in many physical systems. Many phase transitions observed in nature are first order. Examples are vapour–liquid and liquid–solid transitions, the SU(3) deconfinement transition and others at various stages of our universes evolution. In a first-order phase transition two phases can coexist at the transition point, with a domain wall, whose tension is finite, separating the two phases. Let us denote by f_1 and f_2 the free energies per unit volume of the two phases and by F the free energy of the whole system; the difference

$$F^s = F - (V_1 f_1 + V_2 f_2) > 0, \tag{1}$$

is the free energy associated with the interface. Its value, normalized to unit area f^s, is the surface tension, a quantity of central importance for the theory of first-order phase transitions [1].

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In recent years considerable efforts were devoted to surface-tension calculations. In particular, the two-dimensional 7-state Potts model has served as a testing ground for methods [2,3] which were subsequently applied to SU(3) lattice gauge theory [4,5]. Here we rely on the method of Binder [6] to evaluate again the surface tension for these models. Our surface-tension estimates come out much lower than those of refs. [2–5]. We explain this by showing that their extrapolations were obtained from temperatures for which no true two-phase regions exist. Our SU(3) estimate relies on the $L_t = 2$ data of ref. [7]. For the Potts model we have performed a new high-statistics Monte Carlo (MC) simulation with the recently proposed [8] multicanonical ensemble. For the 10-state Potts model the multicanonical approach had improved standard MC calculations in the two-phase region by almost three orders of magnitude [9]. In our case of the 7-state model, we find the less dramatic improvement of a factor of two to three. This is due to the fact that the first-order transition is considerably weaker than that of the 10-state model.

Besides serving as a testing ground for surface-tension calculations, two-dimensional Potts models have also attracted recent attention through their use as a laboratory for testing finite-size scaling (FSS) concepts. Rigorous work by Borgs et al. [10] has greatly refined the phenomenological two-gaussian-peak model [11], and the question how large the simulated systems must be in order that asymptotic FSS limits are approached has been investigated by a number of MC studies [12–16]. As a by-product of our surface tension investigation, we can supplement these studies with results from our $q = 7$ data.

2. Potts model

The two-dimensional 7-state Potts model [17] is defined on an L^2 lattice by the partition function

$$Z(\beta) = \sum_{\text{configurations}} \exp(-\beta E), \tag{2}$$

$$E = -\sum_{\langle i,j \rangle} \delta_{q_i,q_j}, \quad q_i, q_j = 1, \ldots, 7. \tag{3}$$

Here i,j are labels of the sites of the lattice and $\langle i,j \rangle$ is the sum over nearest neighbours. We always employ the periodic boundary condition. Following ref. [6] we are going to extract the surface tension from the probability density $P_L(E;\beta)$ of the energy E. For β sufficiently close to the transition point $P_L(E;\beta)$ exhibits a double peak structure. We adopt the normalization $P_L^{\max} = 1$ and we define

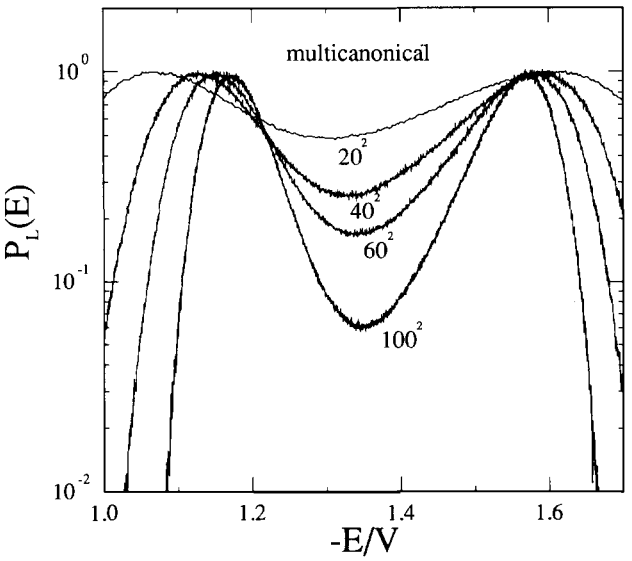

Fig. 1. Energy density distributions $P_L(E)$ for lattices of size $L = 20, \ldots, 100$ on a logarithmic scale. The values of the maxima have been normalized to 1.

