PHYSICS BEYOND INSTANTONS: MEASURING THE PHYSICAL CORRELATION LENGTH

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ABSTRACT

In broken-symmetry phases of models with discrete global symmetry, the physical correlation length can be measured using time-slice correlators projected to non-zero momenta. A transfer matrix based argument is used to construct the finite-size scaling for this quantity. We extract the correlation length for the two-dimensional 10-state Potts model by this means, and the surface tension from the zero-momentum correlator.

Correlation lengths, ξ , are extracted from Monte Carlo simulations by measuring the exponential decay of a correlation function, $C(r)$. When the long-distance limit of $C(r)$ is non-zero, it becomes difficult to measure ξ by the usual methods. These then yield the so-called ‘tunnelling correlation length’, ξ_r , which is unbounded as the system size goes to infinity, and decouples from the physical spectrum in the thermodynamic limit. In a spin model this situation arises in the ferromagnetically ordered phase, where the long-distance limit of $C(r)$ gives the spontaneous magnetisation. Near a first-order phase transition the existence of an unbounded correlation length can make it difficult to pin down the order of the transition based on correlation length measurements alone.

In this letter we present a construction of correlation functions whose long distance properties correctly give the ‘physical’ correlation length, *i.e.*, the one obtained from the connected part of the spin-spin correlation function. This construction uses some symmetry properties of transfer matrices. We present these arguments in the context of the Ising model, and point out the features which can be generalised. We test this method by a measurement of the physical correlation length in the low-temperature (ferromagnetically ordered) phase of the two-dimensional Ising model. Next we present a measurement of the correlation length in the two-dimensional 10-state Potts model at a coupling β just above the order-disorder transition point. Finally we use the zero-momentum correlator to extract the surface tension in this model [1].

Consider the Ising model—

$$Z = \exp(-\beta H), \quad H = \sum_{\langle ij \rangle} (1 - \sigma_i \sigma_j). \quad (1)$$

The known exact result for the asymptotic value of the spin-spin correlation function [2]

$$\langle \sigma_{00} \sigma_{0N} \rangle = (1 - \alpha^2 t)^{1/4} \left[1 + \frac{1}{2\pi N^2} \alpha^{2(N+1)} (\alpha^2 - 1)^{-2} + \dots \right] \quad (2)$$

where $\alpha = 1 / \sinh^2 2\beta$

yields both the spontaneous magnetisation and the correlation length—

$$\begin{aligned} m &= (1 - \sinh^{-4} 2\beta)^{1/8}, \\ \xi &= 1/4 \log \sinh 2\beta. \end{aligned} \quad (3)$$

These results can be obtained by transfer matrix arguments.

We restrict our attention to an $L \times T$ square lattice, with periodic boundary conditions in both directions, and the transfer matrix which propagates states on a time-slice of size L to the next. There are two obvious symmetries of this matrix—the global $Z(2)$ symmetry of the Hamiltonian in Eq. (1), and a symmetry of cyclic permutations of the spins in the time slices. Eigenfunctions of $Z(2)$ are classified according to whether they are even or odd under the transformation. The cyclic permutations, on the other hand, are diagonalised by Fourier modes k on time-slices. Eigenvectors of the transfer matrix carry representations of both these symmetries.

It is known that the largest eigenvalue of the transfer matrix, Λ_0 , belongs to the $k = 0$, $Z(2)$ even, sector. For $\beta > \beta_c$, the $k = 0$ eigenvalue from the $Z(2)$ odd sector becomes degenerate with this (in the thermodynamic limit). On any finite volume this degeneracy is lifted by instantons [3], leading to a splitting which decreases exponentially with L —the tunnelling correlation length. The physical correlation length, on the other hand, depends on the next largest eigenvalue, Λ_2 . This belongs to the $Z(2)$ even sector and $k = 2\pi/L$. These eigenvalues have a simple form for the diagonal to diagonal transfer matrix [4]. For large L we can use the expression

$$1/\xi = 4 \log \left(\frac{\cosh^2 2\beta + c}{\cosh^2 2\beta - c} \right), \quad c = \frac{1}{\alpha} \sqrt{(1 - \alpha)^2 + 4\alpha \sin^2(k/2)}. \quad (4)$$

The masses for other low-lying, $Z(2)$ -even, small- k modes are obtained by simply replacing the corresponding value of k in the argument of the sine [5]. All these eigenvalues are degenerate in the thermodynamic limit, and all yield the correct spin-spin correlation length. For large values of L , the expression above can be expanded as a series in the sine. The leading finite-size correction to the physical mass is thus proportional to the energy of one mode of a free field in the $d - 1$ dimensional slice.

