CRITICAL BEHAVIOUR OF THE 3d ISING MODEL FROM AN EXTENDED LOW-TEMPERATURE EXPANSION OF THE INVERSE CORRELATION LENGTH

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We introduce a new method for the derivation of high-order low-temperature expansions of the inverse correlation length and present an $O(u^8)$ expansion for the Ising model on a 3-dimensional simple cubic lattice. This corresponds to an $O(v^{16})$ high-temperature expansion for the dual model with 4-spin interaction which is equivalent to the 3-dimensional Z_2 lattice gauge theory. The preliminary series analysis admits the rough estimates $u_c = 0.4079(58)$, $u_1 = -0.1368(74)$ and $u_2 = -0.296(11)$ for the location of the physical and two unphysical singularities in the complex u-plane. The critical exponent ν' at u_c , u_1 and u_2 is determined as $2\nu' = 1.255(17)$, $2\nu' = 0.008(1)$ and $2\nu' = 0.80(2)$ respectively. Finally, we indicate further applications of our method.

1. Introduction

As is well known, so far nobody succeeded in an exact solution of the 3-dimensional spin-spin Ising model. Hence the only sources of information about the critical properties of this model have been renormalization group techniques [1] and high- and low-temperature series expansions (for a review see [2]). While in the last 10 years considerable progress has been made in the derivation of longer high-temperature series culminating in the work by Nickel [3], the longest low-temperature series expansion of the inverse correlation length κ in particular has already been published in 1975 [4]. The reason is of course that low-temperature series expansions are more difficult to obtain than their high-temperature counterparts. It is the main intention of this article to introduce a *new method* which enabled the author to extend the low-temperature series expansion of κ of ref. [4] by 3 orders in u.

2. The models

We first fix the notation. We consider two generalized Ising models [5] in zero magnetic field defined on a 3-dimensional simple cubic (sc) lattice Λ with lattice

spacing a. The first model is the usual spin-spin Ising model with the hamiltonian

$$-H/kT = \beta \sum_{\langle ij \rangle} s_i s_j.$$
(1)

The spins $s_i = \pm 1$ are located at the sites *i* of the lattice and the sum runs over all nearest-neighbor pairs. The second model has a generalized 4-spin interaction

$$-H^*/kT = \beta^* \sum_{p} \prod_{\ell \in \partial p} s_{\ell}, \qquad (2)$$

where the spins live on the links ℓ of the lattice and the sum runs over all non-oriented plaquettes p of Λ . The product is to be taken over the 4 links in the boundary of p. We note that this model is equivalent to the Z₂ euclidean lattice gauge theory in 3 dimensions, if we identify $-H^*/kT$ with the lattice action S. The spins correspond to the gauge fields attached to the links of the lattice and the coupling β^* is related to the bare coupling constant g_0 of the theory by $\beta^* = 2/g_0^2$.

Finally, we recall that the two models introduced above are related by the duality transformation. For later use, we will be more specific. If we denote the dual lattice by Λ^* which in our case is isomorphic to Λ because the sc lattice is self-dual, the duality transformation * is a map:

$$*: \begin{pmatrix} \Lambda \to \Lambda^* \\ H \mapsto H^* \end{pmatrix}$$
(3)

Cubes, plaquettes, links and sites of Λ are mapped one-to-one to sites, links, plaquettes and cubes of the dual lattice Λ^* respectively [5]. The dual couplings β and β^* are related by

$$\tanh \beta^* = \exp(-2\beta). \tag{4}$$

In particular, the duality transformation maps the low-temperature phase of the usual spin-spin Ising model to the high-temperature or strong coupling phase of the Z_2 euclidean lattice gauge theory in 3 dimensions.

