

Surprising convergence of the Monte Carlo renormalization group for the three-dimensional Ising model

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We present a surprisingly simple approach to high-accuracy calculations of the critical properties of the three-dimensional Ising model. The method uses a modified block-spin transformation with a tunable parameter to improve convergence in the Monte Carlo renormalization group. The block-spin parameter must be tuned differently for different exponents to produce optimal convergence.

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I. INTRODUCTION

The Monte Carlo renormalization group (MCRG) method is a systematic procedure for computing critical properties of lattice spin models [1,2]. It has been shown to be both flexible and effective in the calculation of critical exponents, critical temperatures, and renormalized couplings constants [3–9]. A particularly interesting application of MCRG is the three-dimensional Ising model [10,11]. This model has proven to be one of the most difficult for which to obtain accurate estimates, because the approach to the fixed point is so slow. Attempts have been made to bring the fixed point closer to the nearest-neighbor model [12], but these have been controversial [13] and have not resulted in improved results.

The most encouraging result has been that of Blöte *et al.* [14], who used a three-parameter approximation to the fixed point along with a modified majority rule for the RG transformation. We have discovered a particularly simple modification of this calculation, which simulates the nearest-neighbor critical point and optimizes the RG transformation for the even and odd exponents separately.

Hasenbusch has done a particularly fine study using Monte Carlo simulations with finite-size scaling [15]. Recently, the conformal bootstrap method has achieved impressive results [16–19]. We will compare our results with theirs in Table VIII.

In the following sections, we recall the MCRG method, illustrate the slow convergence with the majority rule, and introduce a tunable RG transformation in Sec. IV [14]. The improved convergence of the tuned RG transformation is then demonstrated in Secs. V–IX. Finally, we present our conclusions and discuss future work.

II. MCRG COMPUTATIONS

We consider the three-dimensional Ising model on a simple cubic lattice, of size $N \times N \times N$. The Hamiltonian is

given by

$$H = K \sum_{(j,k)} \sigma_j \sigma_k, \quad (1)$$

where $\sigma_j = \pm 1$, and the sum is over all nearest-neighbor pairs. The dimensionless coupling constant K includes the inverse temperature $\beta = 1/k_B T$, so as to make the Boltzmann factor e^H .

We used the Wolff algorithm [20] to simulate the model at an inverse temperature of $K_c = 0.221\,654\,4$ [21]. The renormalized configurations were obtained from these sets. For each configuration, the lattice was divided up into cubes, each containing eight sites, so that the scaling factor $b = 2$. We will denote this block of spins, as well as the renormalized spins associated with them, by ℓ . A value of plus or minus one was assigned to each renormalized spin to represent the original spins in each cube.

We used the ran2 random number generator from Ref. [22]. The lengths of the simulations we used are given in Table I. The renormalized configurations can be described by the set of (unknown) renormalized coupling constants, $K_\alpha^{(n)}$. The subscript α denotes the type of coupling (nearest-neighbor, next-nearest-neighbor, four-spin, etc.). The nearest-neighbor coupling constant K defined earlier is also denoted by $K_{nn}^{(0)}$. All other coupling constants at level $n = 0$ vanish.

To determine the critical exponents, we then wish to calculate the matrix of derivatives of the couplings at level $n + 1$ with respect to the couplings at level n ,

$$T_{\alpha,\beta}^{(n+1,n)} = \frac{\partial K_\alpha^{(n+1)}}{\partial K_\beta^{(n)}}. \quad (2)$$

This matrix of derivatives is then given by the solution of the equation

$$\frac{\partial \langle S_\gamma^{(n+1)} \rangle}{\partial K_\beta^{(n)}} = \sum_\alpha \frac{\partial \langle S_\gamma^{(n+1)} \rangle}{\partial K_\alpha^{(n+1)}} \frac{\partial K_\alpha^{(n+1)}}{\partial K_\beta^{(n)}}, \quad (3)$$

where

$$\frac{\partial \langle S_\gamma^{(n+1)} \rangle}{\partial K_\beta^{(n)}} = \langle S_\gamma^{(n+1)} S_\beta^{(n)} \rangle - \langle S_\gamma^{(n+1)} \rangle \langle S_\beta^{(n)} \rangle \quad (4)$$

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TABLE I. Data for the y_{T1} simulations.