It is well known that finding eigenvalues of the transfer matrix on any finite lattice reduces to solving some quantum mechanics problem. Hence, generalisations of the Ising results can be sought through an effective potential argument. This leads us to believe that the results can indeed be carried over to some other models. When the global symmetry group of the Hamiltonian is discrete, the lowest state belongs to the singlet of this group and $k = 0$. If the system is ordered in the thermodynamic limit, then there are other symmetry-related states (also with $k = 0$) which, on finite lattices, are split by instanton effects. The first excited state above this is split by the ‘rotational energy’ of the Fourier modes. These $k \neq 0$ modes do not couple to the overall magnetisation, and hence are insensitive to tunnellings between the symmetry-related vacua. In the large L limit, the splitting inside this multiplet vanishes as $1/L^2$. Hence measurements of the mass through correlations of

these operators, when coupled with such a finite-size scaling, should yield the physical correlation length. We note that these arguments may fail if the global symmetry group is continuous. However, the physically interesting case of finite-temperature $SU(N)$ gauge theories lies within the scope of this argument.

We have carried out measurements of the correlation functions

$$C_k(t) = \langle \text{Re}[\sigma_k(0)\sigma_k^*(t)] \rangle, \quad (5)$$

on $L \times T$ lattices for the Ising model at $2\beta = 0.95$. The Fourier modes $\sigma_k(t)$ are defined as

$$\sigma_k(t) = \frac{1}{\sqrt{L}} \sum_{r=1}^L e^{ikr} \sigma_r t. \quad (6)$$

The simulations have been run on lattices with $L = 2^n$ ($2 \leq n \leq 6$) and with $L \leq T \leq 4L$. Measurements have been made on configurations separated by 10 to 50 Swendsen-Wang updates. Autocorrelations between measurements are too small to be estimated. We have generated between 1 and 3 million configurations at each of the lattice sizes, and performed a measurement once every 50 sweeps. We have discarded the first 10^4 sweeps for thermalisation. Fourier modes on time slices were constructed by a Fast Fourier Transform. Although this code was run on scalar machines we note that the FFT can be vectorised over time slices. The Fourier transform and the correlation measurement took negligible time compared to the update.

In Fig. 1 we show the local masses obtained from the $k = 2\pi/L$ correlator for $L = 8$ and different values of T . It is clear that the correlation function can be followed to large distances and an asymptotic value for the correlation length can be obtained from these measurements. We have also extracted the correlation length from a two-parameter fit of the form

$$C_k(t) = a \cosh[(L/2 - t)/\xi]. \quad (7)$$

In order to explore the stability of these fits, we have further tried four-parameter fits of the form

$$C_k(t) = a \cosh[(L/2 - t)/\xi_1] + b \cosh[(L/2 - t)/\xi_2], \quad (\xi_1 > \xi_2). \quad (8)$$

We have usually been able to follow the correlation function out to $t \simeq 7\xi_1$, and, even in the worst case, to $t \simeq 5\xi_1$. The values of ξ obtained from fits to Eq. (7) match those obtained for ξ_1 in Eq. (8); only the errors are somewhat larger. We

have been able to use all data for $t \geq 2$ in the four-parameter fits. We found that a stable two-parameter fit could always be made after cutting out the data on the lowest $2-3\xi_2$ time separations. The efficiency of the cluster algorithm shows up even in the magnetised phase of the Ising model through the fact that covariances between measurements of $C(t)$ at different separations t are extremely small. This leads, in turn, to the happy situation that the ‘correlated- χ^2 ’ [6] fits yield the same results as the usual fits.

The best-fit values of the correlation length are shown in Table 1. The deviation of the measured result from the infinite volume value, $\xi = 2.64$, obtained from Eq. (3), shows the presence of substantial finite size corrections. In order to verify that the measurement indeed yields the correct correlation length, we show in Fig. 2 our results along with those obtained from Eq. (4). The good agreement between the two indicates that finite-size effects are under control.

We have used this method to extract the correlation length in the 10-state Potts model. In terms of integer-valued site spins σ_i ($0 \leq \sigma_i \leq 9$), the Hamiltonian is

$$H = \sum_{\langle ij \rangle} (1 - \delta_{\sigma_i \sigma_j}). \quad (9)$$

This model undergoes a first-order phase transition at $\beta_c = \log(\sqrt{10} + 1)$. We have simulated this model on $L \times T$ lattices at a coupling $\beta = \beta_c$. On any finite lattice the system is ordered at this coupling. Hence measurements of ξ , extrapolated to the thermodynamic limit, should give us the physical correlation length of this model for $\beta \rightarrow \beta_c^+$.

Configurations have been generated using the Swendsen-Wang algorithm. The longest autocorrelation time in this system is dictated by order-disorder flip rates [7], and is fairly large. However, we found that integrated autocorrelation times for the $k \neq 0$ correlators seem to be rather insensitive to flips. In Table 2 we display the lattice sizes, statistics and estimates of the tunnelling autocorrelation time in our runs. We observed that the integrated and exponential autocorrelation masses for the energy are equal within errors, and both are related to the flip rate through the formalism of [7].