3. Calculation of series expansion

We now describe the essential features of our method. First we note that the inverse correlation length κ along a lattice axis of the spin-spin Ising model is mapped to the mass gap *m* of the lattice gauge theory which can be determined via the asymptotic decay of the connected correlation function Γ [6]: we denote x_3 to be the time coordinate; for two local operators O_1, O_2 we get

$$\Gamma(x_3) \coloneqq \langle O_1(x_3) O_2(0) \rangle - \langle O_1(x_3) \rangle \langle O_2(0) \rangle \underset{x_3 \to \infty}{\to} \operatorname{const} \times \exp(-mx_3), \quad (5)$$



Fig. 1. The leading-order contribution in the cluster expansion of Γ stretching in time direction x_3 .

where we choose for O_1 , O_2 the gauge-invariant product of the gauge fields attached to the links in the boundary of two space-like plaquettes p_1 and p_2 separated x_3 lattice spacings in time direction. In addition we sum over all possible space-like positions of p_1 and p_2 separately, in order to project out the zero-momentum part. As described in ref. [6], Γ can now be calculated in a *cluster expansion*, which is valid to all orders in the expansion parameter β^* . The clusters are sets of *plaquetteconnected polymers*, the *polymers* themselves being *connected graphs* on the lattice [7]. Geometrically, the polymers are *closed surfaces* on Λ which for gauge group Z_2 have no branch-lines.

The leading-order contribution to the cluster expansion of Γ is the 1-polymer cluster X_0 , the long straight tube connecting p_1 and p_2 (fig. 1). For the leading order term $m^{(0)}$ of the mass gap $m := m^{(0)} + \Delta m$ this yields in lattice units

$$m^{(0)}a = -4\log v \equiv -2\log u,$$
(6)

in terms of the high-temperature/strong coupling variable v or the low-temperature variable u defined by

$$v := \tanh \beta^*,$$

$$u := \exp(-4\beta) = v^2.$$
 (7)

If we take only those clusters into account, which can be obtained by local modifications of X_0 , the cluster expansion of Γ exponentiates in the form

$$e^{-mx_3} = e^{-m^{(0)}x_3} e^{-\Delta mx_3} = e^{-m^{(0)}x_3} \left\{ 1 - \Delta mx_3 + \frac{1}{2!} (\Delta m)^2 x_3^2 \dots \right\},$$
(8)

and corrections Δm to the leading-order term $m^{(0)}$ of the mass gap can be determined from the term linear in x_3 in the cluster expansion of Γ . The problem is to generate these corrections systematically in a unique way. For this purpose the use of a computer is inevitable, if one aims at a reliable, high-order determination of Δm .

First we reformulate the cluster expansion of ref. [6] in terms of geometrically local quantities. If we introduce the concept of the *decoration*, which roughly speaking is a local modification of the leading-order cluster X_0 , any cluster C contributing to the cluster expansion of Γ can be represented as a set of decorations (fig. 2). Due to a *partition theorem*, this representation is *unique*, which is a very



Fig. 2. Two clusters contributing to the cluster expansion of Γ and the corresponding sets of decorations.

important feature of our method because double-counting of contributions is avoided by construction. We note for completeness that there is a special type of decorations which are treated separately. They are obtained by cutting X_0 into several rings of 1-plaquette diameter and closing these rings with additional plaquettes at their open ends. However, these decorations can be taken into account in closed form for any (multiply) decorated X_0 and are therefore not discussed in further detail now. For details we refer to [8].

What can be learned from fig. 2 is that clusters which transform into each other by translation of one or more decorations are represented by the same set of decorations. Hence, mapping clusters to sets of decorations induces a *class decomposition* of the set of clusters contributing to the cluster expansion of Γ . The cardinality of any class of clusters is easily calculated from the geometrical properties of the associated set of decorations. Therefore the cluster expansion of Γ is mapped to the determination of the *set* \mathfrak{N} of *all non-equivalent decorations D*. As the correction to the mass gap due to a given class of clusters can be determined from the cardinality of that class and the properties of the associated set of decorations, the evaluation of \mathfrak{N} is also sufficient for a systematic computation of Δm .

Next we want to sketch how the determination of \mathfrak{D} is related to the even simpler problem of the cluster expansion of the *free energy* log Z.

Every decoration D has an entrance and an exit side where tube parts enter which may carry additional decorations but ultimately connect D to p_1 and p_2 . Entrance



Fig. 3. A 4-point configuration $K^{(4)}$, its dual envelope and some of the associated decorations.

and exit sides are called p_{in} and p_{out} and are indicated by dashed lines (fig. 2). Closing *D* at p_{in} and p_{out} , i.e. adding p_{in} and p_{out} to the *support* of *D* (which is the set of plaquettes carrying the non-trivial representation of Z_2), results in a *cluster* \hat{C}_D contributing to the cluster expansion of log *Z*.

