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Analytic and Numerical Evidence from Quantum Field Theory for the Hyperscaling Relation $d\nu = 2\Delta - \gamma$ in the $d = 3$ Ising Model

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The hyperscaling relation $d\nu = 2\Delta - \gamma(d = 3)$ for the Ising model has been shown to follow from a constructive approach proposed by one of the authors (R.S.) of a relativistic theory of self-interacting Bosons in d space-time dimensions. We present evidence that the two assumptions made in this approach are valid: On a finite Euclidean (hyper-) cubical lattice in d dimensions the renormalization map from the bare to the renormalized parameters should have nonvanishing Jacobian everywhere. We show this analytically and numerically on the boundary set of the parameters. The numerical analysis involves Monte Carlo calculations in the region where the bare coupling constant g_0 is infinite, giving the Ising model. The linear size n of the lattice (with periodic boundary conditions) was taken to be 5, 6, and 10. There we also checked the second assumption saying that the correlation length for the Ising model is a monotonic function of the temperature. We also comment on the possible numbers of zeros of the Callan–Symanzik β function of this theory.

KEY WORDS: Ising model; hyperscaling, relativistic, self-interacting Boson quantum field theory; renormalization; Monte-Carlo calculations; multispin coding.

1. INTRODUCTION

The question whether the hyperscaling relation

$$d\nu = 2\Delta - \gamma$$

holds for the Ising model in $d = 3$ dimensions remains one of the controversial issues in the theory of critical phenomena. It is known that the

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dimensionless renormalized coupling constant remains bounded,[1-3] whence

$$d\nu \geqslant 2\Delta - \gamma \tag{1}$$

holds rigorously for all d. High-temperature expansions combined with Padé techniques numerically favor a strict inequality in relation (1) when $d = 3$. For a recent review of this, see, e.g., Ref. 4.

There are, however, also attempts to reconcile high-temperature series for $d = 3$ with scaling relations; see, e.g., Ref. 5.

Within renormalization group theory relation (1) is of course an equality; see, e.g., Ref. 6.

In a series of articles[4,7-10] one of the present authors (R.S.) proposed a constructive approach to a relativistic ϕ^4 theory in d space-time dimensions within the following frame:

(a) Euclidean formulation,

(b) intermediate renormalization,

(c) lattice approximation.

We briefly explain this approach, the assumptions involved, and how it leads to a prediction on the hyperscaling relation (1).

The Euclidean approach has the advantage of allowing a discussion in the framework of measure theory in terms of functional integration.[11,12] The intermediate renormalization,[13] which is a renormalization at momentum zero, allows the application of Griffiths' inequalities (see, e.g., Ref. 14) and Lebowitz inequalities.[15,16] Sufficient conditions are then known to ensure that the moments thus obtained are the Wightman functions of a relativistic theory at the Euclidean points.[17]

The lattice approximation is a convenient cutoff which furthermore allows us to relate this approach to critical phenomena. Two of the renormalization conditions fix the two-point function and thus the field strength and a typical length, whereas the third gives the coupling constant by fixing the truncated four-point function at momentum zero.

On a finite lattice this renormalization map is real analytic in the bare parameters. In Refs. 7–9 the following assumptions for a finite hypercubical lattice were made:

(i) The renormalization map has everywhere nonvanishing Jacobian (local injectivity). This was combined with a relative mild assumption on the behavior when g_0, the bare coupling constant, tends to infinity, which leads to the Ising model. This assumption would in particular be satisfied if the following were true:

(ii) The Ising model correlation length on a finite lattice given by the second moment of the two-point function is a monotonically decreasing function of the temperature.

These assumptions evidently do not involve the lattice distance. In

Refs. 1–3 they were shown to imply the following:

(α) The renormalization map is globally injective, i.e., the renormalized parameters uniquely specify the theory on a finite lattice.

(β) Therefore, under the renormalization map the boundaries $g_0 = 0$ (Gaussian theory), $g_0 = \infty$ (Ising model), $Z = 0$ (ultralocal theory) (Z = amplitude renormalization constant), and $Z = \infty$ (strongly coupled modes) are mapped onto the boundary of the image.

We will call the images of the sets $g_0 = 0$ and $g_0 = +\infty$ under the renormalization map the Gaussian and Ising surface, respectively. In particular (β) implies the following:

(γ) For fixed renormalization of the two-point function (two conditions) the renormalized coupling constant takes its maximal value at the Ising surface. It does not seem unreasonable to assume that for fixed renormalization of the two-point function, the renormalized coupling constant is a monotone function of the bare coupling constant. This assumption trivially also implies (γ); on the other hand, this assumption is *not* necessarily a consequence of (i) and (ii): maps which define diffeomorphisms, but where certain matrix elements of the Jacobian change sign, may easily be found. In other words: Conjecture (i) is compatible with the possibility that the renormalized coupling constant is not a monotonic function of the bare coupling constant g_0 for fixed normalization of the two-point function.

Now it is known that there exists nontrivial infinite volume continuum ϕ^4 theories for $d = 3$ within the framework given by (a)–(c).[18–20] Hence by (β) in the thermodynamic limit (lattice tending to infinity) followed by the scale limit (lattice distance going to zero) the Ising surface cannot fall into the Gaussian surface. This again implies that relation (1) has to be an equality for $d = 3$ giving a hyperscaling relation. There is a subtlety in this argument, which we want to comment on, namely, the order in which the limits are taken. In Ref. 20, e.g., first the lattice spacing tends to zero for fixed volume and then the thermodynamic limit is taken. The phase space cell expansion and cluster expansion of Glimm, Jaffe, and Spencer[21] as used in Refs. 19 and 20, however, may be used to show that (for small coupling constants), the order of taking the limits is irrelevant (K. Osterwalder, private communication).

Now in a recent paper[23] G. A. Baker, Jr. and J. M. Kincaid presented numerical evidence that the renormalized coupling constant does not take its maximal value at the Ising surface (see, however, another analysis of the same data given by B. G. Nickel and B. Sharpe[24]). Previous numerical evidence in the same direction was also found by K. G. Wilson and J. Kogut for $d = 4$.[25]

With these conflicting results, it is of interest to take a closer look at conjectures (i) and (ii). It is the aim of this paper to present direct evidence for these assumptions, which we stress are assumptions involving arbitrary large but finite lattices.

For the case $d = 1$, numerical evidence for assumptions (i) to hold has previously been given by D. Marchesin.[26]

In Section 2 we check assumption (i) on the boundary of the set of bare parameters. More precisely, we show that the Jacobian is nonzero when $g_0 = 0$ or when $Z = 0$. For $g_0 = 0$ this is of course not surprising since it is related to the well-known fact that in the continuum infinite volume limit theory intermediate renormalization works in perturbation theory.