For $k = 2\pi/L$, we have been able to follow $C(t)$ upto $t \sim 5\xi$. In this case we performed the analysis of correlation function by minimising

$$\chi^2 = \sum_{ij} \left(\frac{y_i - f(t_i)}{\sigma_i} \right) (C^{-1})_{ij} \left(\frac{y_j - f(t_j)}{\sigma_j} \right), \quad (10)$$

where C is the covariance matrix of the data [6] $\{y_i\}$, and $f(t)$ is the fitting function. The matrix C was inverted through a singular-value decomposition (SVD). Given the matrix of covariances, this method consists of writing its decomposition as

$$C = UDV, \quad C^{-1} = V^T D^{-1} U^T,$$

where U and V are orthogonal matrices and D is diagonal. Numerical instabilities in the fitting procedure set in when some pieces of data, for example, at the tail of the correlation function, are badly determined. This is usually dealt with by removing the data from the fit altogether. SVD provides us with an alternative procedure. The same instability shows up as a large condition number for D . This can be controlled by the removal of large elements of D^{-1} , corresponding to linear combinations of the data which are strongly correlated. We set $1/D_{ii} = 0$ whenever D_{ii} is small enough that it would yield a condition number larger than some preset limit c_0 , unless removed. We have used values of c_0 varying between 0.05 and 0.1, in conjunction with the two-parameter fitting function of Eq. (7).

For lattices with L upto 48 the resulting inverse covariance matrix C^{-1} is diagonal dominated, and the results of the fits are not changed appreciably in going to the usual definition of χ^2 . In Fig. 3 we show the data obtained on the 48×48 lattice along with the best fit. Data from the two lattices with $L = 64$, on the other hand, contain strong covariances. The major effect of this is to introduce some covariance between the best-fit values of a and ξ (Eq. (7)). We believe that larger statistics would reduce this problem. In all these cases we have checked that the values of ξ obtained remain stable when using four parameter fits. These yield a crude measure of the next higher mass in this channel; it turns out to be of the order of one lattice spacing. The best fit values of ξ are shown in Table 3. We note that it is not necessary to use extremely long lattices to extract ξ —a square lattice seems to yield quite acceptable results. Furthermore, the statistics used is quite sufficient to bound the errors to a few percent.

We have extracted the physical correlation length in the thermodynamic limit using the finite-size scaling ansatz presented earlier. We constructed a fit of the form

$$\xi(L) = \xi + \frac{a}{L^2}. \quad (11)$$

Data for $L = 32, 48$ and 64 can be extremely well described by this form. The quality of the fit may be judged from Fig. 4. We obtain the estimate

$$\xi = 5.66 \pm 0.09, \quad 10 - \text{state Potts model.} \quad (12)$$

A previous measurement [8] yielded $\xi = 5.9 \pm 0.7$, in agreement with our results.

It has recently been pointed out [1] that a finite-size analysis of the tunnelling correlation length can be used to measure the surface tension σ in broken-symmetry phases of different models. The argument is perfectly general [4]. A useful ansatz is provided by a dilute instanton gas approximation. This yields the large- L result [3] that

$$\xi_r(L) \sim \exp(\sigma L). \quad (13)$$

We have tried to extract the tunnelling mass from the zero-momentum correlators using two-parameter fits of the form shown in Eq. (7). The inverse covariance matrix of the data is not diagonal-dominated on any of lattices we have studied. The reason is well-understood: when T is not much larger than ξ_r , the lattice does not break up into domains in the T direction, but flips, as a whole, between different vacua. Thus measurements of $C(t)$ at different t are strongly correlated. It is clear that the rapid growth of ξ_r with L implies that T/L should increase exponentially with L in order to permit reliable measurements of this correlation length. We find that the relative errors in ξ_r are typically two to three times those obtained for ξ ; it would require four to ten times as much CPU effort to reduce these errors to the same level. Four-parameter fits yield statistically meaningless results for the next higher mass in this channel.

With the limited values of T/L at our disposal, we have been able to perform reliable measurements only till $L = 32$. The resulting correlation lengths do seem to scale exponentially with L (Fig. 5). Our estimate for the surface tension from a fit to measurements of ξ_r on the $8 \times 32, 16 \times 32$ and 32×64 lattices is

$$\sigma = 0.09 \pm 0.01, \quad 10 - \text{state Potts model.} \quad (14)$$

This result is compatible with a direct measurement of the barrier height in the effective potential [9], yielding $\sigma = 0.0978 \pm 0.0008$. We find it interesting to note that the relation $2\sigma\xi = 1$, proven for the Ising model, seems to hold also in this case. A generalisation of the methods of Ref. 10 would lead to a relation between σ at any coupling in the ordered phase and ξ at the duality-related coupling in the disordered phase. If, further, the relation observed here could be proved, then one would have a relation between the physical correlation lengths at duality-related couplings above and below the transition temperature.