Conversely, starting from a cluster \hat{C}_D , in general there exist several candidates for p_{in} and p_{out} . Making use of the geometrical properties of \hat{C}_D and the partition theorem which fixes the properties the p_{in} and p_{out} have to fulfill, we can evaluate the set of all p_{in} and p_{out} in a uniquely determined way. As this is equivalent to the determination of the set of all decorations D associated with \hat{C}_D , the determination of \mathfrak{P} is mapped to the computation of the cluster expansion of $\log Z$.

The first step in the cluster expansion of $\log Z$ is the classification of all \hat{C}_D according to the supports of the included polymers. As Z_2 has only one non-trivial representation, this step is trivial in the case under consideration, because we have a one-to-one mapping from the supports of the included polymers to the corresponding polymers. However, in the case of gauge groups with a more complicated structure, this step becomes essential [8].

Next we classify the supports $|\hat{C}_{\rm D}|$ according to their *envelope* E. The envelope of some $|\hat{C}_{\rm D}|$ is loosely speaking $|\hat{C}_{\rm D}|$ with the inner plaquettes removed (fig. 3). Because in d = 3 dimensions, to each envelope E which is a closed surface on Λ , there exists exactly one volume V with the property $\partial V = E$, the classification of all $|\hat{C}_{\rm D}|$ according to their envelopes is equivalent to their classification according to their volumes.

For the reconstruction of all $|\hat{C}_D|$ which have identical volume, it is advantageous to recall that the volumes may be considered as *chains of plaquette-connected cubes* on the lattice. Making use of the cell structure of the volumes, the determination of $\{\hat{C}_D\}$ causes no principal difficulties, and the remaining step in the cluster expansion of log Z and therefore in the cluster expansion of Γ as well as the strong coupling expansion of the mass gap m is the unique generation of all volumes needed in a calculation of a given order in the expansion parameter β^* . In particular for a high-order computation of Δm , the volumes may be of considerable extent and may have a complicated geometry. Even the topology may become non-trivial at already rather low order. Moreover, as we expect a very large number of non-equivalent volumes to be needed in a high-order computation of Δm , the requirements on an useful method are a compact *and* complete description as well as an a priori unique generation of each volume. It must be emphasized that this second demand is absolutely necessary, because due to computer time *and* storage requirements one cannot afford to store the data of all volumes and to scan through this set each time a new volume is generated in order to avoid double-counting.

For the solution of this problem, we again make use of the cell structure of volumes of Λ and also use the duality between cubes on Λ and sites or lattice points on Λ^* . By duality, each volume which is a chain of plaquette-connected cubes is mapped to a *nearest-neighbor point configuration* on Λ^* . To fulfill the uniqueness requirements mentioned above, we therefore constructed an algorithm which generates every nearest-neighbor point configuration $K^{(n)}$ with n points (n = 1, 2, 3, ...) through a *unique sequence*

$$K^{(1)} \to K^{(2)} \to \cdots K^{(n-1)} \to K^{(n)} \tag{9}$$

of 1-point, 2-point, ..., (n-1)-point nearest-neighbor point configurations on Λ^* . This means that we have a *tree structure on the set of point configurations on* Λ^* . Besides avoiding double-counting by construction, our algorithm meets the speed requirements naturally.

In closing this section, we note that the application of our algorithm is not restricted to the problem discussed above, but it is in particular perfectly suited for the derivation of high-order strong coupling expansions of the mass spectrum of pure Yang-Mills theories in 3 and 4 dimensions. In fact, this is the main purpose our algorithm has been invented for. Moreover, as it is already clear from the above description, a subset of this algorithm can be used to get high-order expansions of the free energy log Z.

4. Series analysis

Making use of our algorithm we have been able to generate correction terms up to $O(u^8)$. In lattice units, we get for κ along a lattice axis

$$\kappa a = -2\log u + F(u) = -2\log u + \sum_{k=0}^{8} m_k u^k + O(u^9), \qquad (10)$$

with the coefficients m_k given in table 1. To obtain these coefficients, more than 1.5×10^6 point configurations on Λ^* have been generated, mapped to volumes on Λ and investigated within a total amount of CPU time of approximately 12.5 h on an IBM 3081-D. For comparison, we quote the corresponding numbers for a u^5 calculation, which are about 1800 point configurations and roughly 20 s of CPU time.

