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# Finite size effects on measures of critical exponents in d = 3O(N) models

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## Abstract

We study the critical properties of three-dimensional O(N) models, for N=2,3,4. Parameterizing the leading corrections-to-scaling for the  $\eta$  exponent, we obtain a reliable infinite volume extrapolation, incompatible with previous Monte Carlo values, but in agreement with  $\epsilon$ -expansions. We also measure the critical exponent related with the tensorial magnetization as well as the  $\nu$  exponents and critical couplings.

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## 1. Introduction

The study of continuous spin models in low dimensions has been very useful either for the knowledge of some physical systems directly associated (mainly in condensed matter), or as toy systems for studying relativistic field theories.

The O(4) model in three dimensions has been conjectured to be on the same universality class as the finite-temperature chiral phase transition of QCD with massless flavors [1]. The O(4) universality class has also appeared in perturbation-theory studies of spin-systems for which the O(3) symmetry of the action is fully broken on the low temperature phase [2]. It is well known that the O(3) model in two dimensions of-

The O(N) nonlinear sigma models in three dimensions have been extensively studied either with analytical [7–9] or numerical methods, obtaining very accurate results in the determination of the critical properties. In particular the critical exponents have been measured for  $N \le 4$  with a precision greater than a 1% [10–12]. However, the finite-size effects have not been considered in a systematic way. We find this pro-

fers a play-ground to explore asymptotic freedom [3], although there has been recently some controversy on this point [4]. Regarding the applications to condensed matter physics, let us remind that the three-dimensional O(3) model is the low-temperature's effective-model for a bidimensional quantum antiferromagnet [5]. It also appears as a limiting case of a  $Z_2$ -gauge lattice model for nematic phase transitions of liquid crystals [6]. Finally, the O(2) model in three dimensions is known to be in the same universality class as superfluid  $^4$ He.

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cedure not harmful for  $\nu$  exponent measures, but quite dangerous for  $\eta$  exponents determinations.

Another point we focus on, is the study of the second-rank tensorial magnetization. This composite operator is needed as an order-parameter in some applications, for instance when the usual magnetization vanishes, as in studies of nematics [6]. It is also the relevant order parameter for systems where the O(3) symmetry is fully broken [2]. Naively one could expect that the tensorial magnetization scales just as the square of the vectorial one, that is,  $\beta_T$  is twice  $\beta$ , as a mean field calculation predicts (it was also assumed in Ref. [6]). Nevertheless we shall show that this is not so. A somehow related question, which has aroused interest lately, is the presence of some pathologies in the renormalization of composite operators in  $2 + \epsilon$  expansions [13].

In this paper we consider the O(2), O(3) and O(4) models, centering mainly in the measures of magnetic exponents using a finite-size scaling method which is specially useful for observables that change rapidly at the critical point. In addition to the standard magnetic exponents we measure those related with tensorial excitations. The critical couplings and  $\nu$  exponents are also studied. We are specially interested in the measure of  $\nu$  in the O(4) case in order to compare with the results obtained in the antiferromagnetic RP<sup>2</sup> model [14], which is related with O(4) when there is a total breakdown of its O(3) symmetry.

# 2. The model

We consider the usual Hamiltonian

$$\mathcal{H} = -\beta \sum_{\langle i,j \rangle} v_i \cdot v_j,\tag{1}$$

where  $v_i$  is a N components normalized vector, and the sum is extended over first neighbor pairs.

It is well known that this model undergoes a second order phase transition for which the normalized magnetization  $M = \frac{1}{V} \sum_{i} v_{i}$  is an order parameter (V is the lattice volume). As this model can be simulated using cluster algorithms [15], it is possible to thermalize very large lattices.

