VACUUM TUNNELING IN THE FOUR-DIMENSIONAL ISING MODEL

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In the broken phase of the four-dimensional Ising model tunneling between the two degenerate minima of the effective potential takes place in a finite volume. We study this phenomenon numerically. The energies of the lowest zero momentum states are determined on both sides of the phase transition and their different correspondence to particle states in the infinite-volume limit is discussed. A Z_2-invariant definition of the field expectation value and susceptibility is exploited for calculation of these quantities in finite volumes.

The numerical study of spontaneous symmetry breaking is an interesting but delicate problem, because the symmetry is never spontaneously broken in a finite volume where the numerical simulation is done. In this letter we investigate a prototype model with spontaneously broken discrete symmetry, the four-dimensional Ising model. Variables $\phi_x = \pm 1$ are associated with the points x of a hypercubical lattice in four dimensions. The action

$$S = -2\kappa \sum_x \sum_{\mu=1}^{4} \phi_x \phi_{x+\hat{\mu}} \tag{1}$$

couples nearest neighbour points. This model is equivalent to the single-component ϕ^4 theory in the limit of an infinite bare quartic self-coupling $\lambda = \infty$ for fixed hopping parameter κ. For values of κ above a certain critical κ_c the Z_2-symmetry $\phi \to -\phi$ of the action is broken spontaneously by the non-zero vacuum expectation value of the field: $v = \langle \phi_x \rangle \neq 0$ in an infinite volume. This "spontaneous magnetization" can be defined by applying an external magnetic field h and taking first the limit of an infinite volume $V \to \infty$ and then $h \to 0$. In a numerical simulation, however, this extrapolation procedure would be demanding and introduces an additional source of systematic errors. Therefore other equivalent definitions which avoid the introduction of a magnetic field are more appropriate. We choose a definition of v in terms of the long-distance behaviour of the two-point function, which has a clear conceptual and field theoretic meaning and can be determined unambiguously in finite volumes. From the point of view of four-dimensional euclidean quantum field theories, besides the vacuum expectation value of the field, other expectation values with odd field parity like the cubic coupling are also of interest. In numerical simulations an important question is the influence of the finite volume on the results. Usually a careful investigation of the finite-size effects has to be done in order to extract the required infinite-volume information.

This letter is a continuation of previous work in the symmetric phase of the four-dimensional Ising model [1,2]. We report on a detailed study of finite-size effects in the broken phase. It is shown that on medium-size lattices (which occur quite often in four-dimensional Monte Carlo investigations) the finite-size effects are dominated by tunneling of the system between the two degenerate minima of the finite-volume effective action. The spectrum of low-lying states on a finite-size lattice is investigated in the critical region near the phase transition, and the possible rel-

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evance of the obtained results to the numerical simulation of other quantum field theories is briefly discussed.

In a finite volume spontaneous symmetry breaking does not occur, as is well known. However, the spontaneous symmetry breaking in the infinite-volume limit manifests itself on finite lattices in the distribution of the average value of the field [3]. If the value of κ is larger than the critical value κ_c, this distribution is doubly peaked with two maxima near $+v$ and $-v$. In a Monte Carlo simulation the distribution is sampled with an efficiency which can strongly depend on the choice of the algorithm. In standard algorithms based on sequences of local updating steps global changes resulting in a transition between $+v$ and $-v$ are suppressed. Far away from the phase transition or on very large lattices overall sign changes practically never occur. This fact can even be used for a rough determination of expectation values with odd Z_2-parity, which appear to be non-zero due to the inefficiency of the updating procedure.