1 2 3	4 5	6 7	8
$1 - \frac{15}{2} - \frac{7}{3}$	$-\frac{87}{4}$ $\frac{251}{5}$	$-\frac{331}{2}$ $\frac{8793}{7}$	$-\frac{55927}{8}$
-1 10 -3	14 93 -201	972 - 347	0 17254
-1 9 -1	12 74 -159	719 - 278	8 14022

 TABLE 1

 Coefficients m_k , g_k and h_k of the series expansion of κa , Λ'_2 and Λ'_1 as defined in eqs. (10), (14) and (15)

To begin with, we analyse F(u) defined in (10). As the expansion coefficients m_k alternate in sign, the dominant singularity lies on the real negative u-axis as expected.

To obtain quantitative results, we applied ratio methods, Neville tables [9], Shanks extrapolation [10] and Padé approximants. Whereas ratio methods and Neville tables applied to the series expansion of F(-u) do not admit an estimate of the location of the dominant singularity, Shanks extrapolation yields the prediction $0.17 \le \hat{u} \le 0.29$



Fig. 4. The poles of all the Padé approximants to F(u). Open circles represent poles which have been found in one approximant only. Poles indicated by a full circle, a full triangle or a full box have been obtained in two, three or four and more Padé approximants respectively.

for the modulus \hat{u} of the dominant singularity. This is in agreement with the results from ref. [11], where an *unphysical singularity* has been found to be located at $u_2 = -0.2860(2)$.

The singularity structure of F(u) is displayed in fig. 4: as a single open circle at some position in the complex *u*-plane indicates that only a single Padé approximant to F(u) has a pole at that location, the significant items are accumulations of poles.

We observe such accumulations around $u \approx -0.31$ and along a circle with radius $|u| \approx 0.13$ open towards the real positive *u*-axis, which indicates stable, unphysical singularities u_2, u_1 in the low-temperature series of κ at $u_2 \approx -0.31$ and $u_1 \approx -0.13$. Whereas the existence of u_2 is in accordance with the results from [11], u_1 has so far not been reported in the literature.

Finally, as can be seen from fig. 4, we note that the analysis of F(u) is not particular useful for the determination of the physical singularity $u_c = 0.412045(5)$ [12].

To obtain independent estimates for u_1 and u_2 and to get predictions for the location of u_c as well as estimates for the *critical exponent* ν' at u_c and the unphysical singularities, we investigated in addition the quantities Λ'_2 and Λ'_1 [4,13]:

$$\Lambda'_{2} := \frac{1}{2[\cosh(\kappa a) - 1]} = \frac{\exp(-\kappa a)}{\left[1 - \exp(-\kappa a)\right]^{2}} = (\xi/a)^{2} \left[1 + O((\xi/a)^{-2})\right], \quad (11)$$

$$\Lambda'_{1} := \frac{1}{1 - \exp(-\kappa a)} = (\xi/a) \left[1 + O((\xi/a)^{-1}) \right], \tag{12}$$

where ξ is the *true* or *exponential correlation length* along a lattice axis (x_3) defined by

$$\xi^{-1} = \kappa \coloneqq \lim_{x_3 \to \infty} x_3^{-1} \log \Gamma(x_3).$$
(13)

As can be read off from eqs. (11) and (12), in the critical region Λ'_2 and Λ'_1 behave asymptotically like positive powers of the true correlation length ξ . Hence we expect them to be more useful in our analysis than κa itself.

Using the expansion of κa , we obtain

$$\Lambda'_{2}(u) = u^{2}G(u) = u^{2}\sum_{k=0}^{8} g_{k}u^{k} + O(u^{11}), \qquad (14)$$

$$\Lambda'_{1}(u) = 1 + u^{2}H(u) = 1 + u^{2}\sum_{k=0}^{8}h_{k}u^{k} + O(u^{11}).$$
(15)

The coefficients g_k and h_k can be found in table 1.

We first try to determine the location of the singularities and apply the same methods of series analysis as previously. Ratio methods and Neville tables still do



Fig. 5. The poles of all the Padé approximants to G(u). Symbols as defined for fig. 4.

not admit an estimate of the location of the dominant singularity and Shanks extrapolation makes only a very crude judgement which is, however, in agreement with the result from the κa analysis.

