

C-Periodicity and the Physical Mass in the 3-State Potts Model

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Abstract

The standard infinite-volume definition of connected correlation function and particle mass in the 3-state Potts model can be implemented in Monte Carlo simulations by using C-periodic spatial boundary conditions. This avoids both the breaking of translation invariance (cold wall b.c.) and the phase-dependent and thus possibly biased evaluation of data (periodic b.c.). The numerical feasibility of the standard definitions is demonstrated by sample computations on a $24 \times 24 \times 48$ lattice.

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The 3-dimensional 3-state Potts model has been extensively studied in particle physics context because of its relation to the finite-temperature $SU(3)$ Yang-Mills theory [1]. Both have phase transitions which are characterised by spontaneous breaking of a global $Z(3)$ -symmetry. A controversial issue for the latter has been the order of the deconfinement phase transition [2, 3]. While two coexisting states, typical of a first order phase transition, were reported in Ref. [3], long-range correlations reminiscent of a second order phase transition were observed in Ref. [2]. The resolution of this controversy was first proposed in the context of the Potts model in Ref. [4]. Using finite size scaling theory for bulk quantities, a first order phase transition was established although the correlation length displayed identical behaviour to that seen in Ref. [2]. It was argued that the diverging correlation length was not due to a massless physical particle, but rather due to the finite-size effect of vacuum tunnelling. Subsequently, simulations of $SU(3)$ gauge theory at finite temperature confirmed [5] such an interpretation. The problem of determination of the physical correlation length was, however, left almost unsolved. Since the physical picture of a phase transition appears intuitively much clearer in terms of the physical correlation length, it appears desirable to devise a method of separating it from the tunnelling correlation length. Indeed, various physics applications, such as the Early Universe or heavy ion collisions, need a precise value of the physical correlation length in the critical region.

Most simulations employ periodic spatial boundary conditions to minimise surface effects. These, however, give rise to a rather complicated low-energy level structure in the broken phase of a theory with a spontaneously broken discrete symmetry. For both the Potts model and the finite temperature $SU(3)$ theory, one has three ordered vacua and tunnelling occurs between them in a finite volume. Close to the transition temperature there is order-disorder tunnelling as well. Thus, if the mass of the physical particle were small, it would be hard to separate it from the multitude of tunnelling levels. Indeed, various prescriptions [4, 6, 7] have been used to extract the physical mass in the Potts model. These are, however, not satisfactory since the results can be sensitive to various assumptions and parameters. Thus, e.g., Ref. [6] claimed a discontinuity in the physical mass which was shown to decrease with increasing volume in Ref. [7]. We therefore agree with the authors of Ref. [2] that a useful strategy is to single out one of the three ordered ground states by imposing a suitable boundary condition, thus sim-

plifying the low-energy level structure. Our boundary condition will emulate spatial infinity in two respects: breaking the global $Z(3)$ symmetry (without an external field) while preserving translational invariance.

A $Z(3)$ -symmetry breaking spatial boundary condition already extensively studied for $SU(3)$ Yang-Mills theory is the cold wall [2]: all links lying *in* the wall are set to their trivial values. The Potts model analogue is to put $s_w = 1$ for all spins on the wall. The cold wall, however, breaks the translational invariance. In order to reduce surface effects, one is forced to obtain results away from the wall where one sees little difference from the periodic boundary conditions.

The virtue of periodic b.c., on the other hand, is their preservation of translational invariance, and avoidance of any surface interactions. With a cold wall b.c. the very concept of particle mass is only an approximation. Furthermore, particles with any kind of charge will induce anticharges on the wall and will thus incur surface interactions.

Recently, C-periodic spatial boundary conditions have been developed for Monte Carlo simulations of (generalized) non-zero charges on finite lattices [9, 10, 11]. A numerical study of the $SU(3)$ Polyakov loop using those b.c. has already been carried out [11]. In this Letter, we propose C-periodic spatial boundary conditions for extracting the physical mass of the 3-dimensional 3-state Potts model in Monte Carlo simulations. As translational invariance is preserved, the concept of physical mass is clearly defined, and a precise determination by standard methods of statistical mechanics is possible. Connected correlation functions can be defined without any ad-hoc prescriptions (such as phase separation or arbitrary subtraction).