L-dependent pseudo-transition points β_L^c by the requirement that both maxima are of equal height:

$$P_L^{1,\max} = P_L\left(E_L^{1,\max}\right) = P_L\left(E_L^{2,\max}\right) = P_L^{2,\max} = 1 \quad \left(E_L^{1,\max} < E_L^{2,\max}\right). \tag{4}$$

As in this equation we suppress in the following β in the argument of $P_L(E;\beta)$ when the probability density is considered at its pseudo-transition point. Once the energy probability density $P_L(E)$ is known, the interfacial free energy per unit area follows [6] from the $L \to \infty$ limit of *

$$2f_L^s = -\frac{1}{L}\ln\left(P_L^{\min}\right). \tag{5}$$

Here $P_L^{\min} = P_L(E_L^{\min})$, where $E_L^{\min}$ is the position of the minimum which the probability density takes in the range $E_L^{1,\max} \leqslant E \leqslant E_L^{2,\max}$. The factor 2 accounts for the fact that for periodic boundary conditions the minimum of the probability density is governed by at least two interfaces. Our empirical results of $P_L(E)$ for lattices in the range $L = 20, \ldots, 100$ are depicted in fig. 1 on a logarithmic scale. To enhance the MC statistics at the minima of the probability densities, we have simulated the multicanonical ensemble as described in refs. [8,9]. The multicanonical probability densities $P_L'(E)$ of our "raw" data are fairly flat in E and the

* To comply with refs. [2–5] our present definition differs by a factor of two from ref. [9].

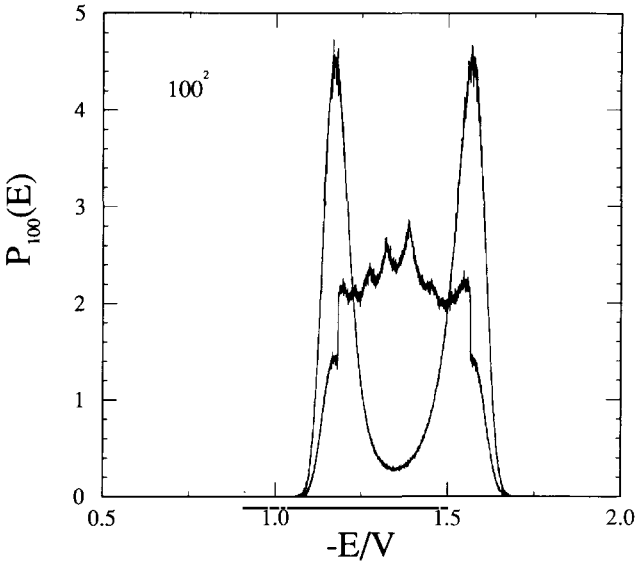

Fig. 2. Multicanonical energy distribution $P'_{100}(E)$ together with its reweighted distribution $P_{100}(E)$. Both distributions are normalized to unit area.

results of fig. 1 are obtained by reweighting for the correct Boltzmann factor. For our $L = 100$ lattice this procedure is illustrated by fig. 2. Table 1 gives an overview of our data and results. The statistics is given in sweeps, a sweep being defined as updating each spin in the lattice once. The other quantities given are β_L^c, $e_L^{1,\max}$, $e_L^{\min}$, $e_L^{2,\max}$ and f_L^s, where we denote by $e = E/V$ the energy density and $e_L^{1,\max}$, $e_L^{\min}$ and $e_L^{2,\max}$ are the densities belonging to the corresponding extensive quantities as introduced above.