When $Z \to \infty$, the Jacobian tends to zero. However, after an appropriate rescaling, we obtain a quantity which we show to be nonvanishing. The same situation occurs when g_0 tends to infinity: By an appropriate rescaling, we obtain a quantity which essentially only depends on $\beta = (kT)^{-1}$ through Ising model quantities.

In Section 3 we present Monte Carlo calculations for this (scaled) Jacobian on an $n \times n \times n$ lattice ($n = 5, 6$, and 10) with periodic boundary conditions and T above the critical temperature. (Since we work with untruncated two-point functions, our constructive approach aims at a theory in the one-phase region, in other words, in the thermodynamic limit only the part of the Ising surface above the critical temperature survives.)

The Monte Carlo method employed is a combination of the Metropolis method[27] and the so-called heat bath method, by which the importance sampling is achieved by successively putting each lattice site variable into a heat bath of temperature T while freezing the remaining lattice variables. Standard references for this method, which also quote earlier contributions, are Refs. 28–30.

To make the computation fast, we employed the technique of storing many spins in a single memory word of the computer. This method has now received the name multispin coding (MSC).[31] In contrast to the work of Creutz, Jacobs, and Rebbi,[31–33] e.g., our MSC procedure leaves the single lattice variable updating procedure intact.

The results obtained are all in agreement with conjecture (i) and conjecture (ii). It remains to check conjecture (i) in the interior of the set of allowed parameters.

However, the results obtained so far allow to make another conclusion:

Since in all cases the (scaled) Jacobian has the same sign and since this sign gives the orientation of the image of an infinitesimal volume element at the corresponding point, this indicates that the Ising surface is approached from the correct side when $g_0 \to \infty$. If this persists for all lattice sizes in three dimensions, it can only be reconciled with the result in Ref. 23, if the renormalized coupling constant together with a maximum beyond the Ising surface also exhibits at least one minimum. Note that such stationary points correspond to zeros of the β function of Callan and Symanzik.[33–35]

In other words: If the Ising model and the ϕ^4 theory in three dimensions are described by different zeros of the Callan–Symanzik β functions these zeros should be separated by an odd number of additional zeros. This again conforms with standard wisdom, according to which the Ising model and the ϕ^4 theory are described by an infrared stable fixed point.

2. ANALYTIC RESULTS

To establish the notation, we recall the conventions used in Ref. 1. Let $\mathfrak{T}$ be a unit lattice on a torus in d dimensions, i.e.

$$\mathfrak{T} = \mathbb{Z}_{n_1} \times \mathbb{Z}_{n_2} \times \cdots \times \mathbb{Z}_{n_d}$$

where $\mathbb{Z}_n$ denotes the set of integers modulo n. $|\mathfrak{T}| = \pi_{e=1}^{d} n_e$ is the number of points on $\mathfrak{T}$.

For $i = (i_1, \ldots, i_d)$, $j = (j_1, \ldots, j_d) \in \mathfrak{T}$, $(i-j)^2$ is the translation invariant distance square on $\mathfrak{T}$, i.e.,

$$(i-j)^2 = \sum_{e=1}^{d} (i_e - j_e)^2$$

where $(i_e - j_e)^2 = \min[|i_e - j_e|^2, (|i_e - j_e| - n_e)^2]$. i, j are called nearest-neighbors (NN), if $(i-j)^2 = 1$. In d dimensions, obviously each point has $2d$ nearest neighbors whenever $n_e > 2$ for all e. For fixed $\mathfrak{T}$ and each $\alpha = (\alpha_1, \alpha_2, \alpha_3) \in \mathbb{R}^+ \times \overline{\mathbb{R}^+} \times \mathbb{R}$ we define a probability measure $\mu(\alpha)$ on $\mathbb{R}^{|\mathfrak{T}|}$ by

$$d\mu(\{x_j\}_{j\in\mathfrak{T}}) = \frac{1}{N} \underset{i,jNN}{\pi} \exp(\alpha_2 x_i x_j) \underset{i\in\mathfrak{T}}{\pi} \exp(-\alpha_1 x_i^4 + \alpha_3 x_i^2)\, dx_i \qquad (2)$$

Here and in what follows N will always denote a normalizing factor which makes the measure in question a probability measure.

$\langle \cdot \rangle$ will denote expectations w.r.t. μ and ; denotes truncation. To each $\mathfrak{T}$ (and lattice spacing $a = 1$) we define a mapping

$$T : \mathbb{R}^+ \times \overline{\mathbb{R}^+} \times \mathbb{R} \to \overline{\mathbb{R}^+} \times \overline{\mathbb{R}^+} \times \overline{\mathbb{R}^+}$$
$$\alpha \to y = T(\alpha)$$

called the renormalization map, which is given by

$$y_1 = \frac{1}{|\mathfrak{T}|} \sum_{i,j} \langle x_i x_j \rangle$$
$$y_2 = \frac{1}{|\mathfrak{T}|} \sum_{i,j} (i-j)^2 \langle x_i x_j \rangle \qquad (3)$$
$$y_3 = -\frac{1}{|\mathfrak{T}|} \sum_{i,j,k,l\in\mathfrak{T}} \langle x_i ; x_j ; x_k ; x_l \rangle$$

The relations $y_1 \geqslant 0$, $y_2 \geqslant 0$ are a consequence of Griffiths' first inequality (see e.g., Ref. 14), $y_3 \geqslant 0$ follows from the Lebowitz inequality.[15]

$y_2 y_1^{-1}$ is then the correlation length squared as given by the second moment of the two-point function. In Ref. 5 it was furthermore shown that the estimate

$$\frac{y_2}{y_1} \leqslant D(\mathfrak{T}) \tag{4}$$

holds where

$$D(\mathfrak{T}) = \frac{1}{|\mathfrak{T}|^2} \sum_{i,j \in \mathfrak{T}} (i-j)^2$$

Whenever the lattice $\mathfrak{T}$ is a cubical box, i.e., whenever $n_e = n$ for all $1 \leqslant e \leqslant d$, then an easy calculation shows that

$$D(\mathfrak{T}) = \begin{cases} \dfrac{d}{12}(n-1)(n+1) & (n \text{ odd}) \\ \dfrac{d}{12}(n^2+2) & (n \text{ even}) \end{cases} \tag{5}$$

The variable α_1 corresponds to the coupling constant and α_2 to the amplitude renormalization constant.

Let

$$\mathrm{Det}(\alpha) = \frac{\partial(y_1, y_2, y_3)}{\partial(\alpha_1, \alpha_2, \alpha_3)}$$

be the Jacobian of the renormalization map at α. Our first result is the following.

Proposition 1. At the Gaussian surface the Jacobian $\mathrm{Det}(\alpha)$ never vanishes: The inequality

$$\mathrm{Det}(\alpha)|_{\alpha_1=0} < 0 \tag{6}$$

holds for all α with $-\alpha_3 - d\alpha_2 > 0$.