The Hamiltonian of the Potts model with nearest-neighbour couplings is

$$H = - \sum_{\langle j,k \rangle} \delta_{\sigma_j, \sigma_k}$$

where $\sigma_i \in \{0, 1, 2\}$ defines the spin on site i . The partition function is

$$Z = \sum_{\{\sigma\}} e^{-\beta H}$$

Link by link, H is invariant under the charge-conjugation operation

$$s \rightarrow \bar{s} \quad \text{where} \quad s = e^{2\pi i \sigma/3} \quad \text{and} \quad \bar{s} = e^{-2\pi i \sigma/3}.$$

In terms of the σ s,

$$0 \xrightarrow{C} 0 \quad 1 \xrightarrow{C} 2 \quad 2 \xrightarrow{C} 1.$$

We consider C-periodic spin configurations on an L^3 lattice,

$$\sigma_{i+L} = \bar{\sigma}_i \quad , \quad (1)$$

where $i + L$ denotes the site i translated by the lattice length L in a spatial direction. Such configurations are conveniently visualized as a chess-board array of copies and C-conjugate copies of the L^3 configuration stored in the computer. Under translation $\sigma_i \rightarrow \sigma_{i+1}$ of a C-periodic σ configuration the Hamiltonian is invariant.

The ground state of the ordered phase is characterized by $\sigma_i = 0$ on all sites i and is C-invariant. It is the same vacuum as with periodic boundary conditions and has the same energy. There are no other C-periodic vacua: if $\sigma_i = 1$ for some i then $\sigma_j = 2$ must also occur, so the minimum excitation energy is that of six $\langle ij \rangle$ bonds which corresponds to a *particle* excitation. A configuration with all $\sigma_i = 1$ on the L^3 lattice will have all $\sigma_j = 2$ on the adjacent C-conjugate lattices and will have the excitation energy of $n_{\text{cbc}}L^2$ bonds (n_{cbc} = number of C-periodic directions). It is a many-particle state rather than another vacuum.

The infinite-volume definition of the connected spin-spin correlation function

$$C(x - y) = \langle \bar{s}_x s_y \rangle - \langle \bar{s}_x \rangle \langle s_y \rangle$$

makes sense with C-periodic boundary conditions, too, since translation invariance is preserved. Due to C-conjugation invariance of the Hamiltonian, the correlation function is real. Furthermore,

$$\begin{aligned} C &= R + I \\ \text{where } R(x - y) &= \langle \text{Re } s_x \text{Re } s_y \rangle - \langle \text{Re } s_x \rangle \langle \text{Re } s_y \rangle \\ \text{and } I(x - y) &= \langle \text{Im } s_x \text{Im } s_y \rangle \end{aligned}$$

In any coordinate direction with a C-periodic boundary condition, $\text{Re } s$ is periodic while $\text{Im } s$ is *antiperiodic* [9, 11]. Thus the R and I parts of the correlation function C are clearly distinguished here. By contrast, both R and I would be periodic functions if purely periodic b.c. were imposed.

The Fourier decomposition of $C(x - y)$ can be interpreted in terms of “particle” excitations of the two-dimensional quantum field theory underlying the three-dimensional Potts model. This requires that a direction of Euclidean time is singled out in which the boundary condition is periodic (finite temperature). Of the two remaining spatial directions, at least one should be C-periodic for lifting the degeneracy of the ordered vacua.

For particles generated by $\text{Re } s$ the projection onto zero spatial momentum can be implemented as usual with periodic b.c. The masses of such particles are best obtained from the correlation function of $\text{Re } s$ averaged over the two-dimensional time slices.