The results from the Padé analysis are shown in figs. 5 and 6. The majority of the poles can now be found to lie on the real *u*-axis. Moreover, we recognize three points of accumulation of poles which in fig. 6 are not as pronounced as in fig. 5 and which correspond to the physical and the two unphysical singularities. If we simply average over all the members of the appropriate accumulation, we find that the corresponding predictions from the Λ'_2 and Λ'_1 analysis do not agree within the standard deviation in the mean. We take this as an indication that this naive error determination might be misleading. Taking all estimates from the Padé analysis into account simultaneously, we compute weighted averages for u_1 , u_2 and u_c . We weigh according to the number of values the different single estimates rely on and obtain the predictions $u_1 = -0.1368(74)$, $u_2 = -0.296(11)$ and $u_c = 0.411(12)$. The errors quoted in parentheses (as always in this article) are the standard deviations in the mean.



Fig. 6. The poles of the Padé analysis of Λ'_1 . Symbols as defined for fig. 4.

In addition, we tried to obtain an improved estimate for u_c by mapping away the unphysical singularities located on the real negative *u*-axis. We performed a *conformal transformation*:

$$u = \frac{z}{1 - \mu z},$$

$$z = \frac{u}{1 + \mu u}, \qquad \mu \in \mathbb{R}_+,$$
(16)

where we choose $\mu = 1/\hat{u}$ with $\hat{u} = |u_{1,2}|$ or some value from a neighborhood of u_1 and u_2 . Now we can make profit by ratio methods and Neville tables. The quality of the estimates depend strongly on the choice of μ and best estimates are obtained, if we choose $\mu^{-1} = |u_1|$ with u_1 as determined by the Padé analysis of Λ'_2 and Λ'_1 respectively.

Qualitatively, we find that the different methods when applied to the transformed series of Λ'_1 result in better convergent estimates than when applied to the transformed series of Λ'_2 .

Finally we comment on the Padé analysis. The obtained values for z_c are now stable under the variation of μ . However, the computed estimates for u_c are systematically shifted to lower values and the statistical errors of u_c are not substantially smaller than in the original analysis of Λ'_2 and Λ'_1 in the variable u. Because we believe that these estimates contain *large systematical errors*, they are omitted in the final estimate. Instead we combine the results from the ratio methods and Neville tables as applied to the transformed series with those from the Padé analysis of Λ'_2 and Λ'_1 in the variable u and compute a weighted average with the weighting procedure already described above. The final estimate for u_c is $u_c = 0.4079(58)$.

We now turn to the determination of the critical exponent ν' . Concerning the ratio methods, we only get an estimate for ν' at u_c from the analysis of the transformed series of Λ'_2 with $\mu^{-1} = |u_1|$. We observe reasonable convergence for the last five members of the sequence $g_n(0)$ [9] and predict $2\nu' = 1.225(12)$. The recent Monte Carlo renormalization group analysis of Pawley et al. [1] yields $2\nu(=2\nu') = 1.258(8)$.

Applying the method of Padé approximants, we first have to make an assumption on the critical behaviour of ξ . The simplest assumption is that ξ has a *pure power law singularity* at the corresponding value $u = u^*$ and that the amplitude function A(u) is *analytic* at $u = u^*$. This implies for example for Λ'_2 :

$$\Lambda'_{2}(u) = (u^{*} - u)^{-2\nu'} A(u)^{2}.$$
(17)

Taking the logarithmic derivative and multiplying by $(u^* - u)$ we obtain

$$\left[(u^* - u)(d/du) \log \Lambda'_2 \right](u) = 2\nu' [1 + O(u^* - u)].$$
 (18)

Then evaluating Padé approximants at $u = u^*$ to the function on the left-hand side give estimates for $2\nu'$ at u_c , u_1 , u_2 , if we choose $u^* = u_c$, u_1 , u_2 respectively.

This works of course quite analogously for Λ'_1 . However, it turns out that in this case most of the Padé approximants have nearby zeros and/or poles at the singularity under consideration and are therefore unreliable. Hence we restrict to the Padé analysis of Λ'_2 .