Remark. Only when the last condition in Proposition 1 is satisfied, the renormalization map is defined.

Proof. We have

$$\left.\frac{\partial y_1}{\partial \alpha_1}\right|_{\alpha_1=0} = \left.\frac{\partial y_2}{\partial \alpha_1}\right|_{\alpha_1=0} = 0$$

Hence

$$\mathrm{Det}(\alpha)|_{\alpha_1=0} = \left.\frac{\partial y_3}{\partial \alpha_1}\right|_{\alpha_1=0} \cdot \det \left. \begin{pmatrix} \dfrac{\partial y_1}{\partial \alpha_2} & \dfrac{\partial y_2}{\partial \alpha_2} \\ \dfrac{\partial y_1}{\partial \alpha_3} & \dfrac{\partial y_2}{\partial \alpha_3} \end{pmatrix} \right|_{\alpha_1=0} \tag{7}$$

It was shown in Ref. 5 that the last factor in relation (7) is always < 0.

Furthermore, a simple calculation using translation invariance gives

$$\left.\frac{\partial y_3}{\partial \alpha_1}\right|_{\alpha_1=0} = 4!\, y_1^4\big|_{\alpha_1=0} > 0$$

This concludes the proof of Proposition 1. Next we discuss ultralocal theories. ■

Proposition 2. For ultralocal theories the Jacobian $\mathrm{Det}(\alpha)$ never vanishes: The inequality

$$\mathrm{Det}(\alpha)\big|_{\alpha_2=0} < 0$$

holds for all $(\alpha_1, \alpha_2) \in \mathbb{R}^+ \times \mathbb{R}$.

Proof. An easy argument shows that

$$\left.\frac{\partial y_2}{\partial \alpha_1}\right|_{\alpha_2=0} = \left.\frac{\partial y_2}{\partial \alpha_3}\right|_{\alpha_2=0} = 0$$

and

$$\left.\frac{\partial y_2}{\partial \alpha_2}\right|_{\alpha_2=0} = \frac{1}{|\mathcal{T}|} \sum_{i,j NN} \sum_{k,l} (k-l)^2 \langle x_k x_l ; x_i x_j \rangle\big|_{\alpha_2=0}$$

$$= 2d \langle x_0^2 \rangle^2\big|_{\alpha_2=0} > 0$$

Also

$$\det\left.\begin{pmatrix} \dfrac{\partial y_1}{\partial \alpha_1} & \dfrac{\partial y_1}{\partial \alpha_3} \\ \dfrac{\partial y_3}{\partial \alpha_1} & \dfrac{\partial y_3}{\partial \alpha_3} \end{pmatrix}\right|_{\alpha_2=0} = \det\left.\begin{pmatrix} -\langle x_0^2 ; x_0^4 \rangle & \langle x_0^2 ; x_0^2 \rangle \\ \langle x_0^4 ; x_0^4 \rangle & -\langle x_0^2 ; x_0^4 \rangle \end{pmatrix}\right|_{\alpha_2=0} \tag{8}$$

We claim the expression (8) is < 0.

Indeed, there is no real τ such that $x_0^4 + \tau x_0^2 = \text{const}$ almost everywhere with respect to $\mu|_{\alpha_2=0}$. Hence in the next expression the Schwarz inequality must be strict, i.e., for no real τ can we have the equality:

$$\left\langle \left(x_0^4 + \tau x_0^2 \right) \right\rangle^2 \Big|_{\alpha_2=0} = \left\langle \left(x_0^4 + \tau x_0^2 \right)^2 \right\rangle \Big|_{\alpha_2=0}$$

But this is a quadratic expression in τ. Solving this for τ must lead to nonreal solutions. This, however, is equivalent to the fact that the expression in relation (8) is < 0, q.e.d. This concludes the proof of Proposition 2. ■

Next we study the behavior when $\alpha_2 \to \infty$. For this purpose we introduce new bare parameters $(\alpha_1', \tau, \alpha_3')$ by

$$\alpha_1' = \alpha_1, \quad \tau = (\alpha_2)^{-1/2}, \quad \alpha_3' = \alpha_3 - d\alpha_2$$

The Jacobian of this transformation is evidently

$$\frac{\partial(\alpha_1', \tau, \alpha_3)}{\partial(\alpha_1, \alpha_2, \alpha_3)} = -\frac{\tau^3}{2}$$

Expressed in terms of α_1', τ, α_3' we introduce the scaled Jacobian

$$\begin{aligned}\mathrm{Det}'(\alpha_1', \tau, \alpha_3') &= \tau^{-4}\mathrm{Det}(\alpha)\\ &= -\frac{1}{2}\tau^{-1}\frac{\partial(y_1, y_2, y_3)}{\partial(\alpha_1', \tau, \alpha_3')}\end{aligned}$$

Our next result is as follows.

Proposition 3. When $\tau \to 0$ the scaled Jacobian Det′ has a limit which is everywhere negative, i.e.,

$$\mathrm{Det}'(\alpha_1', 0, \alpha_3') < 0$$

for all $\alpha_1' > 0$, $\alpha_3' \in \mathbb{R}$.

Proof. We first replace the set of random variables $\{x_i\}_{i\in\mathfrak{T}}$ by the new set of random variables x_0, $\{\xi_i\}_{i\in\mathfrak{T}_{i\neq 0}}$ with

$$\xi_i = (x_i - x_0)(1/\tau), \qquad i \in \mathfrak{T}, \quad i \neq 0$$

Agreeing ξ_0 to be zero, the measure may then be written as

$$d\mu(x_0, \{\xi_i\}_{i\in\mathfrak{T}, i\neq 0}) = \frac{1}{N}\exp - \alpha_1' \sum_{j\in\mathfrak{T}} (x_0 + \tau\xi_j)^4 \exp - \frac{1}{2}\sum_{k,lNN} (\xi_k - \xi_l)^2$$

$$+ \alpha_3' \sum_{j\in\mathfrak{T}} (x_0 + \tau\xi_j)^2 \prod_{\substack{j\in\mathfrak{T}\\ j\neq 0}} d\xi_j\, dx_0 \tag{9}$$

Finally let $\mu' = \mu'(\alpha_1', \alpha_3')$ be the probability measure on $\mathbb{R}$ given by

$$d\mu'(x_0) = \frac{1}{N}\exp(-\alpha_1'|\mathfrak{T}|\, x_0^4 + \alpha_3'|\mathfrak{T}|\, x_0^2)\, dx_0 \tag{10}$$

and denote by $\langle\cdot\rangle' = \langle\cdot\rangle'(\alpha_1', \alpha_3')$ the expectations with respect to μ'. For any function F depending on x_0 only, we therefore have

$$\langle F\rangle|_{\tau=0} = \langle F\rangle'$$

by comparison of (9) and (10).