In the long run, however, tunneling between the field averages $+v$ and $-v$ takes place. Configurations with an average field somewhere between $+v$ and $-v$, although suppressed, sometimes do occur. Typically they have a domain structure, where regions with average field values around $+v$ and $-v$ are separated by more or less sharp surfaces. The exponential suppression of these configurations is proportional to the area of the separating surface. This situation can be visualized in a simulation on elongated lattices of space–time volume $L^3 \cdot T$ with $T \gg L$. As an example, the distribution of the timeslice averages of the field

$$S_t \equiv \frac{1}{L^3} \sum_{\boldsymbol{x}} \phi_{\boldsymbol{x},t}, \quad x=(\boldsymbol{x}, t) \tag{2}$$

is shown in fig. 1 on an $8^3 \cdot 240$ lattice at $\kappa=0.076 > \kappa_c \simeq 0.0748$. As it can be seen in fig. 1, the transition regions separating the positive and negative domains are well defined even on the moderately large 8^3 volume. For larger volumes the transition is even sharper and the fluctuations inside the domains are smaller. We checked this on a $12^3 \cdot 240$ lattice with antiperiodic boundary conditions.

Most of our results presented in this paper were obtained by the percolation cluster algorithm [4]. This

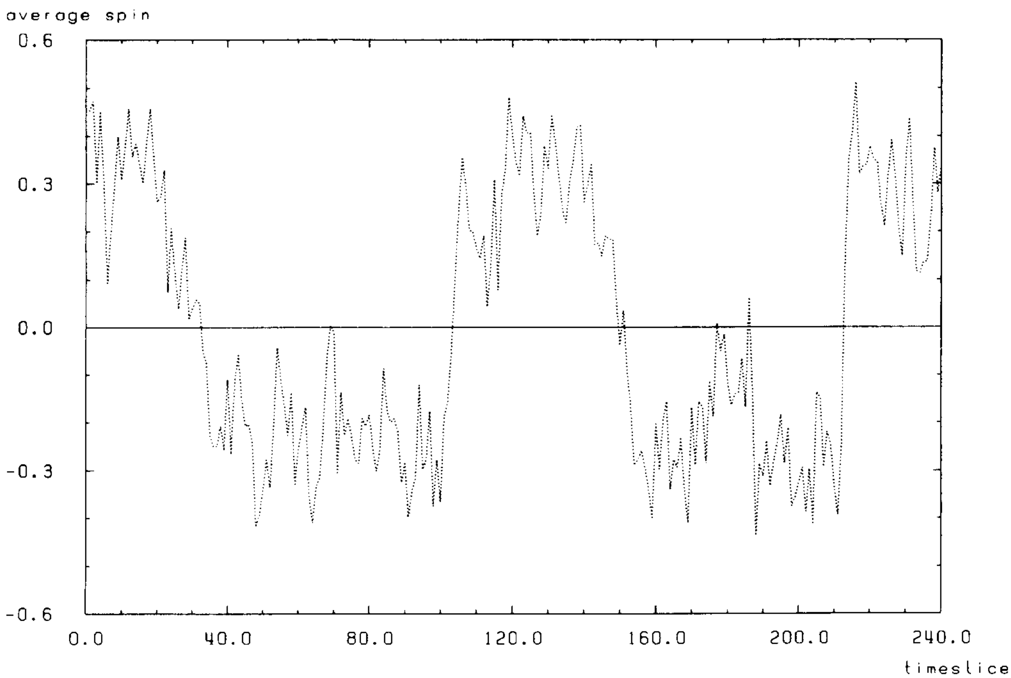

Fig. 1. The timeslice averages of the field on a $8^3 \cdot 240$ lattice at $\kappa=0.076$.

algorithm turned out to be very efficient in the symmetric phase of the four-dimensional Ising model for fighting critical slowing down and for variance reduction [2]. In the present context it is advantageous because of the global character of the updating. It makes the algorithm particularly suitable for a study of tunneling. The algorithm also allows to get quick thermalization on elongated lattices, which are crucial for a precise calculation of energy splittings and other quantities related to tunneling. The typical situation in the broken phase on a large enough lattice is that there is a single large "background cluster" corresponding to the non-zero field expectation value and a large number of small clusters with random signs. During the cluster updating whole clusters are assigned to +1 or −1 with 50% probability, therefore the sign of the average field can change from one sweep to the next. On medium-size lattices, where tunneling between the two minima is important, there are a few large clusters and many small ones. Since the large clusters are changed globally, the cluster algorithm exploits the tunneling configurations very effectively. Pictures like fig. 1 can also be obtained by a local Metropolis algorithm, but the change of the configuration is much slower, i.e. the autocorrelation time is much longer, as we checked in a few runs.