TABLE 2 The table of Padé approximants to the function $[(u_c - u)(d/du)\log \Lambda_2](u)$ evaluated at $u = u_c$

		1	М	
L	1	2	3	4
1	1.291	1.457	1.071	1.063
2	1.428	1.331	1.063	1.072
3	1.137	0.604	1.378	2.221
4	0.937	1.161	1.703	1.319

TABLE 3 The table of Padé approximants to the function $[(u_1 - u)(d/du)\log A'_2](u)$ evaluated at $u = u_1$

	М						
L	1	2	3	4	5	6	7
1	0.2274	0.1631	0.1297	0.1073	0.0918	0.0803	0.0713
2	0.0541	0.0150	0.0040 ^b	0.0080	0.0083	-0.0057^{b}	
3	0.0417	0.0010 ^b	0.0070	0.0080	0.0080		
4	0.0110	0.0093	0.0079	0.0071			
5	0.0089	0.0384 ^{a, b}	0.0096				
6	0.0018 ^b	0.0092					
7	0.0104						

'a' indicates a spurious pole whereas 'b' indicates a nearby zero of the numerator polynomial.

	М						
L	1	2	3	4	5	6	7
1	0.9246	0.8121	0.7965	0.8214	1.0980	19.483 ^a	- 8.8108 ^a
2	0.7661	0.7936	0.8060	0.7931	0.7207	-6.5528^{a}	
3	0.8019	0.6920	0.7870	0.8283	0.8114		
4	0.8451	0.7942	0.7613	0.8102			
5	0.5118	-0.2662	0.8452				
6	0.0355 ^b	0.5389					
7	2.0563						

TABLE 4 The table of Padé approximants to the function $[(u_2 - u)(d/du)\log \Lambda'_2](u)$ evaluated at $u = u_2$

The symbols 'a' and 'b' are defined as for table 3.

Qualitatively, the Padé approximants at $u = u_1$ and $u = u_2$ are better convergent than at $u = u_c$ as expected. The corresponding Padé tables are presented in tables 2-4.

We first come to the determination of $2\nu'$ at $u = u_c$. As can be learned from table 2, the convergence is very poor but a possible stabilization of the estimates in the series analysis of an extended series expansion along the diagonal of the Padé table might be concluded. Simple averaging gives $2\nu' = 1.265(89)$. Taking also into account the estimate from the ratio method analysis above, the weighted average is $2\nu' = 1.255(17)$.

For the determination of $2\nu'$ at $u = u_1$, where we choose u_1 as determined in the Padé analysis of Λ'_2 , we note that there is no convergence for [1/M] Padé approximants and [L/M] approximants with L + M < 6. Averaging over the re-

maining set of approximants which have no spurious poles or zeros yields $2\nu' = 0.008(1)$. As already discussed previously, the true error might be larger, but this can only be judged from a more detailed analysis of a longer series expansion.

Finally we discuss the critical exponent at $u = u_2$. For u_2 we take the best value from the literature [11] to be compatible with the analysis of Itzykson et al. [14] who predict $\nu' = 0.4 \pm 0.1$ from the analysis of the O(u^5) series. Our estimate from the diagonal and near-diagonal Padé approximants is $2\nu' = 0.80(2)$. As all estimates lie in the interval $0.69 \le 2\nu' \le 0.93$, a more conservative guess for $2\nu'$ would be $2\nu' = 0.80^{+0.13}_{-0.11}$.

5. Summary and conclusion

We gave a description of the main features of a fast computer algorithm which allows an arbitrary high-order low-temperature expansion of the inverse correlation length in the Ising model or strong coupling expansion of the mass gap in the Z_2 euclidean lattice gauge theory in 3 dimensions respectively. This algorithm can be generalized without any principal difficulties to be applicable to the interesting case of 4-dimensional lattice gauge theory with non-abelian gauge groups.

As an application of our method, we presented an $O(u^8)$ low-temperature series expansion for the spin-spin Ising model. A preliminary series analysis resulted in rough estimates for the location of the physical singularity u_c and two unphysical singularities u_1 and u_2 lying on the real negative axis in the complex *u*-plane. The critical exponent ν' at u_c , u_1 and u_2 has also been investigated.

The new observation is the singularity u_1 , whose existence implies a violation of the *empirical relation*

$$n = \frac{1}{2}(q-4), \tag{19}$$

which relates the number of poles in the disk $|u| \leq |u_c|$ to the *lattice coordination* number q. In [15], this equation was found to hold for various 3-dimensional lattices.

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