Our aim is to obtain the leading terms of

$$\frac{\partial(y_1, y_2, y_3)}{\partial(\alpha_1', \tau, \alpha_3')}$$

in an expansion in τ around $\tau = 0$. This necessitates a corresponding analysis of all the matrix elements involved in this determinant. A lengthy but straightforward calculation gives

$$\frac{\partial y_1}{\partial \alpha_1'} = -\langle x_0^2; x_0^4\rangle' |\mathfrak{T}|^2 + O(\tau^4)$$

$$\frac{\partial y_1}{\partial \tau} = \frac{1}{\tau} \sum_{k,lNN} \left\langle x_0^2; (\xi_k - \xi_e)^2 \right\rangle |\mathfrak{T}|$$

$$- \frac{\tau}{|\mathfrak{T}|} \sum_{\substack{p,j \in \mathfrak{T} \\ k,lNN}} \left\langle \xi_j \xi_p; (\xi_k - \xi_l)^2 \right\rangle + O(\tau^3)$$

$$\frac{\partial y_1}{\partial \alpha_3'} = \langle x_0^2; x_0^2\rangle' |\mathfrak{T}|^2 + O(\tau^4)$$

$$\frac{\partial y_2}{\partial \alpha_1'} = -\langle x_0^2; x_0^4\rangle' D(\mathfrak{T}) |\mathfrak{T}|^2 + O(\tau^4)$$

$$\frac{\partial y_2}{\partial \tau} = \frac{1}{\tau} \sum_{k,lNN} \left\langle x_0^2; (\xi_k - \xi_l)^2 \right\rangle D(\mathfrak{T}) |\mathfrak{T}|$$

$$- \frac{\tau}{|\mathfrak{T}|} \sum_{\substack{p,j \in \mathfrak{T} \\ k,lNN}} j^2 \left\langle \xi_j \xi_p; (\xi_k - \xi_l)^2 \right\rangle + O(\tau^3)$$

$$\frac{\partial y_2}{\partial \alpha_3'} = \left\langle x_0^2; x_0^2 \right\rangle' D(\mathfrak{T}) |\mathfrak{T}|^2 + O(\tau^4)$$

$$\frac{\partial y_3}{\partial \alpha_1'} = \left(\langle x_0^4; x_0^4\rangle' - 6 \langle x_0^2; x_0^4\rangle' \langle x_0^2\rangle' \right) |\mathfrak{T}|^4 + O(\tau^4)$$

$$\frac{\partial y_3}{\partial \tau} = O(\tau^2)$$

$$\frac{\partial y_3}{\partial \alpha_3'} = \left(6 \langle x_0^2; x_0^2\rangle' \langle x_0^2\rangle' - \langle x_0^4; x_0^2\rangle' \right) |\mathfrak{T}|^4 + O(\tau^2)$$

Hence we obtain

$$\frac{\partial(y_1, y_2, y_3)}{\partial(\alpha_1', \tau, \alpha_3')} = \tau |\mathfrak{T}|^5 A(\tau) \left\{ \left(\langle x_0^2; x_0^4\rangle' \right)^2 - \langle x_0^2; x_0^2\rangle' \langle x_0^4; x_0^4\rangle' \right\} + O(\tau^3) \tag{11}$$

with

$$A(\tau) = \sum_{\substack{j,p \\ k,lNN}} \left[D(\mathfrak{T}) - j^2 \right] \left\langle \xi_j \xi_p; (\xi_k - \xi_l)^2 \right\rangle \tag{12}$$

By the arguments used to prove Proposition 2, it is enough to show that $A(\tau = 0) < 0$. First we want to put $A(\tau = 0)$ into another form, so let

$$\langle \cdot \rangle(\rho) = N^{-1} \int \cdot \exp\left[-\frac{\rho^2}{2} \sum_{\substack{k,l \\ N.N}} (\xi_k - \xi_l)^2 \right] \prod_{\substack{1 \in \mathfrak{T} \\ 1 \neq 0}} d\xi_e$$

and for arbitrary j, p consider

$$H(\rho) = \langle \xi_j \xi_p \rangle(\rho)$$

By scaling

$$H(\rho) = \frac{1}{\rho^2} H(\rho = 1)$$

such that

$$-\sum_{k,lNN}{}' \left\langle \xi_j \xi_p ; (\xi_k - \xi_l)^2 \right\rangle(\rho = 1) = \left.\frac{\partial H(\rho)}{\partial \rho}\right|_{\rho = 1}$$

$$= -\frac{1}{2} H(\rho = 1)$$

Comparison with (12) therefore shows that

$$A(\tau = 0) = \frac{1}{2} \sum_{j,p} \left[D(\mathfrak{T}) - j^2 \right] \langle \xi_i \xi_p \rangle(\rho = 1)$$

Now we reintroduce the old random variables x_j ($j \in \mathfrak{T}$) and define a new expectation parametrized by $\kappa > 0$:

$$\langle \cdot \rangle(\kappa) = \frac{1}{N} \int \cdot \exp\left[-\kappa_i \sum_{i \in \mathfrak{T}} x_i^2 - \frac{1}{2} \sum_{k,lNN} (x_k - x_l)^2 \right] \prod_{l \in \mathfrak{T}} dx_l$$

such that for expectations involving only ξ variables

$$\langle \cdot \rangle(\kappa = 0) = \langle \cdot \rangle(\rho = 1)$$

Next let

$$F(j, \kappa) = \sum_{p \in \mathfrak{T}} \langle \xi_j \xi_p \rangle(\kappa)$$

In terms of the x_j

$$F(j, \kappa) = -|\mathfrak{T}| \left[\langle x_j x_0 \rangle(\kappa) - \langle x_0 x_0 \rangle(\kappa) \right]$$

due to translation invariance.