We are also interested in studying the behavior of composite operators that could be related with bound states from a quantum field theory point of view. One can construct orthogonal states to that generated by the fundamental field, just ensuring that the composite operator transforms as a higher order irreducible representation. The simplest representation beyond the fundamental one is the second rank tensorial representation. The associated tensorial magnetization can be written as

$$\mathcal{M}^{\alpha\beta} = \frac{1}{V} \sum_{i} (v_i^{\alpha} v_i^{\beta} - \frac{1}{N} \delta^{\alpha\beta}). \tag{2}$$

As it happens with the vectorial magnetization, the mean value of  $\mathcal{M}$  is zero in a finite lattice, so, in the Monte Carlo simulation we have to construct an estimator that avoids the tunneling effects. We define the (normalized) magnetizations as

$$M = \left\langle \sqrt{M^2} \right\rangle, \quad M_{\rm T} = \left\langle \sqrt{{\rm tr} \mathcal{M}^2} \right\rangle.$$
 (3)

We also define the associated susceptibilities as

$$\chi = V \langle \mathbf{M}^2 \rangle$$
,  $\chi_{\rm T} = V \langle \text{tr} \mathcal{M}^2 \rangle$ . (4)

The critical behavior of those quantities is expected to be

$$M \propto t^{\beta}$$
,  $M_{\rm T} \propto t^{\beta_{\rm T}}$ ,  
 $\chi \propto |t|^{-\gamma}$ ,  $\chi_{\rm T} \propto |t|^{-\gamma_{\rm T}}$ , (5)

where t is the reduced temperature. We expect the tensorial exponents to be also related through the (hyper) scaling relation  $\gamma_T + 2\beta_T = \nu d$ .

#### 3. The method

To compute the critical exponents we have used a finite-size scaling analysis. Specifically, we have used the method of Refs. [14] that consists in the comparison of observables on several pairs of lattices at the same coupling. The mean value for the operator O, measured in a length L lattice, at a coupling  $\beta$  in the critical region, is expected to behave as

$$\langle O(L,\beta) \rangle = L^{x_O/\nu} \left[ F_O(\xi(L,\beta)/L) + L^{-\omega} G_O(\xi(L,\beta)/L) + \ldots \right], \tag{6}$$

where  $F_O$  and  $G_O$  are smooth scaling functions for this operator,  $\xi$  is a measure of the correlation length and  $x_O$  is the critical exponent associated with O. Let

us recall that  $\omega$  is an universal exponent related with the first irrelevant operator. The dots stand for further scaling corrections. We have also dropped a  $\xi^{-\omega}$  term, negligible in the critical region. To eliminate the scaling functions we compare the measures in two different lattice sizes  $(L_1, L_2)$  at the same coupling. Let be

$$Q_{O} = \frac{\langle O(L_{2}, \beta) \rangle}{\langle O(L_{1}, \beta) \rangle}$$

$$= s^{x_{O}/\nu} \frac{F_{O}\left(\xi(L_{2}, \beta)/L_{2}\right)}{F_{O}\left(\xi(L_{1}, \beta)/L_{1}\right)} + O(L^{-\omega}), \tag{7}$$

where  $s = L_2/L_1$ . It is easy to find the coupling value where  $Q_{\xi} = s$ . Measuring O at that point we obtain the critical exponent from

$$Q_O|_{O_{\varepsilon=\delta}} = s^{x_O/\nu} + O(L^{-\omega}). \tag{8}$$

We remark that even if O is a fast varying function of the coupling in the critical region, as the magnetization, the statistical correlation between  $Q_O$  and  $Q_{\xi}$  allows a very precise determination of the exponent.

For the correlation length, we use a second momentum definition [16] which is easy to measure and permits to obtain an accurate value:

$$\xi = \left(\frac{\chi/F - 1}{4\sin^2(\pi/L)}\right)^{1/2},\tag{9}$$

where F is defined as the Fourier transform of the two-point correlation function at minimal momentum  $((2\pi/L,0,0))$  and permutations).

## 4. Critical exponents

For the Monte Carlo simulation, we have used the Wolff's embedding algorithm with a single cluster update [15]. We have simulated in lattice sizes from L=8 to L=64 on the critical coupling reported on Refs. [10–12]. We have used the spectral density method to extrapolate to the neighborhood of these couplings. We have updated 25 million clusters for O(2) and O(3) and 50 million in the O(4) case. The autocorrelation times are very small in all cases (not larger than a hundred of clusters). The runs have been performed on several workstations.