	256 ³	128 ³	64 ³	32 ³	16 ³
No. _{sites} / N^3	2.2×10^5	2.2×10^5	2.2×10^5	4×10^7	4×10^8
No. _{Wolff} / N^3	22	91	420	3.2×10^4	1.2×10^6
Δ No. _{Wolff}	164	87	50	26	15
Cluster	1.0×10^5	2.4×10^4	5.2×10^3	1.2×10^3	2.7×10^2

and

$$\frac{\partial \langle S_\gamma^{(n+1)} \rangle}{\partial K_\alpha^{(n+1)}} = \langle S_\gamma^{(n+1)} S_\alpha^{(n+1)} \rangle - \langle S_\gamma^{(n+1)} \rangle \langle S_\alpha^{(n+1)} \rangle. \quad (5)$$

For our calculations, we have included $N_e = 30$ even and $N_o = 20$ odd interactions. We have followed [23], who calculated all 53 even and 46 odd interactions that fit in either a 3×3 square or a $2 \times 2 \times 2$ cube of spins, and we used their first 34 even operators (excluding the 25th, 29th, 31st, and 32nd) and their first 20 odd operations. The eigenvalues of the T -matrix in Eq. (2) are found separately for the even and odd operators. The critical exponents are then obtained from the usual equations.

III. THE SLOW CONVERGENCE OF THE MAJORITY RULE

The usual majority rule performs very well for the two-dimensional Ising model, which converges to the fixed point values of the exponents by the second iteration of the RG transformation [2]. For the three-dimensional Ising model, however, convergence is very slow, as shown in Table II. Reading across at each level n of RG iterations, the values of the approximations for y_{T1} are quite consistent. There is no problem with finite-size effects on the RG trajectories, indicating that the range of the renormalized Hamiltonian is limited. However, even after five iterations of the renormalization group, the value of y_{T1} does not seem to have converged. Anticipating our final result of $y_{T1} \approx 1.591$, Table II is very far from convergence.

TABLE II. The eigenvalue exponent y_{T1} for majority transformation, which is equivalent to using a large w in Eq. (6).

n	N_e	256 ³	128 ³	64 ³	32 ³
1	10	1.4189(7)	1.4202(5)	1.4203(2)	1.4206(1)
	20	1.4230(7)	1.4241(5)	1.4240(2)	1.4241(1)
	30	1.4224(7)	1.4243(5)	1.4237(2)	1.4238(1)
2	10	1.5093(6)	1.5106(3)	1.5108(1)	1.5120(1)
	20	1.5076(6)	1.5088(3)	1.5086(1)	1.5084(1)
	30	1.5072(6)	1.5084(3)	1.5082(1)	1.5076(1)
3	10	1.5521(5)	1.5534(5)	1.5544(2)	
	20	1.5508(5)	1.5515(5)	1.5507(2)	
	30	1.5504(5)	1.5512(5)	1.5501(2)	
4	10	1.5733(7)	1.5745(5)		
	20	1.5721(7)	1.5711(5)		
	30	1.5718(7)	1.5702(5)		
5	10	1.5825(11)			
	20	1.5797(11)			
	30	1.5788(11)			

TABLE III. The eigenvalue exponent y_{T1} . The parameter $w = 0.4314$.

n	N_e	256 ³	128 ³	64 ³	32 ³	16 ³
1	10	1.5870(6)	1.5864(2)	1.5865(1)	1.5872(1)	1.58835(4)
	20	1.5923(7)	1.5914(3)	1.5916(1)	1.5920(1)	1.59266(5)
	30	1.5930(8)	1.5924(3)	1.5922(2)	1.5927(2)	1.59308(5)
2	10	1.5908(5)	1.5903(2)	1.5907(1)	1.5920(1)	
	20	1.5917(5)	1.5912(2)	1.5915(1)	1.5923(1)	
	30	1.5919(5)	1.5914(2)	1.5916(1)	1.5921(1)	
3	10	1.5910(5)	1.5904(2)	1.5922(1)		
	20	1.5912(5)	1.5905(2)	1.5920(1)		
	30	1.5912(5)	1.5905(2)	1.5918(1)		
4	10	1.5906(6)	1.5918(3)			
	20	1.5906(6)	1.5914(3)			
	30	1.5906(6)	1.5912(3)			
5	10	1.5911(6)				
	20	1.5909(6)				
	30	1.5908(7)				