We would now like to discuss the model, in particular the spectrum of states, in a more field theoretic context. In the infinite volume the model has a phase transition at $\kappa_c=0.0748$. For $\kappa<\kappa_c$ there is a unique ground state which is symmetric with respect to the reflection $\phi\to-\phi$. The spectrum above this vacuum state corresponds to that of multi-particle states which are symmetric(s) or antisymmetric (a) under field reflection. The mass gap m_a is given by the energy E_{0a} of the antisymmetric one-particle state with zero momentum. For $\kappa>\kappa_c$ the ground state as well as all higher states are doubly degenerate. In the two vacua $|0_\pm\rangle$ the field has expectation values $+v$ and $-v$, respectively. They yield two sectors of the system such that matrix elements of local operators between different sectors vanish. The reflection $\phi\to-\phi$ transforms the sectors into each other. The spectra in both sectors are identical and again correspond to multiparticle states. The mass gap $m_+=m_-$ is the single-particle mass. As $\kappa\to\kappa_c$ the mass gap m_a (for $\kappa<\kappa_c$) or m_+ (for $\kappa>\kappa_c$) approaches zero.

In a finite spatial volume L^3 there is always a unique symmetric ground state $|0_s\rangle$. For $\kappa>\kappa_c$ transitions between the two sectors occur and the degeneracy of states is lifted by tunneling. The ground state and the lowest antisymmetric state can be written as

$$|0_s\rangle\equiv\frac{1}{\sqrt{2}}(|0_+\rangle+|0_-\rangle),$$

$$|0_a\rangle\equiv\frac{1}{\sqrt{2}}(|0_+\rangle-|0_-\rangle), \tag{3}$$

where $|0_+\rangle$ and $|0_-\rangle$ are states which go over into the above mentioned degenerate vacua in the infinite-volume limit. The energy E_{0s} of the ground state is usually defined to be zero, whereas $|0_a\rangle$ has a small energy $E_{0a}>0$. Similarly, the symmetric and antisymmetric one-particle states with momentum zero in the broken phase are denoted by $|1_s\rangle$ and $|1_a\rangle$ and their energies by E_{1s} and E_{1a}, respectively.

The small energy splitting E_{0a} in the broken phase can be estimated in a semiclassical instanton-type calculation. The tunneling configurations are described by continuous instanton ("kink") solutions of an effective ϕ^4 theory, which interpolate between the two minima of the effective action at $+v$ and $-v$ [5]. Expanding around those solutions a one-loop calculation yields [5,6] (see also ref. [7])

$$E_{0a}\simeq C\cdot L^{1/2}\exp(-\sigma L^3), \tag{4}$$

where the "surface tension" σ is given to leading order by

$$\sigma=2m_R^3/g_R\equiv\tfrac{2}{3}m_R v_R^2. \tag{5}$$

Here m_R is the renormalized mass, g_R the renormalized coupling defined by the second equality and v_R is the renormalized vacuum expectation value. Some details of this calculation and many other things related to the finite-size effects in the broken phase of the four-dimensional Ising model will be published in a longer paper [6].

In the Monte Carlo simulation the transition regions between two domains in fig. 1 correspond to the instanton solutions mentioned above. The small tunneling energy E_{0a} results in a long range correlation, which is represented in fig. 1 by the domain structure. The average length of the domain is roughly of the same order as the correlation length. For local Metropolis or Langevin updating procedures the autocorrelation time (relevant for observables with odd parity) is proportional to the square of this correlation length [8].