For particles generated by $\text{Im } s$, there is a minimal spatial momentum of π/L for each C-periodic direction [9]. Hence, averaging $\text{Im } s$ over a time slice would mean to project onto an *antiperiodic continuation* of the constant function— an oscillatory step function with a strong contamination of higher momenta. The closest approximation to zero momentum in the antiperiodic case is a projection onto functions of minimal spatial momentum: $\cos x\frac{\pi}{L}$ and $\sin x\frac{\pi}{L}$ for C-periodicity in the x direction, and analogously for the y direction. As a consequence, the mass m_- of such a particle is not directly observable in the $\text{Im } s$ correlation function; rather, its correlation length is given by the energy E which depends on the spatial momentum according to some dispersion relation. Exploiting the cubic symmetry of the Hamiltonian, which includes space inversion and rotations by $\pi/2$ about the coordinate axes, one finds that an inverse propagator for the Potts model must take the form $m^2 + p_1^2 + p_2^2 + p_3^2 + \mathcal{O}(p^4)$. Hence, identifying $p_3 = iE$, the exponential decay of the correlation function is related to the particle mass and the spatial momentum by

$$E^2 = m^2 + p_1^2 + p_2^2 + \mathcal{O}(p^4, p^2 E^2, E^4) \quad (2)$$

In this Letter, eq. (2) will be used only at minimal momentum: $p_{i \min} = 0$ or $\pi/24$, depending on whether a periodic or C-periodic boundary condition is imposed in the corresponding direction. Furthermore, the energy levels we consider will be of order 0.1 in lattice units. Thus $\mathcal{O}(p^4, p^2 E^2, E^4)$ amounts to a correction in the 1% range. This is unresolvable within our statistical errors and will be neglected.

Since the C-periodic boundary conditions allow only one ordered state for $\beta > \beta_c$, vacuum tunnelling can take place only in the coexistence region of width σ_L around $\beta_{c,L}$ on a finite L^3 lattice. As a consequence, possible

contamination of physical mass by the tunnelling mass is restricted to this region only. Figure 1 shows schematically the expected behaviour of the lowest excitation energy, near the phase transition, as a function of β . Also shown is the corresponding behaviour for the periodic boundary case [4].

Following Wang and DeTar [8], we estimate the tunnelling effects for our version of the Potts model in terms of a simple model. Compared to their case, the Potts model with C-periodic boundary conditions has a much reduced symmetry—only charge conjugation symmetry is left. We, therefore, choose an extensive “ordered” state $|O\rangle$ which derives from the exact ordered vacuum at infinite β , and another extensive state $|D\rangle$ which derives from the exact disordered vacuum at $\beta = 0$ to describe our model. Both these states are assumed to be invariant under charge conjugation. In case of $|O\rangle$ this is because all spins s are equal to the real number 1; in case of $|D\rangle$ it is due to the superposition of all spin eigenstates with equal amplitudes. We furthermore assume the following relations to hold for the matrix elements of the real part \hat{r} of the spin operator:

$$\langle O|\hat{r}|O\rangle = 1 \quad \langle O|\hat{r}|D\rangle = \langle D|\hat{r}|D\rangle = 0$$

When restricted to the Hilbert space spanned by $|O\rangle$ and $|D\rangle$ the Hamiltonian will take the form

$$\begin{pmatrix} E_O & c \\ c & E_D \end{pmatrix}$$

where $c \geq 0$ as a matter of phase convention for the two states. At the point of order-disorder coexistence the energies E_O and E_D are equal. More generally, they depend on β and are proportional to the spatial volume V except for boundary effects. The matrix element c describes the vacuum tunnelling to be expected for $V < \infty$; it will depend on β and will decrease with $V \rightarrow \infty$. For $c \neq 0$ the eigenstates of the Hamiltonian are superpositions of the form

$$\begin{aligned} |+\rangle &= \sin \alpha |O\rangle + \cos \alpha |D\rangle \\ |-\rangle &= \cos \alpha |O\rangle - \sin \alpha |D\rangle \end{aligned}$$

$$\text{where } \tan \alpha = \sqrt{1 + x^2} + x \quad \text{with } x = \frac{E_O - E_D}{2c} \quad (3)$$

Hence we have

$$\langle +|\hat{r}|+\rangle = \cos^2 \alpha \quad \langle -|\hat{r}|-\rangle = \sin^2 \alpha \quad \langle +|\hat{r}|-\rangle = \langle -|\hat{r}|+\rangle = \sin \alpha \cos \alpha$$