For lattices of size up to $L = 60$ we have also performed simulations with a standard heat-bath algorithm to evaluate the improvements due to the multicanonical method. The relative performance of the two algorithms is best evaluated by comparing the tunneling times. As in refs. [12,16] we define four times the tunneling time $4\tau_L^t$ as the average number of sweeps needed to get from a configuration with energy $E_L^{1,\max}$ to a configuration with $E_L^{2,\max}$ and back. This

TABLE 1
Results of multicanonical simulations

L	Statistics	β_L^c	$e_L^{1,\max}$	$e_L^{\min}$	$e_L^{2,\max}$	$2f_L^s$
20	4000000	1.284692	1.066(10)	1.3124(24)	1.602(38)	0.03645(48)
40	4000000	1.291051	1.127(18)	1.327(24)	1.578(15)	0.03387(59)
60	8000000	1.292283	1.1525(03)	1.3369(87)	1.575(02)	0.02997(60)
100	16000000	1.293089	1.1736(29)	1.3466(12)	1.570(02)	0.02816(58)

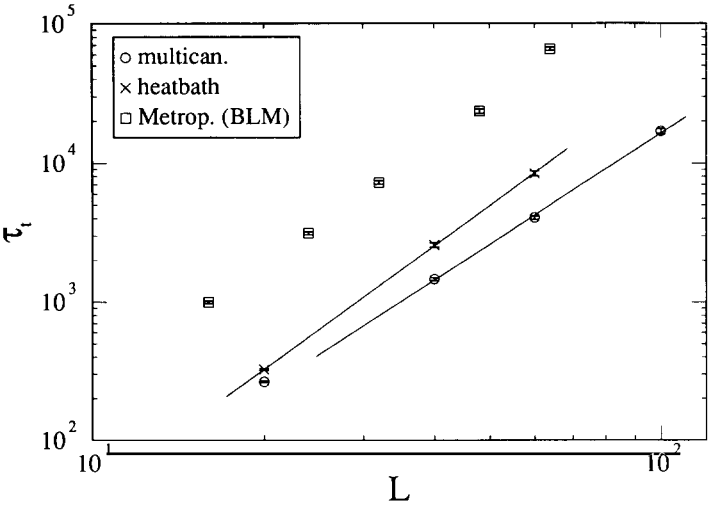

Fig. 3. Tunneling times for the multicanonical, for the standard heat-bath, and for the Metropolis [13] simulation on a double log scale.

definition has the advantage that tunneling time and exponential autocorrelation time in general agree with good precision (exactly in a simple model). In fig. 3 we display on a log–log scale the divergence in the tunneling times for the multicanonical algorithm (circles) and for the heat bath algorithm (crosses). Notice that the tunneling times for the single-hit Metropolis algorithm (squares) are larger by a factor of about seven [13]. The fit to the multicanonical data is $\tau_L^{\mathrm{t}} = 0.082(17) \times L^{2.65(5)}$. Incidentally, this is the same power law which was observed in ref. [9] for the 10-state model. Due to the weakness of the transition, the exponential divergence of the canonical tunneling times is not yet obvious in the present case. Still the multicanonical improvement should be appreciated as we spent most of our CPU time simulating the 100^2 lattice.

In the forthcoming fits we rely only on our multicanonical data, as otherwise the small lattices would get too large a weight as compared with out $L = 100$ lattice. A major point of this paper is the analysis of the f_L^{s} data given in table 1. The FSS fit

$$2f^{\mathrm{s}} = 2f_L^{\mathrm{s}} + \frac{c}{L} \tag{6}$$

is depicted in fig. 4 and gives

$$2f^{\mathrm{s}} = 0.0241 \pm 0.0010, \tag{7}$$

with $c = 0.384 \pm 0.055$ for the constant. Our result (7) is about a factor of ten smaller than the estimates given in refs. [2,3]. We like to argue that their methods analyze properties of rigid domain walls which have no connection to the statistical