We have used the operator  $\mathrm{d}\xi/\mathrm{d}\beta$  to obtain the  $\nu$  exponent  $(x_{\mathrm{d}\xi/\mathrm{d}\beta}=1+\nu)$ . For the magnetic exponents, we use the total magnetization  $(x_M=\beta)$  as well

as the corresponding susceptibility  $(x_{\chi} = \gamma)$ . From them we obtain the  $\eta$  exponent using the scaling relations  $\gamma/\nu = 2 - \eta, 2\beta/\nu = d - 2 + \eta$ . For the tensorial channel we obtain a different set of exponents that we denote as  $\beta_T, \gamma_T, \eta_T$  respectively.

In Table 1 we report the results for the exponents displaying also the used operator. We have checked other observables as well as other definitions of the correlation length but, in all cases, either the corrections-toscaling or the statistical errors are greater.

## 5. Infinite volume extrapolation

In Table 1 corrections-to-scaling are clearly visible for the  $\eta$  exponent. To control them, we need an estimation of the  $\omega$  exponent. To measure this index and the critical coupling [14], we study the crossing between the Binder cumulant of the magnetization for different lattice sizes, as well as the corresponding for  $\xi/L$ . The shift from the critical coupling of the crossing point for lattices of sizes  $L_1$  and  $L_2$  behaves as [17]

$$\Delta \beta^{L_1, L_2} \propto \frac{1 - s^{-\omega}}{s^{\frac{1}{\nu}} - 1} L_1^{-\omega - \frac{1}{\nu}}.$$
 (10)

As the crossing point for the Binder cumulant and  $\xi/L$  tends to the critical coupling from opposite sides, it is convenient to fit all the data together. We have carried out two types of fits, one fixing the smaller lattice and the other fixing the  $L_2/L_1$  ratio. In Table 2 we present the results obtained using the full covariance matrix, for  $L_1 = 8$  and s = 2.

We observe a value for the  $\omega$  exponent compatible with the 0.78(2) value obtained from g-expansions for the O(2) and O(3) models [7]. In the O(4) case the result is almost twice. Lacking a theoretical prediction, this could be interpreted in two ways, the exponent could truly be so big, or it might be that the coefficient of the leading corrections-to-scaling term is exceedingly small.

The values obtained for the critical couplings are extremely precise, and compatible with the most accurate previous determinations by Monte Carlo simulations [18,11,12]. Let us remark that the conjectured value for the critical coupling of the O(3) model [19],  $\beta_c = \log 2$ , is ten standard deviations away from our measures.

Table 1 Critical exponents obtained from a finite-size scaling analysis using data from lattices of sizes L and 2L for the O(N) models. In the second row we show the operator used for each column

		$ u \ d \xi / d eta$	$\eta$		$\eta_T$	
N	L		X	M	Хт	$M_T$
2	8	0.683(3)	0.0252(10)	0.0297(11)	1.499(2)	1.506(2)
	12	0.678(3)	0.0303(11)	0.0333(13)	1.496(3)	1.500(3)
	16	0.672(3)	0.0329(12)	0.0355(12)	1.494(2)	1.497(3)
	24	0.676(4)	0.0344(12)	0.0355(13)	1.494(3)	1.495(3)
	32	0.670(3)	0.0366(12)	0.0387(13)	1.494(3)	1.496(3)
3	8	0.724(3)	0.0300(10)	0.0317(10)	1.432(2)	1.437(2)
	12	0.712(4)	0.0337(9)	0.0352(10)	1.4312(17)	1.4342(17)
	16	0.712(4)	0.0344(11)	0.0354(12)	1.428(2)	1.429(2)
	24	0.716(5)	0.0378(12)	0.0385(13)	1.4320(18)	1.4335(18)
	32	0.711(5)	0.0371(11)	0.0377(12)	1.428(2)	1.430(2)
4	8	0.752(2)	0.0307(6)	0.0316(6)	1.3735(10)	1.3767(11)
	12	0.747(3)	0.0338(5)	0.0345(6)	1.3771(10)	1.3790(10)
	16	0.754(4)	0.0341(7)	0.0344(7)	1.3770(14)	1.3781(13)
	24	0.757(4)	0.0348(5)	0.0349(5)	1.3771(10)	1.3774(11)
	32	0.753(5)	0.0359(9)	0.0361(10)	1.3753(18)	1.3759(18)

To control finite-size effects the most common procedure is to pick the smaller lattice for which there is no scaling corrections. That is, one uses a log-log plot, discard small lattices, and stop when the value of critical index stabilizes. Using this method, it has been determined that for the O(2) model it is enough to use lattices with sizes  $L \geq 16$  [10],  $L \geq 12$  for the O(3) model [11], and  $L \geq 8$  for the O(4) model [12]. We shall confirm this assumption for the  $\nu$  exponent but no for the magnetic ones.