IV. TUNABLE BLOCK-SPIN TRANSFORMATION

Instead of using the usual majority rule, the renormalized spin was assigned a value according to the following probability [14]:

$$P(\sigma'_\ell) = \frac{\exp(w \sigma'_\ell \sum_{j \in \ell} \sigma_j)}{\exp(w \sum_{j \in \ell} \sigma_j) + \exp(-w \sum_{j \in \ell} \sigma_j)}. \quad (6)$$

For $w = \infty$, this becomes identical to the majority rule.

A special feature of the present calculation is that the RG transformation in Eq. (6) was optimized separately for the even and odd operators. The determination of the optimal value of the parameter w was also done much more carefully than in earlier work. The value of w was adjusted so that the largest eigenvalue (for the even and odd operators separately) was nearly constant for $n > 1$.

V. THE LARGEST EVEN EIGENVALUE EXPONENT, y_{T1}

The results for the largest even eigenvalue are given in Table III. In contrast to the slow convergence seen in Table II, the convergence is striking. For $n = 1$, the majority rule has $y_{T1} \approx 1.422$, changes to $y_{T1} \approx 1.507$ for $n = 2$, and increases to $y_{T1} \approx 1.579$ for $n = 5$. The tuned RG transformation in Table III starts with $y_{T1} \approx 1.593$ for $n = 1$, moves to $y_{T1} \approx 1.592$ for $n = 2$, and stays at $y_{T1} \approx 1.591$ for $n = 3, 4$, and 5. Our best estimate for the largest even eigenvalue is $y_{T1} = 1.591(1)$.

VI. THE LARGEST ODD EIGENVALUE EXPONENT, y_{H1}

Table IV shows the convergence of y_{H1} for the tuned renormalization group. Reading along the rows, we see that there is virtually no effect of the size of the lattice on the estimated values of y_{H1} . Only for a renormalized lattice of $4 \times 4 \times 4$ can a decrease in the value of y_{H1} of about 0.000 14 be seen. Neither is there a noticeable dependence on the number of operators for a given number of RG iterations n .

TABLE IV. The eigenvalue exponent y_{H1} . The parameter $w = 0.555$.

n	N_o	256^3	128^3	64^3	32^3	16^3
1	5	2.50830(8)	2.50831(3)	2.50829(1)	2.50828(1)	2.50823(1)
	10	2.50853(14)	2.50869(4)	2.50860(2)	2.50860(2)	2.50856(1)
	15	2.50844(15)	2.50871(5)	2.50859(2)	2.50861(2)	2.50859(1)
	20	2.50843(15)	2.50871(5)	2.50860(2)	2.50862(2)	2.50860(1)
2	5	2.48503(2)	2.48504(1)	2.48503(1)	2.48503(2)	2.48481(1)
	10	2.48507(3)	2.48506(1)	2.48505(1)	2.48506(2)	2.48498(1)
	15	2.48508(3)	2.48507(1)	2.48506(1)	2.48507(2)	2.48493(2)
	20	2.48508(3)	2.48507(1)	2.48506(1)	2.48507(2)	2.48494(2)
3	5	2.48285(3)	2.48287(2)	2.48286(1)	2.48267(4)	
	10	2.48284(3)	2.48287(2)	2.48288(1)	2.48279(4)	
	15	2.48285(3)	2.48288(2)	2.48288(1)	2.48274(4)	
	20	2.48285(3)	2.48288(2)	2.48288(1)	2.48274(4)	
4	5	2.48300(5)	2.48293(4)	2.48279(3)		
	10	2.48299(5)	2.48295(4)	2.48290(3)		
	15	2.48300(5)	2.48295(4)	2.48283(3)		
	20	2.48300(5)	2.48294(4)	2.48282(3)		
5	5	2.48271(12)	2.48250(9)			
	10	2.48272(12)	2.48259(9)			
	15	2.48273(12)	2.48251(9)			
	20	2.48274(12)	2.48251(9)			
6	5	2.48223(23)				
	10	2.48234(24)				
	15	2.48234(25)				
	20	2.48231(25)				

The first iteration of the renormalization group ($n = 1$) gives an estimate of about $y_{H1} \approx 2.5086$. For $n = 2$, it has dropped slightly to $y_{H1} \approx 2.48507$, and for $n = 3, 4$, and 5 , it is $y_{H1} \approx 2.4829$. Our best estimate is $y_{H1} = 2.4829(2)$.