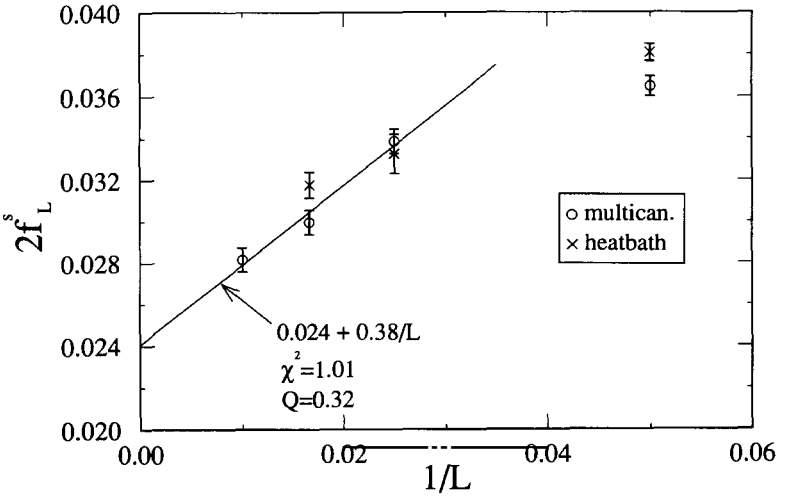

Fig. 4. Finite-size scaling fit for the interfacial free energy $2f^s$. For comparison also the data from the standard heat-bath simulations are shown.

fluctuations of the systems at their pseudo-transition points β_L^c. To enhance the signal for the surface free energy, the methods [2–5] have in common that they introduce domains corresponding to temperatures $\beta^c \pm \delta$, where in the case of the two-dimensional 7-state Potts model the exactly known [17] transition temperature $\beta^c = \ln(1 + \sqrt{7}) = 1.293562\ldots$ is used. Then, it is tried to extract the surface tension through carefully monitoring the limit $\delta \to 0$. This seems precisely why their methods fail. The signal is lost before the relevant δ-region of adiabatic distortions is reached. For instance, the smallest δ-value on which the extrapolation of ref. [2] relies is $\delta = 0.01$ on a large 128×256 lattice, where also an unused data point with $\delta = 0.005$ exists. The $\delta = 0.005$ data point had to remain unused as it exhibits a cross-over to much smaller surface tension values, interpreted then as a finite-lattice size effect. Our fig. 5 reveals that even the $\delta = 0.005$ value is still too large in the sense that $\beta^c \pm 0.005$ cannot be associated with the phase transition region. When we reweight the canonical energy density distribution from our 100×100 lattice (where the transition is less sharp than on the 128×256 lattice) to the values $\beta^c \pm 0.005$ the double-peak structure disappears: for $\beta^c - 0.005$ the system is completely in the disordered, and for $\beta^c + 0.005$ it is completely in the ordered phase.

Finally, in this section, we summarize our FSS analysis of standard quantities like various pseudo-transition temperatures, the Binder cumulant, the specific heat and the latent heat. Conventionally, pseudo-transition temperatures $T^{B,min}$ and $T^{c,max}$ are defined by the location of the Binder-parameter minimum and specific-heat maximum, respectively. Fig. 6 shows the FSS of these quantities, together with the exactly known [10,14] asymptotic expansions to first order. Fig. 7 gives the FSS

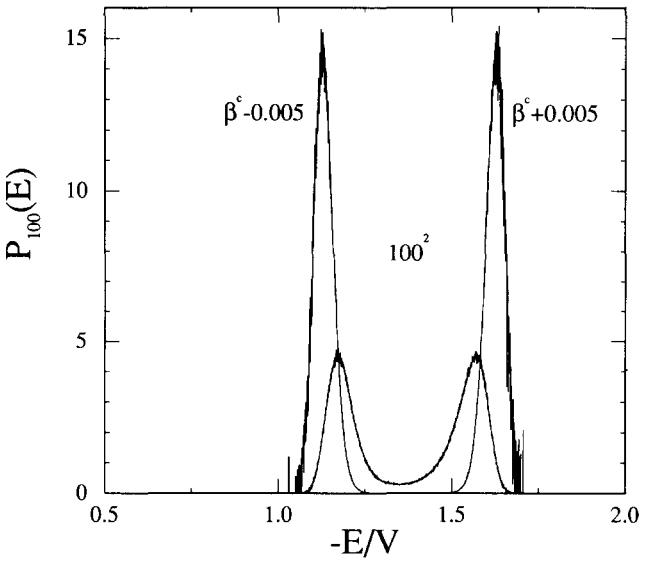

Fig. 5. Reweighting of our $P_{100}(E)$ probability density to $\beta^c - 0.005$ (high left peak alone) and $\beta^c + 0.005$ (high right peak alone).