On a lattice of finite spatial extension L the spectrum is similar to the infinite-volume spectrum if $|\kappa-\kappa_c|$ is sufficiently large, namely for m_a^{-1} or $m_\mp^{-1}<L/2$. For κ near κ_c the spectrum interpolates continuously between these two spectra. The qualitative nature of the spectrum of low-lying zero momentum states can be illustrated by a quantum mechanical system. The finite-size scaling theory for cylindrical geometry [5] asserts that for $\kappa\approx\kappa_c$ the behaviour of the model is governed by the Fourier component of ϕ_x with vanishing three-momentum. In such an approximation the system is described by a quantum mechanical model with one degree of freedom and a single-well ($\kappa<\kappa_c$) or a double-well ($\kappa>\kappa_c$) quartic potential, whose spectrum is well known [9]. For $\kappa<\kappa_c$ it is similar to the harmonic-oscillator spectrum, whereas for $\kappa>\kappa_c$ it is the spectrum belonging to two potential wells separated by a barrier, and each pair of energies E_{ns} and E_{na} of the nth symmetric and antisymmetric state is nearly degenerate. A schematic picture of the dependence of the zero-momentum spectrum on κ is shown in fig. 2, where scattering states with non-zero relative momenta have been neglected.

The contribution of the lowest zero-momentum states to the partition function in the case of periodic boundary conditions is given by

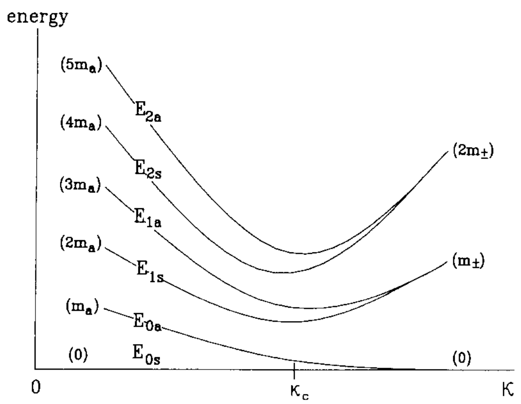

Fig. 2. Schematic picture of the spectrum of low-lying states in the one-component ϕ^4 theory on a finite lattice. States with non-zero momentum and scattering states with non-zero relative momentum are neglected. The energies result from an effective quantum-mechanical hamiltonian for the zero momentum field mode; see the discussion in the text.

$$Z\equiv\mathrm{Tr}\,\exp(-TH)$$
$$=1+\exp(-TE_{0a})+\exp(-TE_{1s})$$
$$+\exp(-TE_{1a})+\ldots\,. \tag{6}$$

Here H is the hamiltonian, $\exp(-H)$ the transfer matrix and the dots stand for higher contributions. The vacuum expectation value of the product of timeslice field averages is given by

$$\langle S_0S_t\rangle Z\equiv\mathrm{Tr}\{S_0\exp(-tH)S_t\exp[-(T-t)H]\}$$
$$=v^2\{\exp(-tE_{0a})+\exp[-(T-t)E_{0a}]\}$$
$$+c_{01}^2\{\exp(-tE_{1a})+\exp[-(T-t)E_{1a}]\}$$
$$+c_{10}^2\{\exp[-tE_{0a}-(T-t)E_{1s}]$$
$$+\exp[-(T-t)E_{0a}-tE_{1s}]\}$$
$$+c_{11}^2\{\exp[-tE_{1a}-(T-t)E_{1s}]$$
$$+\exp[-(T-t)E_{1a}-tE_{1s}]\}$$
$$+\ldots\,. \tag{7}$$

Here the matrix elements are defined as

$$v\equiv\langle 0_s|S_t|0_a\rangle\,, \tag{8}$$

and

$$c_{01}\equiv\langle 0_s|S_t|1_a\rangle,\quad c_{10}\equiv\langle 1_s|S_t|0_a\rangle\,,$$
$$c_{11}\equiv\langle 1_s|S_t|1_a\rangle\,. \tag{9}$$

Eq. (8) is a possible definition of the vacuum expectation value of the field in a finite volume. In the infinite-volume limit this is equivalent to the definition by an external magnetic field. This "invariant" definition was, to our knowledge, first introduced in the two-dimensional Ising model by Yang [10]. (For a discussion of other possible finite-volume definitions of the vacuum expectation value see refs. [11,3,12].) Using eq. (7) one can also define an "invariant" susceptibility χ_2 in the broken phase by subtracting from the sum of the two-point function the contribution proportional to v^2:

$$\chi_2\equiv\sum_x\langle\phi_0\phi_x\rangle_c$$
$$\equiv L^3\sum_t\left(\langle S_0S_t\rangle-v^2\,\frac{\{\exp(-tE_{0a})+\exp[-(T-t)E_{0a}]\}}{1+\exp(-TE_{0a})}\right). \tag{10}$$