The energy eigenvalues are

$$E_{\pm} = \frac{E_O + E_D}{2} \pm \frac{\epsilon}{2} \quad \text{where} \quad \epsilon = \sqrt{(E_O - E_D)^2 + 4c^2}$$

Let $|-\rangle$ correspond to the lower energy level which we put to zero, and let $|+\rangle$ be the first excited state at energy ϵ . The partition function is

$$Z = 1 + e^{-\beta\epsilon}$$

Evaluating traces in the $|\pm\rangle$ basis we find for the statistical expectation value of the real part of the spin

$$\langle \hat{r} \rangle = \frac{\cos^2 \alpha + e^{-\beta\epsilon} \sin^2 \alpha}{1 + e^{-\beta\epsilon}}$$

To recover the canonical picture, let us assume that the spatial volume is finite but large. At the coexistence point, $\epsilon \approx 0$ so that $\langle \hat{r} \rangle \approx \frac{1}{2}$. Elsewhere, $\epsilon \propto V$, hence the exponential factors are very small, and $\langle \hat{r} \rangle \approx \cos^2 \alpha$. Furthermore, eq. (3) implies $\alpha \approx 0$ for $E_O < E_D$ (broken phase) and $\alpha \approx \frac{\pi}{2}$ for $E_O > E_D$ (symmetric phase). Thus the spin expectation value indeed meets our expectations in this vacuum model. As for the correlation function,

$$\langle \hat{r}(0)\hat{r}(\tau) \rangle = Z^{-1} \text{Tr} \left(\hat{r} e^{-\tau H} \hat{r} e^{\tau H} e^{-\beta H} \right)$$

we have

$$\langle \hat{r}(0)\hat{r}(\tau) \rangle = \frac{\sin^2 \alpha \cos^2 \alpha}{\cosh(\beta\epsilon/2)} \cosh \epsilon \left(\tau - \frac{1}{2}\beta \right) + \frac{\cos^4 \alpha + \sin^4 \alpha e^{-\beta\epsilon}}{1 + e^{-\beta\epsilon}} . \quad (4)$$

Right at the phase transition where $\cos \alpha = \sin \alpha = \sqrt{1/2}$ this expression simplifies to

$$\langle \hat{r}(0)\hat{r}(\tau) \rangle = \frac{1}{4} \frac{\cosh \epsilon \left(\tau - \frac{1}{2}\beta \right)}{\cosh(\beta\epsilon/2)} + \langle \hat{r} \rangle^2$$

As for particle excitations, we assume that one-particle states are generated by acting with the local spin operator $\hat{s}(x)$ on a vacuum state. The real part $\hat{r}(x)$ of the spin field operator has C-parity +1 while the imaginary part $\hat{i}(x)$ has C-parity -1. The Hamiltonian H and the states $|O\rangle$ and $|D\rangle$ are charge-conjugation invariant. In the spin-spin correlations we thus expect to see an excitation scheme whose levels can be classified by their C-parity.

These model considerations suggest that vacuum tunnelling in the C-periodic Potts model (order-disorder tunnelling) only occurs in a narrow region around the phase transition, as illustrated in Figure 1. Outside that region, both in the ordered and disordered phase, the energy spectrum consists of a nondegenerate extensive ground state, followed by particle excitations. In the simplified model described above, ϵ is the energy of the first excited state which corresponds to the physical mass sufficiently away from β_c . In the coexistence region, however, $\epsilon \approx c$ and is thus governed entirely by the finite volume effects. Hence on increasingly larger volumes ϵ becomes vanishingly small at the transition point. On the other hand, the width of the coexistence region also goes down linearly with volume, thus opening the possibility of obtaining the physical mass at β_c in a limiting procedure.

We have simulated the 3-dimensional 3-state Potts model on a $24 \times 24 \times 48$ lattice, imposing C-periodic boundary conditions in *one* of the spatial ($L = 24$) directions, at couplings $\beta = 0.5505$, $\beta = 0.551$ and $\beta = 0.55125$. A total of 40000 measurements were performed at each coupling. At $\beta = 0.5505$ and $\beta = 0.551$ measurements were interspersed with 20 updatings of the spin configuration; at $\beta = 0.55125$ with 100 updatings. Plots of the MC results for those couplings are very similar. We here present plots only for $\beta = 0.5505$.