of the Binder-parameter minimum. The arrow shows the exactly known [12,14] infinite-volume limit. The indicated asymptotic slope uses c_0 as calculated below and relies on a rather lengthy formula which can be found in refs. [14,16]. In fig. 8 we show the FSS of the maxima and the minima of the probability distribution

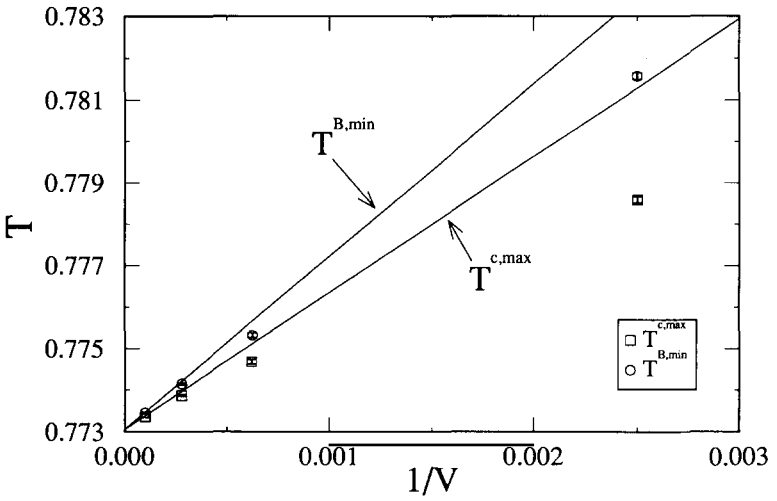

Fig. 6. Scaling of the pseudo-transition temperatures $T^{B,min}$ and $T^{c,max}$. The solid lines are the exactly known asymptotic expansions.

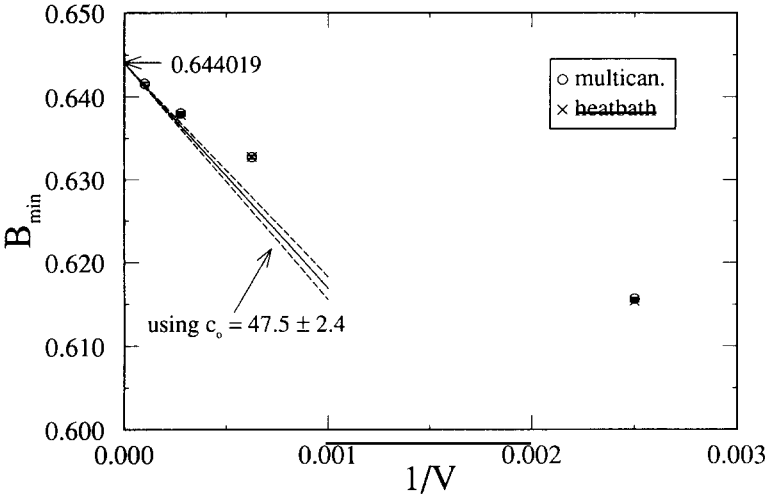

Fig. 7. Results for the Binder-parameter minimum. The arrow shows the exact infinite-volume limit.

$P_L(E)$. Linear fits to the multicanonical data yield $e^{1,\max} = 1.2053 \pm 0.0070$ and $e^{2,\max} = 1.5640 \pm 0.0095$, in good agreement with the exact results [18] 1.2013... and 1.5546..., respectively. For the minimum we find $e^{\min} = 1.3596 \pm 0.0249$. Lastly, the FSS fit of the latent heat is given in fig. 9. The linear fit gives $\Delta e = 0.3574 \pm 0.0087$, in agreement with the exact result 0.3533....