The subtraction here is only meaningful if the spectrum is of the broken symmetry type. The definition (8) can also be generalized to other expectation values in the broken phase which are odd in field parity:

$$\langle \phi_{x_1}\phi_{x_2}\cdots\phi_{x_{2k+1}} \rangle \equiv \langle 0_s | \phi_{x_1}\phi_{x_2}\cdots\phi_{x_{2k+1}} | 0_a \rangle . \quad (11)$$

In a numerical simulation these can, in principle, be extracted from $(2k+2)$ – point functions, if the additional point is separated from the rest by a larger time distance. The separation must be large enough in order to suppress the propagation of the higher states besides $|0_{s,a}\rangle$.

In the broken phase the approximate degeneracy of states in a finite volume has to be taken into account in every correlation function. Another example besides eq. (7) is the connected correlation of the timeslice squared. For large volumes one obtains

$$\langle S_0^2 S_t^2 \rangle_c \equiv \langle S_0^2 S_t^2 \rangle - \langle S_0^2 \rangle^2$$
$$= \Delta^2 \frac{\exp(-TE_{0a})}{[1+\exp(-TE_{0a})]^2}$$
$$+ \frac{a_{01}^2}{1+\exp(-TE_{0a})} \exp(-tE_{1s})$$
$$+ b_{01}^2 \frac{\exp(-TE_{0a})}{1+\exp(-TE_{0a})} \exp[-t(E_{1a}-E_{0a})]$$
$$+ O(\exp(-TE_1), \exp(-tE_2)) , \quad (12)$$

where we define

$$a_{01} = \langle 0_s | S_0^2 | 1_s \rangle, \quad b_{01} = \langle 0_a | S_0^2 | 1_a \rangle , \quad (13)$$

and the small quantity Δ is given by

$$\Delta = \langle 0_a | S_0^2 | 0_a \rangle - \langle 0_s | S_0^2 | 0_s \rangle . \quad (14)$$

For small t the second and third terms are relevant, whereas for large t only the first term survives. This formula can be used to obtain numerical information of the effect of tunneling on the matrix elements of the operator S_t^2.

We have measured the correlation functions $\langle S_0 S_t \rangle$ and $\langle S_0^2 S_t^2 \rangle$ on various lattices of size $L^3 \cdot 120$ in the vicinity of κ_c. The results of the analysis of these functions are listed in table 1 and will be discussed in the following.

The correlation function $\langle S_0 S_t \rangle$ has been fitted by the first two terms in (7), whenever the second term was large enough to be determined reliably. This was the case for $\kappa \geqslant 0.0755$, whereas for smaller κ only the first term was obtained. The third term in eq. (7) is negligible in most of the points due to the suppression factor $\exp(-TE_{0a})$. Exceptions are the points $L=8$, $\kappa=0.077$ and $L=10$, $\kappa=0.076$, where this suppression is only moderate, therefore there is some additional systematic uncertainty in the value of E_{1a}. The fits yield results for v^2 and the energy E_{0a} with rather high precision. The susceptibility χ_2 was then calculated according to (10). It is very small for $\kappa \simeq \kappa_c$ and increases with increasing κ above κ_c. This signals strong finite-size effects because the infinite-volume susceptibility should decrease with increasing κ.

Table 1
The results of the numerical calculation on $L^3 \cdot 120$ lattices. The number of sweeps is given in thousands (ks). Error estimates in last numerals are in parentheses. They were determined by the fluctuation of the best fit parameters from subsamples of our data.