It might not be possible to find a safe  $L_{\min}$  lattice (in fact, to find scaling corrections is just a matter of statistical accuracy), we thus need an extrapolation procedure. With an  $\omega$  estimation, we can extrapolate to the infinite volume limit, with an ansatz for the exponent  $x_0$ :

$$\frac{x_O}{\nu}\Big|_{\infty} - \frac{x_O}{\nu}\Big|_{(L,2L)} \propto L^{-\omega}.$$
 (11)

The situation is fairly different for the  $\nu$  and  $\eta$  exponents, therefore we shall discuss them separately.

## 5.1. $\eta$ type exponents.

Due to the high accuracy that we get from the statistical correlation between the measures of  $\xi$  and  $\chi$ , we

Table 2 Fits for  $\beta_c(\infty)$  and the corrections-to-scaling exponent  $\omega$ . The second error bar in  $\omega$  is due to the variation of  $\nu$  exponent within a 1% interval (the size of previously published error bars)

N	Fit	$\chi^2/\text{d.o.f.}$	ω	$eta_{ m c}(\infty)$
2	$L_1 = 8$ $s = 2$	11 /8 9.8/6	0.86(12)(3) 0.81(12)(1)	0.454169(4) 0.454165(4)
3	$L_1 = 8$ $s = 2$	2.0/8 2.3/6	0.64(13)(2) 0.71(15)(1)	0.693001(10) 0.693002(12)
4	$L_1 = 8$ $s = 2$	11.9/8 8.0/6	1.80(18)(6) 1.85(21)(2)	0.935858(8) 0.935861(8)

are able to resolve finite-size corrections. One could wonder if only the first correction term ( $\propto L^{-\omega}$ ) is needed. To check it we have used an objective criterium: we perform the fit from  $L_{\min}$ , then we repeat it discarding  $L_{\min}$  and check if both fitted parameters (slope and extrapolation) are compatible. If that is the case, we take the central value from the fit with  $L_{\min}$  and the error bar from the fit without it. In the three models, we find that  $L_{\min} = 8$  is enough for this purpose.

For the O(2) and O(3) models, we have a very precise knowledge of  $\omega = 0.78(2)$ , from series analysis. We plot in Fig. 1 our data as a function of  $L^{-\omega}$ . For

Table 3 Infinite volume extrapolation for  $\eta$  from  $\chi$  and M. The second error is due to the uncertainty on  $\omega$ . For the O(4) model, the first column has been calculated with  $\omega = 0.78$  and the second with  $\omega = 1.8(2)$ . In the last three rows we present, respectively, the results for this exponent from  $\epsilon$ , g-expansions and previously published Monte Carlo values

	O(2)	O(3)	O(4)		
χ	0.0424(23)(2)	0.0413(15)(1)	0.0384(12)	0.0359(6)(3)	
M	0.0421(25)(2)	0.0414(18)(1)	0.0381(13)	0.0359(6)(2)	
$\epsilon$ -expansion	0.040(3) [7]	0.040(3) [7]	0.03(1) [21]		
g-expansion	0.033(4) [8]	0.033(4) [8]	-		
Previous MC	0.024(6) [10]	0.028(2) [11]	0.025(4) [12]		

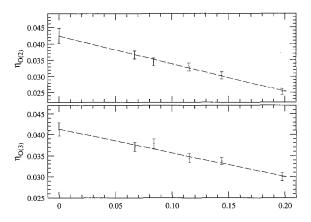


Fig. 1.  $\eta$  estimation from  $\chi$  for pairs of lattices of sizes L and 2L, as a function of  $L^{-\omega}$ ,  $\omega=0.78$ , in the O(2) model (upper part), and O(3) model (lower part). Lines correspond to the  $L_{\min}=12$  fit.