VII. THE SECOND-LARGEST EVEN EIGENVALUE EXPONENT, y_{T2}

Table V shows estimates for the second even eigenvalue as a function of the number of RG iterations, n , and the size of the renormalized lattices. This eigenvalue is negative (“irrelevant”), and controls the leading corrections to scaling.

The second largest eigenvalues are naturally not as accurately determined as the largest. We need about 20 operators to see the asymptotic behavior. There is a slight trend for the values of y_{T2} to increase in magnitude with an increasing number of RG iterations, suggesting that the asymptotic eigenvalue exponent is actually larger. Note that similar slow convergence for the calculation of y_{T2} was already observed and reported by Baillie *et al.* [23]. Perhaps we can estimate $y_{T2} = -0.75(5)$ from the tables, but that might be overly optimistic.

The correction-to-scaling exponent is given by the ratio of $\omega = -y_{T2}/y_{T1}$, so that we would estimate $\omega = 0.75/1.591 = 0.47(3)$.

VIII. THE SECOND-LARGEST ODD EIGENVALUE EXPONENT, y_{H2}

The second-largest odd eigenvalue exponent, like its counterpart in the two-dimensional Ising model, is positive

TABLE V. The eigenvalue exponent y_{T2} . The parameter $w = 0.4314$, the tuned parameter for y_{T1} . The simulations were the same as for y_{T1} , which are given in Table III.

n	N_e	256^3	128^3	64^3	32^3	16^3
1	10	-0.60(2)	-0.548(6)	-0.545(2)	-0.546(3)	-0.5300(10)
	20	-0.70(2)	-0.622(9)	-0.616(3)	-0.622(4)	-0.6081(12)
	30	-0.67(2)	-0.644(12)	-0.626(3)	-0.638(4)	-0.6186(12)
2	10	-0.64(2)	-0.608(5)	-0.611(2)	-0.607(2)	
	20	-0.70(2)	-0.664(7)	-0.668(2)	-0.668(3)	
	30	-0.71(2)	-0.698(10)	-0.691(3)	-0.688(4)	
3	10	-0.66(2)	-0.635(5)	-0.634(2)		
	20	-0.71(2)	-0.691(8)	-0.696(3)		
	30	-0.72(2)	-0.722(10)	-0.725(4)		
4	10	-0.67(1)	-0.658(6)			
	20	-0.74(2)	-0.726(9)			
	30	-0.73(2)	-0.753(10)			
5	10	-0.73(2)				
	20	-0.77(2)				
	30	-0.76(2)				

(“relevant”). It has smaller statistical errors than its even counterpart, but it also shows a slightly slower convergence. As shown in Table VI, the first iteration of the RG transformation ($n = 1$) is $0.287(6)$, and therefore quite far from the best estimate. By $n = 3$ and greater, the value of the second odd eigenvalues has converged to about $y_{H2} = 0.403(4)$.

TABLE VI. The eigenvalue exponent y_{H2} . The parameter $w = 0.555$, the tuned parameter for y_{H1} . The simulations were the same as for y_{H1} , which are given in Table IV.