L	κ	ks	E_{0a}	E_{1s}	E_{1a}	v	χ_2	$\|\Delta\|$
8	0.0740	200	0.2458(7)	0.588(4)		0.1583(5)		
8	0.0745	412	0.1951(4)	0.504(3)		0.1761(2)		
8	0.0750	200	0.1415(3)	0.434(4)		0.2014(4)		
8	0.0755	200	0.0900(3)	0.379(5)	0.70(14)	0.2400(3)	1.9(1.2)	
8	0.0760	528	0.04609(15)	0.352(3)	0.63(4)	0.2898(3)	5.7 (4)	0.04(2)
8	0.0765	200	0.01805(12)	0.40(2)	0.50(4)	0.3415(3)	15.4(6)	
8	0.0770	334	0.00580(5)	0.47(1)	0.521(5)	0.3852(1)	18.5(2)	0.006(2)
6	0.0760	256	0.1281(4)	0.51(1)		0.3083(5)	1.0(4)	
7	0.0760	256	0.0812(3)	0.417(4)		0.2938(4)	1.6(7)	0.2(1)
9	0.0760	256	0.02238(11)	0.316(8)	0.42(4)	0.2921(2)	17(1)	0.016(2)
10	0.0760	361	0.00902(6)	0.329(8)	0.366(8)	0.2958(2)	35.0(6)	0.008(2)

The correlation function $\langle S_0^2 S_t^2 \rangle$ has been fitted with a constant plus an exponentially decreasing term although according to (12) a second exponential should also be present on a finite lattice. It would, however, be difficult to separate the exponentials numerically, because the energies E_{1s} and $E_{1a}-E_{0a}$ are of similar magnitude. Furthermore, the third contribution in (12) is relatively smaller than the second one. Therefore we take the energy extracted from the exponential fit as a measure for E_{1s}. The constant Δ has also been obtained from this fit and is included in table 1. As a measure of the difference between the matrix elements of the states $|0_a\rangle$ and $|0_s\rangle$ it is a quantity characteristic for tunneling.

The energies E_{0a}, E_{1s} and E_{1a} are displayed in fig. 3 as a function of κ. The results are in agreement with the expected behaviour discussed before (fig. 2). In particular it is clearly visible how the double degeneracy in the broken phase is approached. The energy splittings E_{0a}, $E_{1a}-E_{1s}$, which we have been able to determine, are a manifestation of the tunneling phenomenon.

Of particular interest is the volume dependence of E_{0a}, which can be compared with the semiclassical formula (4). A corresponding fit is shown in fig. 4. The predicted form of the volume dependence is confirmed very well. The best fit value for the surface tension between $L=8$, 10 is

$$\sigma=0.00358\pm0.00002\,. \qquad (15)$$

The prediction (5) from the instanton calculation would yield $\sigma=0.0047$ if the values of m_R and v_R in the infinite volume from the analytic calculation of ref. [13] are inserted. If instead we use our measured values of E_{1s}, v and χ_2 on a $10^3\cdot120$ lattice at $\kappa=0.076$ to get estimates for m_R and v_R, the prediction is

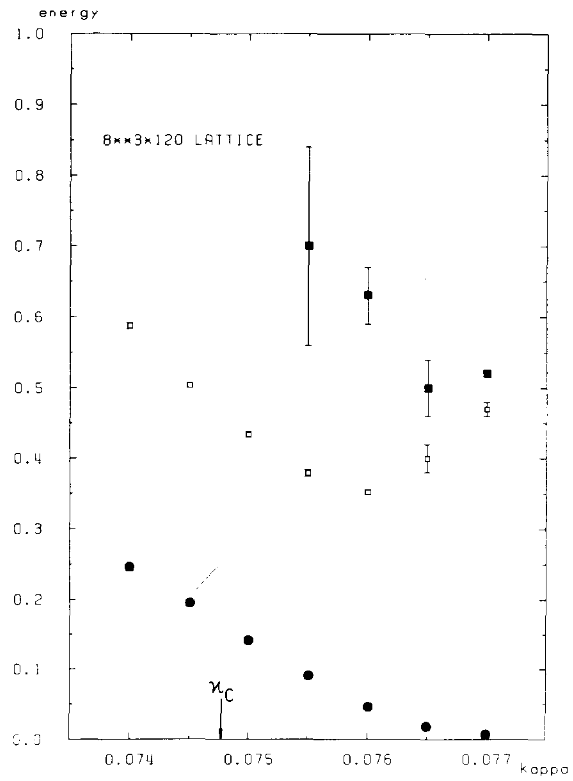

Fig. 3. The lowest zero momentum energy levels as a function of κ on a $8^3\cdot120$ lattice. The full dots stand for E_{0a}, the open squares for E_{1s} and the full squares for E_{1a}.