Besides the surface tension, the only quantities not known exactly are the specific heats c_o, c_d in the ordered and disordered phase, respectively. To

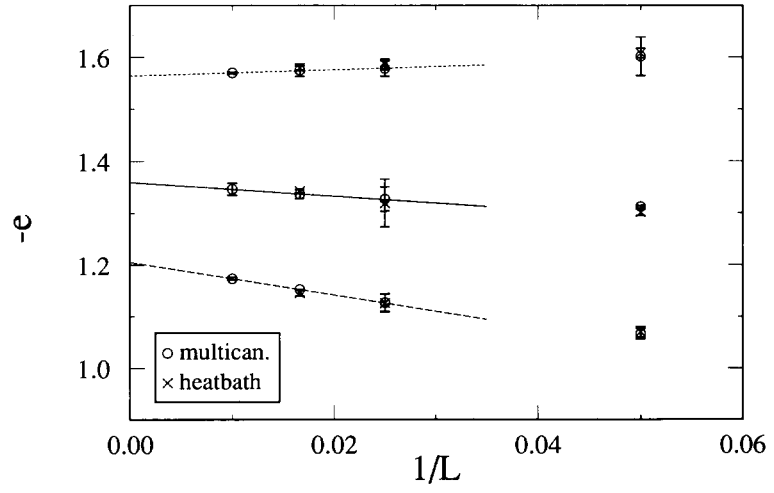

Fig. 8. Finite-size scaling of the extrema of the probability distribution $P_L(E)$.

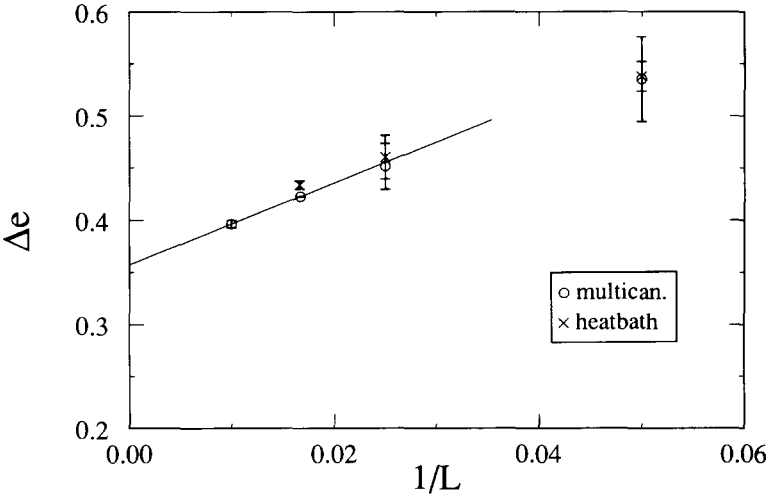

Fig. 9. Finite-size scaling of the latent heat.

calculate these quantities, we use the FSS relation [14,16]

$$c_L^{\max} = L^2\left(\frac{\Delta s}{2}\right)^2 + \Delta c + \tfrac{1}{2}(\Delta c - \Delta s)\,\ln(q) + c_o + O\left(\frac{1}{L^2}\right), \tag{8}$$

where $\Delta c = c_d - c_o$ and $\Delta s = \beta^c\,\Delta e$ is the entropy gap over the transition point. For Potts models $\Delta c = \beta^c\,\Delta s/\sqrt{q}$ [18]. Fig. 10 depicts the FSS of the specific-heat maximum with the exactly known leading term of the asymptotic expansion

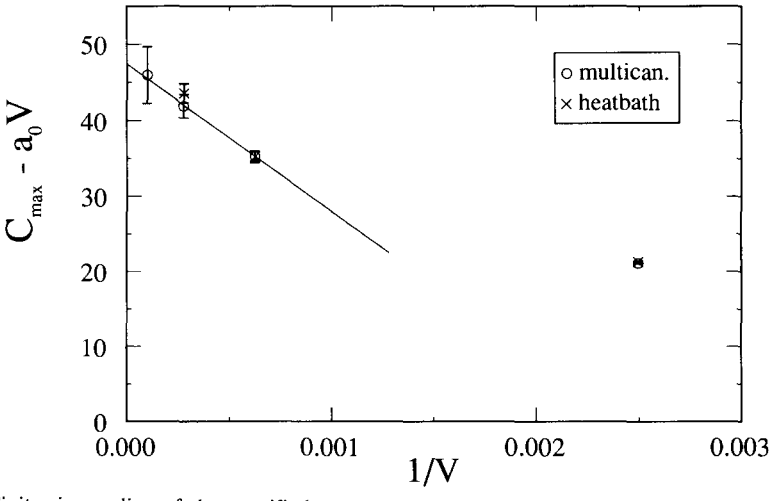

Fig. 10. Finite-size scaling of the specific-heat maximum with the exactly known leading term of the asymptotic expansion subtracted.