By Schwarz inequality and translation invariance

$$F(j, \kappa) \geqslant 0$$

By the results in Ref. 5 $F(j, \kappa)$ is nondecreasing in j for j^2 increasing for any $\kappa > 0$ and therefore also for $\kappa = 0$ by continuity. Hence by Chebychev's inequality $A(\tau=0) \leqslant 0$ with equality only if $F(j,\kappa=0)$ is constant. Now $F(j=0,\kappa=0)=0$, so $F(j,\kappa=0)$ can only be constant if $F(j,\kappa=0)=0$ for all j. However,

$$\sum_{j\in\mathfrak{T}} F(j,\kappa=0) = \left\langle \left(\sum_{j\in\mathfrak{T}} \xi_j \right)^2 \right\rangle (\kappa=0) > 0$$

since $\sum_{j\in\mathfrak{T}}\xi_j$ is a random variable which is not identically zero with respect to the measure in question. By the arguments above, this concludes the proof of Proposition 3. ■

We finally discuss the behavior for $\alpha_1 \to \infty$. For this purpose we now replace the bare parameters $\alpha=(\alpha_1,\alpha_2,\alpha_3)$ by (τ, β, γ) with

$$\tau = \alpha_1^{-1/2}, \qquad \beta = \frac{\alpha_2\alpha_3}{2\alpha_1}; \qquad \gamma = \frac{\alpha_3}{2\alpha_1}$$

such that

$$\frac{\partial(\tau,\beta,\gamma)}{\partial(\alpha_1,\alpha_2,\alpha_3)} = -\frac{\tau^5}{4}\gamma \tag{13}$$

To see what is going on, we rewrite μ in terms of these new bare parameters as

$$d\mu(\{x_j\}_{j\in\mathfrak{T}}) = \frac{1}{N}\exp\left[-\frac{1}{\tau^2}\sum_{i\in\mathfrak{T}}(x_i^2-\gamma)^2 + \frac{\beta}{\gamma}\sum_{i,jNN} x_i x_j \right] \prod_{j\in\mathfrak{T}} dx_j$$

and we see that for $\tau \to 0$ and $\gamma > 0$ we obtain the measure $\mu'' = \mu''(\beta,\gamma)$ with

$$d\mu''(\{x_i\}_{i\in\mathfrak{T}}) = N^{-1}\exp\left\{ \frac{\beta}{\gamma}\sum_{i,jNN} x_i x_j \right\} \times \prod_{j\in\mathfrak{T}} \left[\frac{1}{2}\delta\left(x_j-\sqrt{\gamma}\right) + \delta\left(x_j+\sqrt{\gamma}\right) \right] dx_j \tag{14}$$

This is up to the scale factor γ just the Gibbs measure for an Ising model on $\mathfrak{T}$ at temperature $T=1/k\beta$.

We now define the following scaled determinant:

$$\begin{aligned} \mathrm{Det}''(\tau,\beta,\gamma) &= \tau^{-6}\,\mathrm{Det}(\alpha) \\ &= -\frac{\tau^{-1}}{4}\frac{\partial(y_1,y_2,y_3)}{\partial(\tau,\beta,\gamma)} \end{aligned} \tag{15}$$

In what follows, let $\sigma_j = \pm 1 (j\in\mathfrak{T})$ denote Ising model variables and let $\langle\ \rangle(\beta)$ denote its expectations at temperature $T=(k\beta)^{-1}$. Also set

$$S(m) = \sum_{n\,:\,m,nNN} \sigma_n$$

Note that

$$H(m) = (1/2)\sigma_m S(m)$$

can be considered as the local Hamiltonian. Furthermore let

$$T(m) = S(m) - 2d\sigma_m$$

Then we have the following:

Proposition 4. The following asymptotic relations hold

$$\frac{\partial y_1}{\partial \beta} = \frac{\gamma}{|\mathfrak{T}|} \sum_{\substack{i,j \\ m,nNN}} \langle \sigma_i\sigma_j; \sigma_m\sigma_n\rangle(\beta) + O(\tau^2) \tag{16a}$$

$$\frac{\partial y_2}{\partial \beta} = \frac{\gamma}{|\mathfrak{T}|} \sum_{\substack{i,j \\ m,nN.N}} (i-j)^2\langle \sigma_i\sigma_j; \sigma_m\sigma_n\rangle(\beta) + O(\tau^2) \tag{16b}$$

$$\frac{\partial y_3}{\partial \beta} = -\frac{\gamma^2}{|\mathfrak{T}|} \sum_{\substack{i,j,k,l \\ m,nN.N}} \langle \sigma_i; \sigma_j; \sigma_k; \sigma_l; \sigma_m\sigma_n\rangle(\beta) + O(\tau^2) \tag{16c}$$

$$\frac{\partial y_1}{\partial \gamma} = \frac{1}{|\mathfrak{T}|} \sum_{i,j} \langle \sigma_i\sigma_j\rangle(\beta) + O(\tau^2) \tag{16d}$$

$$\frac{\partial y_2}{\partial \gamma} = \frac{1}{|\mathfrak{T}|} \sum_{i,j} (i-j)^2\langle \sigma_i\sigma_j\rangle(\beta) + O(\tau^2) \tag{16e}$$

$$\frac{\partial y_3}{\partial \gamma} = -\frac{2\gamma}{|\mathfrak{T}|} \sum_{i,j,k,l} \langle \sigma_i; \sigma_j; \sigma_k; \sigma_l\rangle(\beta) + O(\tau^2) \tag{16f}$$

$$\begin{aligned}\frac{1}{2\tau}\frac{\partial y_1}{\partial \tau} &= \left(-\frac{3}{8} + \frac{d}{2}\beta\right)\gamma^{-1}\frac{\partial y_1}{\partial \gamma} - \frac{3}{8}\frac{\beta}{\gamma^2}\frac{\partial y_1}{\partial \beta} + \frac{1}{8\gamma} \\ &\quad + \frac{\beta^2}{16\gamma}\cdot\frac{1}{|\mathfrak{T}|}\sum_{i,j,m}\left\langle \sigma_i\sigma_j; S(m)^2\right\rangle(\beta) + O(\tau^2)\end{aligned} \tag{16g}$$

$$\begin{aligned}\frac{1}{2\tau}\frac{\partial y_2}{\partial \tau} &= \left(-\frac{3}{8} + \frac{d}{2}\beta\right)\gamma^{-1}\frac{\partial y_2}{\partial \gamma} - \frac{3}{8}\frac{\beta}{\gamma^2}\frac{\partial y_2}{\partial \beta} \\ &\quad + \frac{\beta^2}{16\gamma}\cdot\frac{1}{|\mathfrak{T}|}\sum_{i,j,m}(i-j)^2\left\langle \sigma_i\sigma_j; S(m)^2\right\rangle(\beta) \\ &\quad + \frac{\beta}{4\gamma}\cdot\frac{1}{|\mathfrak{T}|}\sum_{i,j}(i-j)^2\left\langle \sigma_i T(j)\right\rangle(\beta) + O(\tau^2)\end{aligned} \tag{16h}$$

$$\begin{aligned}\frac{1}{2\tau}\frac{\partial y_3}{\partial \tau} &= \left(-\frac{3}{8} + \frac{d}{2}\beta\right)\gamma^{-1}\frac{\partial y_3}{\partial \gamma} - \frac{3}{8}\frac{\beta}{\gamma^2}\frac{\partial y_3}{\partial \beta} \\ &\quad - \frac{\beta^2}{16}\cdot\frac{1}{|\mathfrak{T}|}\sum_{i,j,k,l,m}\left\langle \sigma_i; \sigma_j; \sigma_k; \sigma_l; S(m)^2\right\rangle(\beta) + O(\tau^2)\end{aligned} \tag{16i}$$

In particular the scaled determinant given by relation (15) has a finite limit when τ tends to zero.