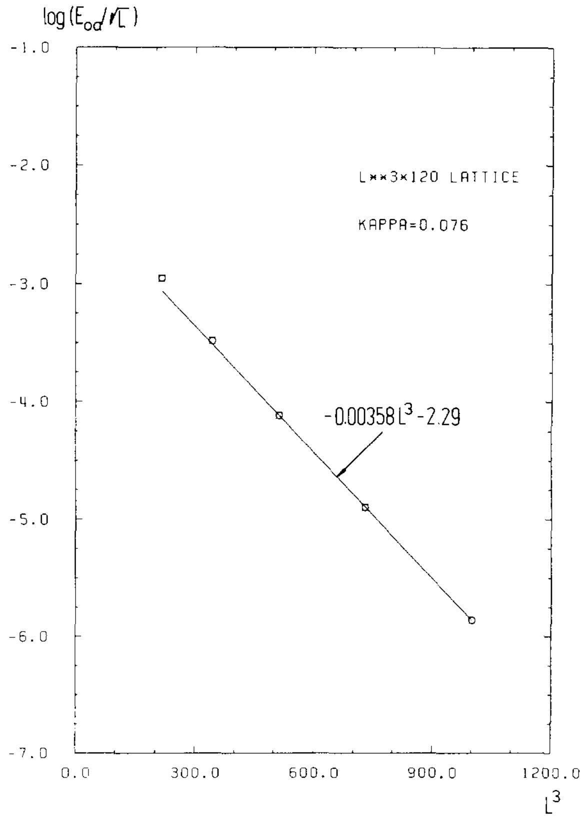

Fig. 4. The quantity log $(E_{0a}L^{-1/2})$ as a function of the volume L^3. The straight line is a fit to the points $L=8$–10

$\sigma = 0.0051$. These values are roughly consistent with the number from our fit in view of the expected higher-loop corrections. At $\kappa = 0.076$ we have determined σ also from the autocorrelation time (inverse flip rates on 8^4, 10^4 and 12^4 lattices in the Metropolis algorithm), as suggested by ref. [8]. We find $\sigma = 0.00289(7)$, which is in reasonable agreement with the value in (15).

On the lattices under consideration tunneling plays a role which is by far not negligible for the study of finite-size effects. Ultimately our aim is to extend our previous work on the symmetric phase of the Ising model [2] to the broken phase and to investigate the scaling behaviour and perturbative finite-size effects [6]. A full control of tunneling is prerequisite for a precise extrapolation to the infinite-volume limit in order to be able to make a comparison with the results of ref. [13]. From the data obtained in the present work we get information on how large the lattices have to be in order for finite-size effects to be dominated by perturbative effects instead of tunneling.

Since tunneling effects in general are fading away exponentially with the volume, once the volume is large enough they quickly disappear. Nevertheless, one has to keep in mind that some more subtle quantities could still be strongly effected even if the vacuum degeneracy is well satisfied (i.e. E_{0a} is very small). As an example, as one can see form table 1 the splitting of the one-particle energies E_{1s} and E_{1a} is still appreciable on volumes where E_{0a} is already very small. In other words, the one-particle mass is still ill-defined, although in a local updating algorithm sign flips of the average spin are very seldom. This can be understood as a consequence of tunneling of local domains even if the configuration as a whole stays in one of the vacua.

It is to be expected that the qualitative features of the finite-size effects due to tunneling are similar also in other systems with two (or more) discrete degenerate ground states. An obvious example is the finite-temperature deconfining phase transition in pure gauge theories (particularly for the SU(2) gauge field, which also has a Z_2-symmetry). More generally, tunneling can also be important near first-order phase transitions, when there are two degenerate minima of the finite-volume effective potential.

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