Figure 2 shows the Monte Carlo history of the real part of the spin averaged over the 3-dimensional lattice. The Figure illustrates the tunnelling between a globally ordered and a globally disordered state.

Our MC data for the Re s two-point correlation function $R(d)$, projected onto zero spatial momentum (Figure 3) are strongly dominated by a constant—presumably the one modelled by eq.(4). The measurement-to-measurement fluctuations in $R(d)$, also, are similar for all values of d , supporting the interpretation as a fluctuating constant. In fact, the errors in the exponentially decaying particle contributions which we are interested in are much smaller. To extract the latter, a better observable, suggested by eq.(4), is the differences $R(d) - R(d + 1)$. The constant part of the spin correlation thus drops out from both the mean values *and* the error bars, as is evident from Figure 4. A one-particle contribution to this difference would be of the form $A \sinh m(\frac{1}{2}N_\beta - \frac{1}{2} - d)$ where N_β is the temporal lattice size. Figure 4 shows the corresponding fit of the data. The mass of the excitation is given in the Table.

Practically the same mass is obtained by a global χ^2 fit of the form

$A \cosh m(N_\beta - d) + B$ to the unsubtracted function $R(d)$. In this latter way one obtains an excessively shallow χ^2 minimum since χ^2 is then mainly based on the fluctuations of the constant. Nevertheless, the agreement of mean excitation energies obtained from our $R(d)$ and from $R(d) - R(d + 1)$ supports the conjecture that C-periodic boundary conditions eliminate order-order tunnelling so that vacuum tunnelling effects must be taken into account only near the phase transition (order-disorder tunnelling).

For the correlation of the imaginary part of the spin, projected onto minimal spatial momentum, Figure 5 shows the differences $I(d) - I(d + 1)$ and a fit of the form $A \sinh E(\frac{1}{2}N_\beta - \frac{1}{2} - d)$. The mass of the $C = -1$ particle as obtained from formula (2) is given in the Table. In view of the non-zero momenta involved, we expect to find, as a consistency check, *no* particle energies in the $\text{Im } s$ correlation

- (a) below π/L if we impose C-periodicity in only one spatial direction,
- (b) below $\sqrt{2\pi^2/L^2}$ if both spatial directions are C-periodic.

In our sample computations of case (a), $L = 24$ so that the physicality bound is 0.131. This bound is consistent with the χ^2 distributions we obtain at all couplings from the *differences* $I(d) - I(d + 1)$. In the unsubtracted correlation functions $I(d)$ we actually observe small *constant* contributions as well. Furthermore, at all three couplings we find error bars consistent with the fluctuations of the mean values *only* in $I(d) - I(d + 1)$ while for $I(d)$ the mean values are overlaid again with the error bars of a fluctuating constant. However, the size of the effect is such that it can easily be understood in terms of mere statistical fluctuations. The constant fitted to $I(d)$ at $\beta = 0.5505$, for example, is 1.2×10^{-4} which is less than a standard deviation, after 40000 measurements, of a fluctuating constant with zero average and an RMS of the same order as in $R(d)$. In the following, we shall form differences $I(d) - I(d + 1)$ with the intention to eliminate from $I(d)$ the artifacts of a finite number of iterations.

At $\beta = 0.551$ and $\beta = 0.55125$, where we expect to be sufficiently deep in the ordered phase, the maximum-likelihood estimates (mean values in Table 1) of $m_- = 0.11$ for both cases indicate a massive particle in the $C = -1$ channel degenerate with the $C = +1$ particle discussed above. Since m_-^2 according to formula (2) involves a difference, $E^2 - p_{i \text{ min}}^2$, the mass estimates in the $C = -1$ channel can be quite sensitive to uncertainties in the correlation length $\xi = E^{-1}$. At the above couplings this results in a rather

large error estimate for m_- . At $\beta = 0.5505$, i.e. near the phase transition, we find an essentially unchanged $m_- = 0.13 \pm 0.02$, while m_+ decreases to 0.07 indicating the increasing dominance of order-disorder tunnelling in this regime.