subtracted. The fit yields then $c_o = 47.5 \pm 2.4$ for the specific heat in the ordered phase. Since $\Delta c \approx 0.2$, this is in good agreement with the estimate [13] $c_\alpha = 50 \pm 10$.

3. SU(3) lattice gauge theory

We considered four-dimensional pure SU(3) lattice gauge theory defined on an $L_t L^3$, $(L_t \leqslant L)$ hypercubic lattice. To each link l of the lattice an element $U_l \in \mathrm{SU}(3)$ is assigned and the partition function is given by [19]

$$Z(\beta) = \int \prod_l \mathrm{d}U_l \exp\left[\frac{2}{g^2} \sum_p \mathrm{Re\ Tr}\ U(\dot{p})\right]. \tag{9}$$

Here Σ_p denotes the sum over all plaquettes of the lattice. For each plaquette p, $U(\dot{p})$ is the ordered product of the four link matrices surrounding the plaquette and $\mathrm{d}U$ is the SU(3) Hurwitz measure. The results of sect. 2 imply, of course, that we cannot have confidence in the SU(3) surface tension estimates [4,5]. The $L_t = 2$ SU(3) deconfining phase transition is sufficiently strong to warrant new MC simulations based on the multicanonical ensemble [8,9]. So far such calculations have not been performed. Nevertheless we are able to give a rough estimate by analyzing the $L_t = 2$ SU(3) data of ref. [7] with regard to the surface tension, although the quality of the SU(3) data is fairly limited. For comparison, in case of the 7-state Potts model we have about 400 tunneling events for our 100^2 lattice,

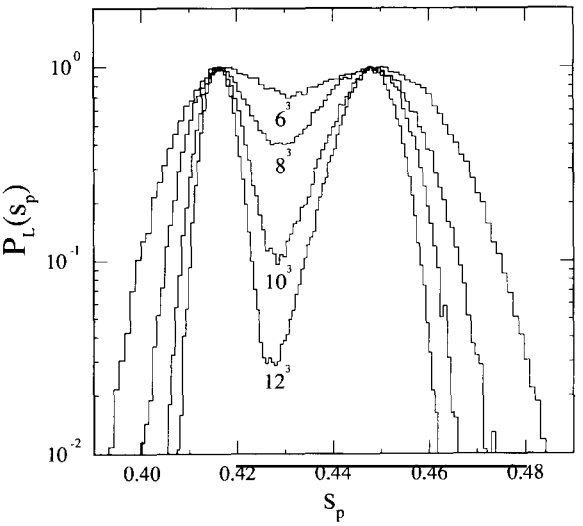

Fig. 11. SU(3) action density distributions $P_L(s_p)$ for lattices of size $2 \cdot 6^3, \ldots, 2 \cdot 12^3$ on a logarithmic scale. The values of the maxima have been normalized to 1.

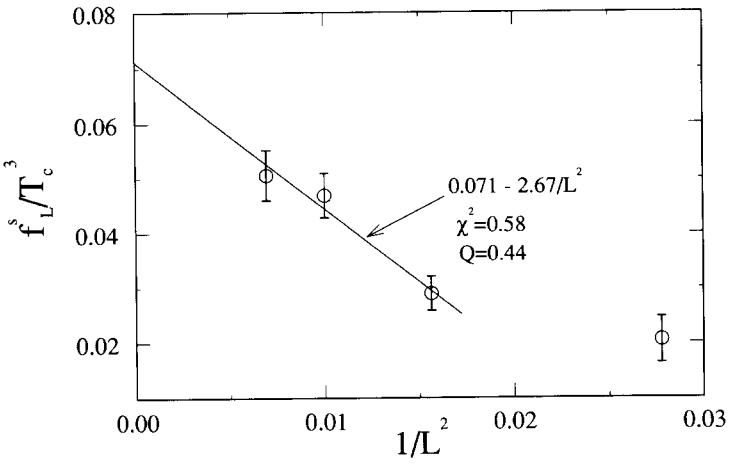

Fig. 12. Finite-size scaling for for the SU(3) interfacial free energy f^s/T_c^3.