O(2), the fit has  $\chi^2/d.o.f. = 0.85/3$ . For O(3) we obtain  $\chi^2$ /d.o.f. = 2.98/3. We then find no reason to expect higher order corrections to be significant. We have also performed a simulation on a L = 6 lattice, finding that, for the O(2) model, the corresponding  $\eta$  value is one standard deviation away from the corresponding point in the fit performed for  $L_{\min} = 12$ . Therefore, it seems even reasonable to keep the error from the  $L_{\min} = 8 \text{ fit } (\eta = 0.0424(14)). \text{ For the O(3) model},$ the L = 6 point is three standard deviations away from the fit for  $L_{\min} = 12$  due to higher order correctionsto-scaling. Notice in Fig. 1 that the slope for O(2)is significantly larger, which could mask higher order corrections. For the O(4) model, lacking a theoretical knowledge of  $\omega$ , there are stronger uncertainties. We find the change from  $\omega = 0.78(2)$  for O(2) and O(3), to  $\omega = 1.8(2)$  for O(4) very surprising (see Table 2). This might arise from an unexpected cancelation of first order scaling-corrections for the Binder cumulant and the correlation length. We show in Table 3 the extrapolated values for  $\eta$  exponents. For the O(4) model we present the extrapolation with  $\omega$  = 0.78 ( $\chi^2$ /d.o.f. = 2.9/3) and with  $\omega$  = 1.8(2) with  $\chi^2$ /d.o.f. = 1.0/3. Both values are hardly compatible.

The determination of  $\eta$  from  $\chi$  and M are of course coincident in all cases due to the strong statistical correlation between both observables. We find that the value for O(2) and O(3) are compatible with  $\epsilon$ -expansions and not too far from g-expansions, but incompatible with the previous Monte Carlo results. High temperature series [9] also predict  $\eta$  values close to the obtained in this letter, but the error bars are large. For O(4) both  $\eta$  values are significantly lower than for the other models which is not surprising because, in the large N limit, this exponent should go to zero.

Let us consider the  $\eta_T$  exponent. From Table 1 corrections-to-scaling are not self-evident. If one adopts this optimistic point of view and performs a mean of all values in the table one finds that only for  $L \ge 16$ ,  $\chi^2/\text{d.o.f.}$  becomes acceptable. Errors for the means are much smaller than for individual measures, and so, maybe smaller than scaling-corrections. We show these mean values on Table 4. We think safer to perform a fit to the functional form (11). We show the extrapolated values on Table 4. Errors coming from the uncertainty on  $\omega$  are smaller than a 10% of the quoted errors. Even more, the two values for O(4) are compatible. The value of  $\chi^2/\text{d.o.f.}$  for O(4) and O(2) models is about 0.6/3. For the O(3) model is higher (about 6/3). Regarding the conjectured relation  $2\beta = \beta_T$  proposed in Ref. [6], notice that it can be formulated equivalently as  $1 + 2\eta = \eta_T$  which is absolutely ruled out by our data.

Table 4 For every model we show in the first column the mean values for  $\eta_T$  from  $\chi_T$  and  $M_T$  for  $L \ge 16$ . The second columns display the infinite volume extrapolation for  $\eta_T$  from  $\chi_T$  and  $M_T$ . For the O(4) model, the second column has been calculated with  $\omega = 0.78$  and the third with  $\omega = 1.8(2)$ 

	O(2)		O(3)		O(4)		
$\chi_T$ $M_T$	1.494(1)	1.489(4)	1.431(1)	1.427(3)	1.3766(5)	1.374(5)	1.376(2)
	1.496(1)	1.491(4)	1.429(1)	1.427(3)	1.3773(5)	1.375(5)	1.376(2)

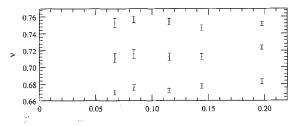


Fig. 2.  $\nu$  estimation from pairs of lattices of sizes L and 2L, as a function of  $L^{-0.78}$ , in the O(4) (upper part), O(3) (middle part), and O(2) model (lower part).