In conclusion, we have shown that the C-periodic boundary conditions, given by eq. (1), eliminate order-order tunnellings and allow numerical implementation of the standard statistical-mechanical definition of connected correlation functions and particle masses in the 3-dimensional 3-state Potts model. This is also true for all $Z(N)$ models, N -state Potts models and $SU(N)$ gauge theories at finite temperature in any dimensions, provided N is odd. In particular, quenched QCD also falls in this category. Furthermore, we suggest a method to obtain the physical mass in all these theories at β_c in the thermodynamic limit. It will be interesting to find out using this method whether the first order phase transition in the 3-dimensional 3-state Potts model or the 3-dimensional $SU(3)$ gauge theory at nonzero temperature manifests itself as a discontinuity in the physical correlation length.

Also, it will be interesting to analyse the dispersion relation (2) beyond the quadratic order in the energy and momenta. For quasi-free actions with a Laplacian structure of derivatives, $E^2 = m^2 + \sum_k \sin^2 p_k$ is a natural extension; it has, in fact, produced satisfactory mass corrections for U(1) monopoles in the Villain approximation on smaller lattices [9]. For the Potts model, the action is of an entirely different form. Here one can study numerically the correlation functions of the real and imaginary parts of the spin after projection onto various non-minimal spatial momenta. However, on lattices large enough so that $\mathcal{O}(p_{\min}^4)$ is negligible, the $\text{Im } s$ correlation function in conjunction with dispersion relation (2) offers perhaps the best possible way to obtain the mass of the lowest $C = -1$ particle as it is not overlaid with any vacuum tunnelling.

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Figure 1: Schematic diagram illustrating the behaviour of the energy of the first excited state as a function of β near the phase transition for two volumes $V_1 < V_2$, using C-periodic (full lines) and periodic (full and dashed lines) boundary conditions.

Figure 2: Monte Carlo history of the real part of the spin (3-dimensional average) at $\beta = 0.5505$.

Figure 3: Monte Carlo data for the $\text{Re } s$ correlation $R(d)$ at $\beta = 0.5505$ and fit of the form $A \cosh m(24 - d) + B$. The error bars are dominated by the fluctuations of the constant B .

Figure 4: Monte Carlo data for the differences $R(d) - R(d+1)$ at $\beta = 0.5505$ and fit of the form $A \sinh m(23.5 - d)$. The χ^2 fit is based on data points $5 \leq d \leq 23$.

Figure 5: Monte Carlo data for the differences $I(d) - I(d+1)$ at $\beta = 0.5505$ and fit of the form $A \sinh E(23.5 - d)$. The χ^2 fit is based on data points $5 \leq d \leq 23$.

Table 1: Inverse correlation lengths ξ^{-1} and particle masses obtained from the spin-spin correlation. R and I refer to the correlation of the real or imaginary parts of the spin, respectively. The form of the fit is $A \sinh \xi^{-1}(23.5 - d)$.

β	Function	ξ^{-1}	Particle Mass
0.55050	$R(d) - R(d + 1)$	0.072 $\begin{smallmatrix} +0.012 \\ -0.014 \end{smallmatrix}$	same as ξ^{-1}
0.55050	$I(d) - I(d + 1)$	0.184 $\begin{smallmatrix} +0.016 \\ -0.014 \end{smallmatrix}$	0.13 ± 0.02
0.55100	$R(d) - R(d + 1)$	0.108 $\begin{smallmatrix} +0.012 \\ -0.014 \end{smallmatrix}$	same as ξ^{-1}
0.55100	$I(d) - I(d + 1)$	0.17 $\begin{smallmatrix} +0.05 \\ -0.045 \end{smallmatrix}$	0.11 $\begin{smallmatrix} +0.07 \\ -0.11 \end{smallmatrix}$
0.55125	$R(d) - R(d + 1)$	0.134 $\begin{smallmatrix} +0.008 \\ -0.007 \end{smallmatrix}$	same as ξ^{-1}
0.55125	$I(d) - I(d + 1)$	0.17 $\begin{smallmatrix} +0.045 \\ -0.055 \end{smallmatrix}$	0.11 $\begin{smallmatrix} +0.06 \\ -0.11 \end{smallmatrix}$

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