Proof. We need an asymptotic expansion in τ of the quantities appearing in

$$\frac{\partial(y_1, y_2, y_3)}{\partial(\tau, \beta, \gamma)}$$

i.e., an expansion around the Ising model. Such expansions have already been performed.[36–40] For our present purpose we make the following variable transformation on the random variables[41]:

$$\{x_j\}_{j\in\mathcal{T}} \to \{\sigma_j, \bar{x}_j\}_{j\in\mathcal{T}}$$

with

$$x_j = \sigma_j\sqrt{\gamma}\,(1 + \tau\bar{x}_j) \tag{17}$$

where

$$\sigma_j = \pm 1 \qquad \text{and} \qquad -\tau^{-1} < \bar{x}_j < \infty \tag{18}$$

We first note that the range of the integration over the $\bar{x}_j$ may be extended to $-\infty$, since this does not affect the coefficients in the asymptotic expansion. The remaining calculations are then standard and we leave the details to the reader. ∎

3. NUMERICAL CALCULATIONS

Since an analytical analysis of the Jacobian (15) is beyond the reach of present methods, we have performed a computer calculation on a CD 175 computer to obtain information on the following quantities for $d = 3$:

$$F(\beta) = \frac{1}{2\tau}\,\frac{\partial(y_1, y_2, y_3)}{\partial(\tau, \beta, \gamma)}\bigg|_{\tau=0,\gamma=1} \tag{19}$$

This is the relevant quantity to consider because

$$\frac{1}{2\tau}\,\frac{\partial(y_1, y_2, y_3)}{\partial(\tau, \beta, \gamma)}\bigg|_{\tau=0} = \gamma F(\beta)$$

so the γ dependence is trivial for the scaled Jacobian.

Also let

$$\xi^2(\beta) = \frac{y_2(\tau, \beta, \gamma)}{y_1(\tau, \beta, \gamma)}\bigg|_{\tau=0} = \frac{\sum_{i,j}(i-j)^2\langle\sigma_i\sigma_j\rangle}{\sum_{i,j}\langle\sigma_i\sigma_j\rangle} \tag{20}$$

be the correlation length squared of the Ising model, defined by the second moment. In order to avoid a six-fold do loop, we used another definition of the distance on a torus, i.e., a modification of the quantity $(i-j)^2$ introduced in Section 2: For a lattice $\mathfrak{T}$ of the form $\mathbb{Z}_{n_1} \times \mathbb{Z}_{n_2} \ldots \times \mathbb{Z}_{n_d}$ we replaced $(i-j)^2$ by

$$\{i-j\}^2 = \frac{1}{\pi^2} \sum_{l=1}^{d} n_l^2 \sin^2(i_l - j_l) \frac{\pi}{n_l} \tag{21}$$

Using the Euler relations, it is easy to see that thus each of the quantities involving $\{i-j\}^2$ may be expressed as a sum of products of quantities which only require three-fold do loops.

The γ-independent quantity

$$\rho(\beta) = y_3(y_1)^{-2}\big|_{\tau=0} \tag{22}$$

is of interest because by the discussion in Refs. 7–9 conjecture (ii) may be replaced by a weaker assumption: The curve obtained by plotting $\rho(\beta)$ and $\xi^2(\beta)$ in the (ρ, ξ^2) plane should lie schlicht over the axis $\rho = 0$.

Finally, the dimensionless renormalized coupling constant

$$g(\beta) = \frac{y_3}{y_1^2(y_2/y_1)^{d/2}} \tag{23}$$

is of interest in the context of the hyperscaling relation (1): F, ξ^2, ρ, and g are of course dependent on the lattice size but have a thermodynamic limit for $\beta < \beta_c$ ($\beta_c \approx 0.22169$ for $d = 3$; see, e.g., Ref. 42). If now

$$g_\infty(\beta) = \lim_{|\mathfrak{T}| \to \infty} g(\beta)$$

satisfies $g_\infty(\beta_c) > 0$, then the discussion in, e.g., Refs. 7–9 shows the existence of a nontrivial ϕ^4 theory in d dimensions. In fact, $g_\infty(\beta_c)$ is that zero of the Callan–Symanzik β function which is related to the Ising model and the cases $g_\infty(\beta_c) = 0$ or $g_\infty(\beta_c) > 0$ decide whether the Ising surface falls into the Gaussian surface or not when the scaling limit is taken.

The numerical analysis consisted in applying Monte Carlo techniques to calculate the expectation values y_1, y_2, and y_3 and partial derivatives thereof in form of suitable averages. We note that the quantities y_1, y_2, and y_3 themselves involve relatively simple expressions in terms of the basic variables σ_i going up to fourth-order moments. The determinant $F(\beta)$ on the other hand is already a complicated sum of products of expectations involving moments of up to sixth-order.

To explain in more detail the techniques we used, we briefly recall the Monte Carlo methods used in the Ising model: The averages are evaluated by generating a sequence ($i = 1, 2, \ldots$) of configurations $\sum_i$, given by specifying the values σ_k, in such a way that a definite configuration $\sum$

appears with a probability proportional to the Gibbs–Boltzmann factor:

$$P(\Sigma) = \exp\left(+\beta \sum_{i,j.N.N.} \sigma_i \sigma_j \right) \tag{24}$$

The expectation value of any function $Y(\Sigma)$ is then approximated by an average over configurations in the sequence

$$\langle Y \rangle \approx \bar{Y} = \frac{1}{M} \sum_{i=i_0}^{i_0+M-1} Y(\Sigma_i)$$

In order to use configurations already close to the statistical equilibrium a number i_0 of configurations at the beginning of the sequence is excluded. In our calculations i_0 was always roughly 100.

Although other choices are possible, in our calculations the sequence $(\Sigma_i)_{i=1,2,3\ldots}$ was constructed as follows:

The configuration Σ_{i+1} is obtained from Σ_i by a succession (specified below) of stochastic processes, one for each lattice point k. For the process associated with k, σ_k is set to a new value σ'_k according to a definite probability

$$P(\sigma'_k) = \frac{\exp[-\beta \Delta E(\sigma'_k)]}{\sum_{\sigma_{k''}=\pm 1} \exp[-\beta \Delta E(\sigma''_k)]}$$

where $\Delta E(\sigma'_k)$ is the interaction energy of σ'_k with the neighboring spins which keep their momentary values σ_j:

$$\Delta E(\sigma'_k) = -\sigma'_k \sum_{j\,:\,j,kN.N.} \sigma_j$$

In other words, this stochastic process corresponds to touching the spin σ_k with a heat reservoir at inverse temperature β while holding all other spin variables fixed. The procedure generated by this choice of $P(\sigma'_k)$ has been called the heat bath algorithm. An alternative possibility for $P(\sigma'_k)$, originally introduced by Metropolis *et al.*[27] consists in changing the sign of the spin σ_k. If the new choice lowers ΔE, σ_k is changed to $\sigma'_k = -\sigma_k$. If not, then this change is only made with the probability

$$\exp\{-\beta[\Delta E(-\sigma_k) - \Delta E(\sigma_k)]\}$$

This procedure is applied successively to all spins in a lattice and constitutes a so-called sweep of the lattice. Thus during one sweep all lattice variables will be probed exactly once. The values of the spins of the end of one sweep, starting from Σ_i, give the configuration Σ_{i+1}.