Previous attempts at measuring the physical correlation length have been concentrated on the zero-momentum propagator. One method [11] has been to try a four-parameter (two-mass) fit in order to extract the tunnelling correlation length as

well as the physical mass. The second [12] method has been to fit a constant plus an exponential, thus trying to obtain the magnetisation and the physical mass. These are expected to work in disjoint situations. When T is large compared to ξ_r one expects the first method to work, otherwise the second may be preferable. The third method [13] relies on local mass measurements using subtractions of the form

$$\mu = \log \left(\frac{C_0(t) - C_0(t+1)}{C_0(t+1) - C_0(t+2)} \right). \quad (15)$$

This local mass coincides with the physical mass gap when the tunnelling correlation length is very large. In all three cases, it has been found necessary to work with reasonably long lattices ($T \geq 4L$) and to use large data samples.

With the lattice sizes and statistics used in our study of the 10-state Potts model, we have been unable to extract statistically meaningful estimates of the physical mass gap from the zero-momentum propagator by any of these three methods. On the other hand, as already shown, the momentum $k = 2\pi/L$ propagator can be used to fix ξ with better than 10% accuracy. We conclude that time-slice correlators projected to non-zero momenta present a simple computational scheme for measurement of physical masses in theories with broken discrete global symmetries.

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TABLE 1

Estimates of the physical correlation length ξ in the two dimensional Ising model obtained on various lattice sizes through two parameter fits to the momentum $2\pi/L$ correlation function.

L	$T = L$	$T = 2L$	$T = 4L$
4			0.64 ± 0.03
8		0.95 ± 0.02	0.97 ± 0.04
16	1.73 ± 0.03	1.69 ± 0.03	1.67 ± 0.02
32	2.50 ± 0.05	2.6 ± 0.2	
64	2.45 ± 0.05	2.51 ± 0.04	

TABLE 2

The number of configurations generated (N , in millions) and estimates of the integrated autocorrelation time for the energy density (τ_E) in the 10-state Potts model for different lattice sizes. The correlation function measurements have been made once every 100 sweeps for $L \leq 16$, and once every 1000 sweeps on the other lattices.

L	$T = L$		$T = 2L$		$T = 4L$	
	N	τ_E	N	τ_E	N	τ_E
4					1.0	$4.5 (2) \times 10^1$
8			2.0	$1.19(7) \times 10^2$	3.0	$1.79(5) \times 10^2$
16	4.0	$4.5 (3) \times 10^2$	3.0	$9.8 (7) \times 10^2$		
32	5.0	$5.3 (7) \times 10^3$	11.0	$1.1 (1) \times 10^4$		
48	11.0	$4.3 (3) \times 10^4$				
64	7.0	$0.8 (2) \times 10^5$	3.5	$1.4 (3) \times 10^5$		

TABLE 3

Estimates of the physical correlation length ξ in the two dimensional 10 state Potts model obtained on various lattice sizes through two parameter fits to the momentum $2\pi/L$ correlation function. χ^2 has been defined in Eq. (10).

L	$T = L$	$T = 2L$	$T = 4L$
4			0.59 ± 0.05
8		0.92 ± 0.02	0.99 ± 0.01
16	2.19 ± 0.03	2.00 ± 0.02	
32	3.54 ± 0.07	3.51 ± 0.02	
48	4.73 ± 0.03		
64	5.1 ± 0.2	5.1 ± 0.1	

FIGURE CAPTIONS

Fig. 1: Local masses in the $k = 2\pi/L$ channel for the Ising model at $2\beta = 0.95$ with $L = 8$. Filled circles denote measurements for $T = 8$, squares for $T = 16$ and open circles for $T = 32$.

Fig. 2: The physical correlation length extracted from the Ising model simulations at $2\beta = 0.95$ along with the exact result on finite lattices.

Fig. 3: Data for the momentum $k = 2\pi/L$ time-slice correlator for the 10-state Potts model on the 48×48 lattice shown along with the result of a two parameter fit. The latter has been obtained with χ^2 defined as in Eq. (10). The covariance matrix of data has been inverted with $c_0 = 0.05$.

Fig. 4: The physical correlation length in the 10-state Potts model at β_c , shown as a function of $1/L^2$. The fit to the three largest values of L is shown by the straight line. Open circles denote measurements on lattices with $T = L$ and filled circles on $T = 2L$.

Fig. 5: The tunnelling correlation length in the 10-state Potts model at β_c , shown as a function of L . The fit yielding the surface tension in Eq. (14) is shown by the straight line.

Figure 1

Figure 2

Figure 3

Figure 4

Figure 5