For the comparison between the critical exponents of the O(4) model and those of the antiferromagnetic RP<sup>2</sup> one, notice that the  $\eta$  value for O(4) is fully compatible with the corresponding exponent for the staggered magnetization of the RP<sup>2</sup> model( $\eta_{\text{stag}} = 0.0380(26)$  [14]). The  $\eta$  exponent associated with the usual magnetization for the RP<sup>2</sup> model ( $\eta_{\text{RP}^2} = 1.339(10)$  [14]) is not compatible with  $\eta_T$ , the difference being of order  $\eta$ .

## 5.2. v exponent.

In Fig. 2, we plot the estimation of  $\nu$  that we get from pairs of lattices of sizes L and 2L as a function of  $L^{-\omega}$ . Indeed one would be tempted to claim that for the O(4) model, finite-size effects are beyond our resolution for  $L \geq 8$ , as stated in Ref. [12]. For the O(3) model this also seems to be the case for  $L \geq 12$  [11]. However the question is not so clear for the O(2) model. Nevertheless, the experimental value is known to be  $\nu^{\rm exp} = 0.6705(6)$  [20], and we do find that for  $L \geq 16$  our  $\nu$  estimation is consistent with it. If we actually believe that the corrections-to-scaling are negligible for  $L \geq L_{\rm min}$ , we can take the mean of the safe lattices, getting

$$\nu_{\rm O(2)} = 0.6721(13)$$
,  $\chi^2/{\rm d.o.f.} = 1.7/2$ ,

$$\nu_{O(3)} = 0.7128(14)$$
,  $\chi^2/\text{d.o.f.} = 0.6/3$ ,  
 $\nu_{O(4)} = 0.7525(10)$ ,  $\chi^2/\text{d.o.f.} = 3.4/4$ . (12)

Error bars decrease strongly compared to the data in Table 1, therefore it is not clear if scaling-corrections are still negligible. A more conservative point of view would ask for the consideration of these corrections. For this we use the ansatz (11). However, from the plot in Fig. 2, it seems clear that the scaling corrections for L=8, 12 in the O(2) model, and L=8 in the O(3) model, could hardly be linear on  $L^{-\omega}$ . Performing the fit suggested by Eq. (11), with  $\omega=0.78(2)$  for O(2) and O(3) [7] from the *safe*  $L_{\min}$ , we get a compatible value, but with a very increased error bar:

$$\nu_{O(2)} = 0.670(10) , \quad \nu_{O(3)} = 0.711(10) .$$
 (13)

In the O(4) case, we perform the extrapolation with both  $\omega$  values. The extrapolation does not increase significantly the error bars. Therefore we consider two values of  $L_{\min}$ . For  $L_{\min} = 8$  we obtain  $\nu = 0.754(3)$  for  $\omega = 0.78$  and  $\nu = 0.7531(15)(3)$  for  $\omega = 1.8(2)$ . On the other hand, with  $L_{\min} = 12$  we get  $\nu = 0.765(8)$  for  $\omega = 0.78$  and  $\nu = 0.7585(34)(7)$ , for  $\omega = 1.8(2)$ .

Regarding the relation with the antiferromagnetic RP<sup>2</sup> model ( $\nu = 0.783(11)$ ), we find it unlikely that both values could coincide, but we cannot rule it out. Notice that if we accept the value  $\omega = 1.8(2)$  we would find a significant difference on this universal exponent from RP<sup>2</sup> ( $\omega = 0.85(5)$ ).

## 6. Conclusions

We have obtained accurate measures of critical exponents and couplings for three dimensional O(N) models. The method used, based on the finite-size scaling ansatz, has a remarkable performance when computing magnetic exponents. The values for  $\eta$  expo-

nents presented are incompatible with previous Monte Carlo results and they have smaller statistical errors. We should point out that our values agree with those obtained with  $4-\epsilon$  expansions, and are not incompatible with those computed by means of g-expansions, in opposition with previous results. We also show that the statistical accuracy that can be reached on three dimensional systems is such that the strongest uncertainties come from finite-size effects, for which a reliable theoretical parameterization would be highly desirable.

We present measures of the exponent corresponding to the tensorial magnetization, which is not twice the corresponding to the usual magnetization as previously stated.

We increase significantly the precision of previous measures of the exponents of O(4), showing that the differences with the  $\nu$  exponent from the values of the antiferromagnetic RP<sup>2</sup> model [14] are two standard deviations appart. However whether they belong to the same universality class or not is not yet completely established.

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