whereas we are down to only (altogether) 10 tunneling events for the largest SU(3) lattice, which is $2 \cdot 12^2$. Available lattice sizes are now $L = 6$, 8, 10 and 12. Fig. 11 depicts the appropriately reweighted probability densities for the lattice averages, called s_p, of the normalized plaquette action Re Tr $U(\hat{p})/3$ (there exist two $L = 12$ data sets which we have combined to one). In contrast to the Potts model there is now some ambiguity in choosing the histogram binning size, but we have checked that within reasonable limits the influence on the final estimates is mild. The interfacial free energy per unit area follows in a similar fashion as in sect. 2. Eq. (5) modifies to

$$2f_L^s = -\frac{a^{-3}}{L_t L^2} \ln\left(P_L^{\min}\right), \tag{10}$$

where a is the lattice constant. It is conventional [4,5] to give final estimates for the dimensionless quantity f^s/T_c^3, where $T_c = a^{-1}L_t^{-1}$ is the physical temperature of the SU(3) deconfining transition. Our estimates of f_L^s/T_c^3 are depicted in fig. 12. The increase of f_L^s with lattice size, as compared to the decrease found in sect. 2 and other Potts model investigations [9,14,16], is remarkable. Presently, we have no theoretical understanding about the circumstances which differentiate an approach of the asymptotic limit from below versus above. The FSS fit of fig. 12 gives the asymptotic estimate

$$\frac{f^s}{T_c^3} = 0.071 \pm 0.008. \tag{11}$$

Of course, in view of the rather small lattice sizes and the somewhat limited quality of the data, this extrapolation is kind of daring. Nevertheless, it is presumably a reasonable starting point. With appropriate CPU time funding of about 1000 CRAY-YMP (or equivalent) supercomputer time, one may perform a multicanonical simulation of a $2 \cdot 24^3$ system to check for consistency by adding f_{24}^{s}/T_c^3 to fig. 12.

Comparison with refs. [4,5] is somewhat subtle, as changing normalizations have to be traced. We believe that their final definitions match with ours and we find our result to be about a factor of two smaller than theirs. The discrepancy is rather mild when compared to the one of sect. 2. Considering the relative weakness of our estimate (11), one may even question whether there is a significant difference at all. However, the investigation of sect. 2 suggests that there is no reason to expect our estimates and those of the methods of refs. [2–5] to converge to the same numbers.

4. Conclusions

We have carried out a fairly detailed FSS investigation for the two-dimensional 7-state Potts model. As far as comparisons with exact analytical results are possible, we find our estimates well consistent. The surface tension is not known exactly. We give an estimate (7) which differs considerably from results reported in previous literature [2,3]. It may look kind of surprising that no problems were noted before, however, the methods of refs. [2–5] seem in some sense to be self-consistently wrong. They rely on simulations far away (in the sense explained in sect. 2) from the relevant pseudo-transition β-values. The orders of magnitude of these deviations from the pseudo-transition points are dictated by the need to increase the signal, and in this region of rigid domains the illusion of a consistent approach is, indeed, suggested by the data. For SU(3) our surface tension estimate (11) should be considered as a first attempt to address the problem, and multicanonical simulations [8,9] on lattices of size up to at least $2 \cdot 24^3$ are suggested.

It had already been noticed some time ago by the authors of ref. [13] that eq. (5) seems to give a smaller estimate than the methods of refs. [2,3], and one of the present authors (BB) likes to thank Alain Billoire for useful discussions. Further, we thank Thomas Neuhaus for contributions at the early stage of the Potts model simulation. The Monte Carlo data were produced on the SCRI cluster of fast RISC workstations and at the Embry-Riddle Aeronautical University.

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