It may easily be shown that this describes an ergodic Markov process with the Gibbs–Boltzmann distribution (25) being the unique stationary distribution. The statistical error δY for the average $\bar{Y}$ of a function $Y(\Sigma)$ is then given by the formula

$$(\delta Y)^2 = \frac{1}{M(M-1)} \sum_{i=i_0}^{i_0+M-1} \left[Y(\Sigma_i) - \bar{Y} \right]^2 \tag{25}$$

This formula, however, is only reasonable if the subsequent $\sum_i$'s are uncorrelated. We have checked empirically that for the quantities we were interested in and for the lattice sizes and β values used, the statistical error does not change if we only use every second or third configuration $\sum_i$. For a more detailed analysis of this problem, see, e.g., Ref. 30. Also during a sweep we moved in a regular way through the lattice, first in the z, then in the y, and finally in the x direction.

A technique of storing many spins in a single memory word of the computer (multispin coding, MCS) to reduce memory requirements and processing time has been used. Besides the spins in the z direction we temporarily store the sum of the spins of five neighbors in a computer word, which reduces the code of the innermost loop to very few statements. They can then be processed very efficiently. For the sixth neighbor we use the last spin value obtained in the preceding step. This guarantees the single spin updating procedure with the above-mentioned properties of a Markov process.

Since this multispin technique turns out to be most efficient for the heat bath method we mainly use this one in our calculations. It has been argued that the sequences of random numbers, obtained from the random number generator in computers, may have long-range correlations (Stoll, private communication). Since in CDC computers the computer word has 60 bit, a large effect of such correlations is unlikely. To randomize small possible effects we change during the time of one sweep with 10% probability from the heat bath method over to the Metropolis method. We expect reduction of possible correlation effects not only because of the difference of the methods but also because of the fact that the Metropolis method makes less use of random numbers.

The computations have been performed on lattices of the form $\mathbb{Z}_n \times \mathbb{Z}_n \times \mathbb{Z}_n$ ($n = 5$, 6, and 10), i.e., with lattices of linear extension n and periodic boundary conditions. The statistical error for the Jacobian and the dimensionless renormalized coupling constant turn out to be rather large, especially for small β values. In particular for $n = 10$ we are only able to compute these quantities with sufficient accuracy for larger β values $< \beta_c$ without excessive processing times. Probably the main reason is, that, as already mentioned, the Jacobian and the coupling constant g are obtained from averages of relatively high moments of the basic variables σ_k. Fortunately, however, in the low-β region volume effects are small, in particular we have the relations:

$$\begin{aligned}
&\lim_{n\to\infty} F(0) = d, &&\lim_{n\to\infty} \frac{\partial F}{\partial \beta}(0) = 12d^2\\
&\lim_{n\to\infty} \xi^2(0) = 0, &&\lim_{n\to\infty} \frac{\partial \xi^2}{\partial \beta}(0) = 2d\\
&\rho(0) = 1, &&\frac{\partial \rho}{\partial \beta}(0) = 8d\\
&g(0) = \infty, &&\frac{\partial g}{\partial \beta}(0) = -\infty
\end{aligned} \tag{26}$$

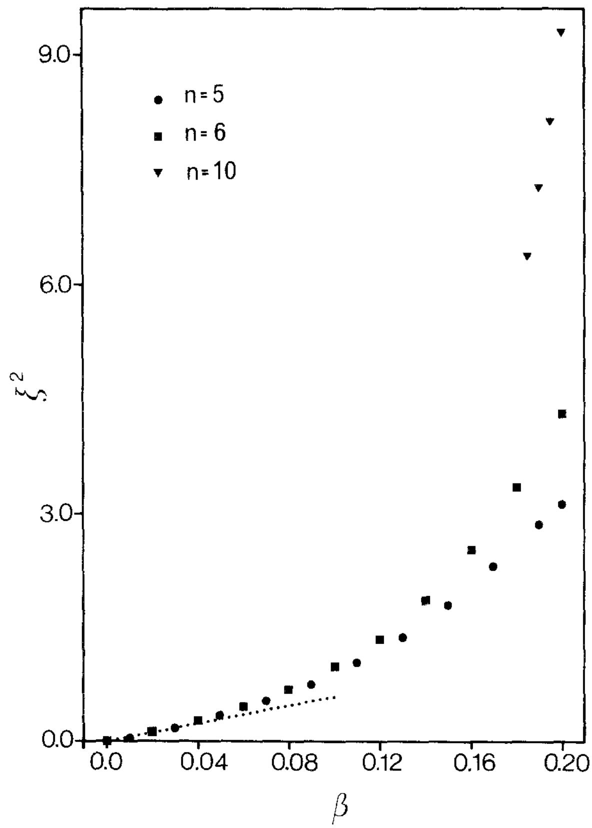

Fig. 1. The square of the correlation length ξ^2 as a function of β for the lattices of linear length $n = 5$ (450000 sweeps), $n = 6$ (600000 sweeps), and $n = 10$ (240000 sweeps). The statistical errors do not appear in the plot, since they are smaller than the plotted symbols. In the region $\beta \leqslant 0.1$ the curves should already represent the thermodynamic limit function. For larger β the curves split up due to finite volume effects. The slope at $\beta = 0$ is taken from relation (26).