n	N_o	256^3	128^3	64^3	32^3	16^3
1	5	0.232(4)	0.236(1)	0.2409(6)	0.2469(7)	0.2561(2)
	10	0.287(5)	0.287(2)	0.2888(7)	0.2910(8)	0.2935(3)
	15	0.287(6)	0.290(2)	0.2911(8)	0.2931(9)	0.2957(3)
	20	0.287(6)	0.297(2)	0.2972(8)	0.2992(9)	0.3012(3)
2	5	0.306(3)	0.307(1)	0.3152(4)	0.3284(5)	0.3405(2)
	10	0.362(4)	0.360(2)	0.3635(5)	0.3689(6)	0.3677(2)
	15	0.366(4)	0.365(2)	0.3680(5)	0.3728(6)	0.3744(2)
	20	0.371(5)	0.372(2)	0.3735(5)	0.3777(6)	0.3770(2)
3	5	0.318(3)	0.331(1)	0.3455(5)	0.3586(5)	
	10	0.379(3)	0.384(1)	0.3900(6)	0.3871(6)	
	15	0.384(3)	0.390(1)	0.3949(6)	0.3949(6)	
	20	0.392(3)	0.396(2)	0.4000(6)	0.3976(7)	
4	5	0.335(3)	0.353(1)	0.3638(4)		
	10	0.390(3)	0.400(1)	0.3935(4)		
	15	0.396(3)	0.406(1)	0.4024(4)		
	20	0.402(3)	0.411(1)	0.4053(5)		
5	5	0.349(3)	0.366(1)			
	10	0.397(3)	0.397(1)			
	15	0.403(3)	0.407(1)			
	20	0.410(3)	0.410(1)			
6	5	0.364(3)				
	10	0.395(3)				
	15	0.406(3)				
	20	0.409(3)				

TABLE VII. Five correlation functions obtained from the same simulations as in Tables III and V, with the parameter $w = 0.4314$. ($a = 000-100$; $b = 000-110$; $c = 000-111$; $d = 000-100-010-110$, and $e = 000-100-010-001$.)

L^3	Σ	256^3	128^3	64^3	32^3	16^3
256^3	a	0.330491(1)				
	b	0.208951(1)				
	c	0.163751(2)				
	d	0.175667(1)				
	e	0.115223(1)				
128^3	a	0.277505(3)	0.330980(2)			
	b	0.193674(4)	0.209600(3)			
	c	0.156671(4)	0.164487(4)			
	d	0.123980(2)	0.176051(2)			
	e	0.096526(2)	0.115679(2)			
64^3	a	0.264324(7)	0.278867(6)	0.332281(2)		
	b	0.189019(8)	0.195345(8)	0.211325(3)		
	c	0.154033(9)	0.158523(8)	0.166440(3)		
	d	0.113330(5)	0.124977(4)	0.177075(2)		
	e	0.091201(5)	0.097588(4)	0.116894(2)		
32^3	a	0.261975(16)	0.267975(16)	0.282485(5)	0.335734(4)	
	b	0.189760(18)	0.193421(18)	0.199785(5)	0.215903(5)	
	c	0.155992(20)	0.158896(20)	0.16350(6)	0.171623(5)	
	d	0.111433(12)	0.115920(11)	0.127626(4)	0.179794(3)	
	e	0.090799(11)	0.093920(12)	0.100414(4)	0.120119(3)	
16^3	a	0.268326(40)	0.271726(37)	0.277684(11)	0.292087(9)	0.344889(3)
	b	0.199029(42)	0.201440(44)	0.205131(12)	0.211566(11)	0.228043(3)
	c	0.166844(46)	0.168865(48)	0.171831(13)	0.176526(12)	0.185370(3)
	d	0.115740(29)	0.118288(26)	0.122836(8)	0.134672(7)	0.187019(2)
	e	0.095977(28)	0.097952(28)	0.101185(8)	0.107933(7)	0.128690(2)
8^3	a	0.291884(85)	0.294200(87)	0.297557(25)	0.303419(22)	0.317542(6)
	b	0.228122(96)	0.229982(95)	0.232453(29)	0.236208(25)	0.242812(7)
	c	0.199280(102)	0.200925(102)	0.203053(32)	0.206160(26)	0.211216(7)
	d	0.132318(70)	0.134094(64)	0.136752(19)	0.141473(17)	0.153630(5)
	e	0.113640(65)	0.115173(63)	0.117304(18)	0.120794(17)	0.128180(5)
4^3	a	0.358390(186)	0.360473(181)	0.362650(60)	0.365979(44)	0.371601(13)
	b	0.307968(197)	0.309833(214)	0.311695(66)	0.314279(50)	0.318110(14)
	c	0.286644(206)	0.288429(226)	0.290147(68)	0.292477(54)	0.295778(14)
	d	0.183398(168)	0.185148(152)	0.187090(51)	0.190036(37)	0.195074(11)
	e	0.167453(156)	0.169101(150)	0.170828(51)	0.173341(38)	0.177337(10)

IX. CONVERGENCE OF THE CORRELATION FUNCTIONS

Note that Blöte *et al.* were able to achieve improved convergence with $w = 0.4$ and a different Hamiltonian, which appeared to be closer to the fixed point [14].