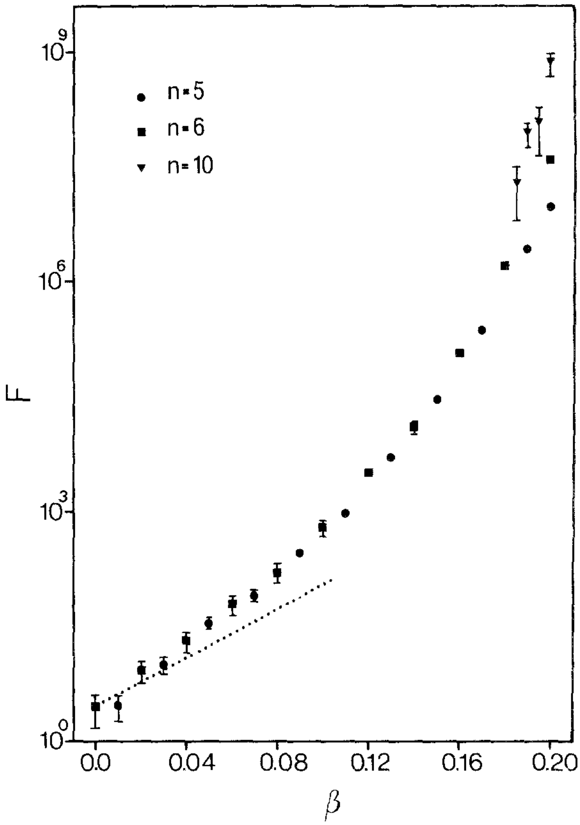

Fig. 2. The scaled Jacobian as a function of β. Because of the logarithmic scale the error bars show the relative error. Values of the $n = 10$ lattice for small β are not given since the statistical errors were too large with the computation time available.

Note that the weak n dependence of these quantities at $\beta = 0$ only comes in through the use of the periodic length definition(22). In the calculations we have taken 450000, 600000 and 240000 sweeps for $n = 5$, 6, and 10, respectively, and for each β value. The processing time on the CDC 175 computer for one β value in the case of $n = 10$ was 1.7 hr, the reduction in computing time due to multispin coding being a factor of roughly 2.

The results of the calculation are plotted in Figs. 1–4. For comparison we also show the linear slopes of the quantities at $\beta = 0$ as they may be read off relation (26) for $d = 3$. Within the error bars the quantities for different n have the same values up to $\beta \approx 0.1$. Indeed, as just mentioned, in this region the curves should already correspond to the thermodynamic

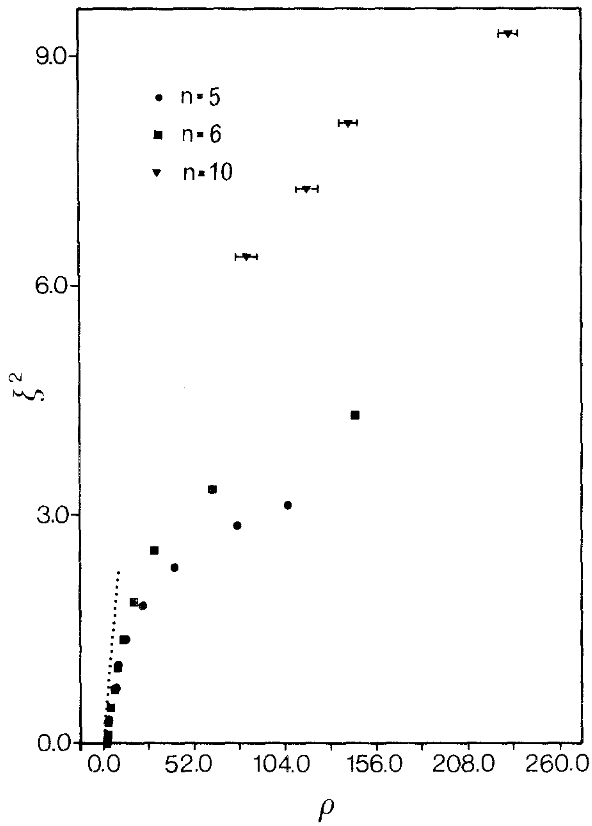

Fig. 3. The squared correlation length ξ^2 plotted as a function of the coupling constant ρ shows the shape of the (ρ, ξ^2) region covered by the ϕ^4 theories on the corresponding lattices.

limit function. By increasing β the curves split up due to finite volume effects.

The correlation length (Fig. 1) increases monotonically with β for the three lattices and confirms conjecture (ii). The Jacobian (Fig. 2) shows the same simple behavior although on a logarithmic scale. In particular since the steepness grows with the lattice size, this result strongly supports conjecture (ii) for all n at the Ising model. It would be interesting to obtain a better theoretical understanding of this quantity, in particular to know the critical exponent.

In Fig. 3 we give the boundary curves of the (ρ, ξ^2) region. Varying the bare parameters for fixed y_1, all (ρ, ξ^2) values of the ϕ_3^4 theory should lie

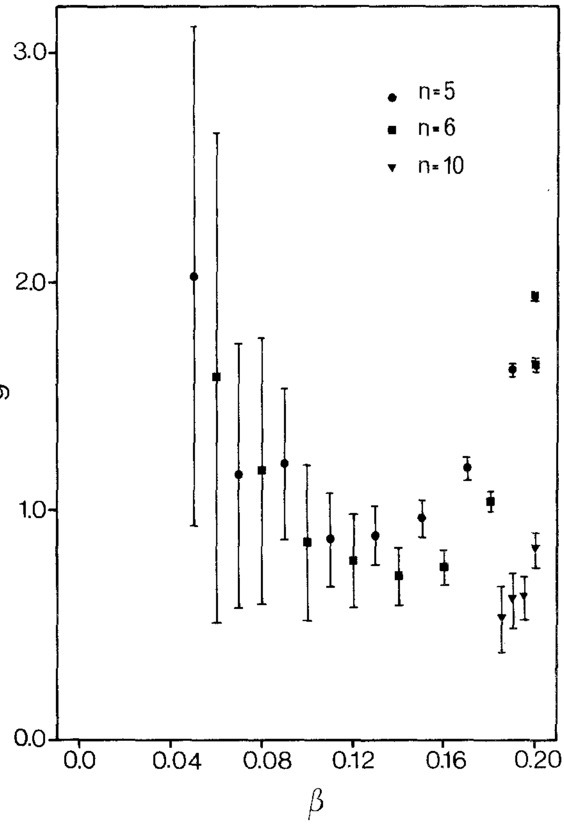

Fig. 4. The dimensionless renormalized coupling constant g as a function of β.

between $\rho = 0$ and these curves. The result shows that they have a simple shape.

Finally, in Fig. 4 we give the dimensionless renormalized coupling constant g plotted versus β. Interpreting this figure, it seems very unlikely to obtain any reliable information on $g_\infty(\beta_c)$ and thus directly on relation (1) with the help of Monte Carlo methods.

We note that the curve $g_\infty(\beta)$ in the form predicted by G. A. Baker, Jr.[4] with a small critical exponent $d\nu - 2\Delta + \gamma = 0.028$ is almost constant up to β_c and goes to zero only within a very small β region.

To conclude, the numerical results obtained so far favor conjecture (i) and conjecture (ii) when the bare coupling constant g_0 becomes infinite. It would be interesting to perform similar calculations for finite g_0 although we expect only lattice sizes up to $n \approx 8$ to be within reach of Monte Carlo methods by present computer facilities.

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