Our results show that the improved convergence came primarily from the choice of RG transformation. Indeed, there is no evidence that the tuned RG transformation brings the renormalized Hamiltonians closer to the fixed point. Apparently, the renormalization trajectory is such that even though it passes through points a significant distance from the fixed point, the convergence of y_{T1} is very good.

The fact that the RG trajectory itself does *not* converge rapidly can be seen in Table VII. This table is organized differently than the tables for the eigenvalue exponents. Rows correspond to equally sized renormalized lattices, with the size indicated by the first column. The entries are the values of the corresponding correlation functions, divided by the size

of the lattice, to facilitate comparisons. It can be seen that although the correlation functions are closer to each other when they correspond to more renormalization iterations, they have not converged for the RG iterations down to 4^3 . A comparison with the entries on the diagonal in Table III shows a relatively weak size effect for the eigenvalue exponent values.

X. SUMMARY AND FUTURE WORK

The results of our computations and a comparison with other works are shown in Table VIII. The agreement between the various methods is generally good, although some differences exist. Since we do not have estimates of the systematic errors in our results, we cannot really say what the source of the differences are.

The most reliable of the estimates shown in Table VIII are probably those of Hasenbusch [15]. This was a very careful Monte Carlo finite-size study that included many effects of corrections to scaling to provide limits on the systematic errors.

TABLE VIII. Estimates of the critical exponents and the eigenvalue exponents from several sources. Values that are marked with an asterisk are calculated to be consistent with the published exponents in the same source. For Refs. [15] and [24], y_{T1} and y_{H1} are obtained for the corresponding values of ν and η .

	This work MCRG	Ref. [14] MCRG	Ref. [15] MC	Ref. [24] ϵ -expansion	Ref. [24] $d = 3$	Ref. [19] bootstrap
y_{T1}	1.591(1)	1.585(3)	1.5872(3)*	1.590(63)*	1.5862(33)*	1.58735(8)
y_{H1}	2.4829(2)	2.481(1)	2.4819(1)*	2.4820(25)*	2.4833(13)*	2.481849(6)
ν	0.6285(4)*	0.6309(2)*	0.63002(10)	0.6290(25)	0.6304(13)	0.62998(3)
η	0.0342(4)*	0.038(2)*	0.03627(10)	0.0360(50)	0.0335(25)	0.036302(12)
β	0.3250(2)*	0.3274(9)*	0.32645(10)*	0.3257(26)	0.3258(14)	0.326423(18)
γ	1.2356(8)*	1.2378(27)*	1.2372(4)*	1.2355(50)	1.2396(13)	1.23708(5)
y_{T2}	-0.75(5)		-0.832(6)*	-0.814(19)*	-0.799(10)*	-0.8303(18)
ω	0.47(3)*		0.524(4)	0.512(12)	0.504(6)	0.5231(12)

There are discrepancies between our estimate of ω and the estimates of Hasenbusch [15] and Guida and Zinn-Justin [24]. Our value $\omega = 0.47(3)$ is substantially lower than the others. This could be partly due to the large fluctuations, but it could be that the estimates for y_{T2} are not yet converged. Table V could be easily viewed as indicating that the absolute values of the estimates of y_{T2} are still increasing with the iterations of the renormalization group.

The most interesting estimates are those in the last column, which were calculated with the conformal bootstrap method [16–19]. The discrepancies with these results are the largest concern, especially when the extremely small errors in conformal bootstrap results are considered.

The most obvious source of systematic error in our calculation of the largest eigenvalue exponents is the uncertainty of the value of the critical coupling that was used in the Monte Carlo simulation. The usual way to estimate the critical coupling from MCRG is to use the convergence of the renormalized correlation functions. Unfortunately, it is clear from Table VII that the convergence of the correlation functions for the tuned RG transformation is not sufficient for that purpose. It might be possible to do the calculation with the assistance of an extrapolation of the values, but it seems more promising to use the convergence of the eigenvalues. Preliminary calculations are very encouraging, but more work is needed.

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