Tricriticality and the Blume-Capel model: A Monte Carlo study within the microcanonical ensemble

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The microcanonical partition function $\Omega_{\alpha,N}(E)$ of a three-dimensional ferromagnetic simple cubic Blume-Capel model is calculated for several coupling ratios α close to and on the first-order side of the tricritical point. To this end a single Monte Carlo simulation of a suitably extended partition function for systems of $L\times L\times L$ spins with $L\in\{8,10,12,14,18\}$ was performed. A finite system analog of the latent heat is introduced in order to define a tricritical point in finite systems as well. An empirical scaling of its coordinates to the thermodynamic limit yields $\alpha^{(t)}=2.844\,79\pm0.000\,30$ for the tricritical coupling ratio, and $k_BT^{(t)}/J=1.4182\pm0.0055$ for the tricritical transition temperature. The results are compared with values obtained on fcc lattices. [S1063-651X(97)04311-0]

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INTRODUCTION

Classical lattice spin models are among the most popular systems of interacting degrees of freedom, since amazingly simple models can account for many characteristic features of phase diagrams occuring in ''real'' experiments. This paper deals with what has become known as the *Blume-Capel model*. It is defined by the Hamiltonian

$$H(x):=-J\sum_{\langle i,j\rangle}s_i(x)s_j(x)+D\sum_i s_i^2(x) \tag{1}$$

$$=:-J\Sigma_J(x)+D\Sigma_D(x), \tag{2}$$

which maps a state x in a phase space $\Gamma_N:=\{-1,0,+1\}^{\times N}$ onto its energy. (Γ_N being the set of all possible configurations of a lattice consisting of N spins, each of which can take on the values -1, 0, or $+1$.) The notation $\Sigma_{\langle i,j\rangle}$ implies summation over all pairs of nearest-neighbor spins (this obviously depends on the topology of the lattice), and $s_i(x)$ denotes the value of the spin being located at the vertex i in the configuration x. J and D are coupling constants, whose ratio $\alpha:=D/J$ controls the thermodynamic behavior of the system. In this paper only the case $J,D>0$ is relevant.

One of the most interesting features of the Blume-Capel model is the occurrence of a *tricritical point*. A qualitative phase diagram in the plane of coupling ratio and temperature is shown in Fig. 1: The spin-ordered phase is separated from the disordered phase by a line of phase transitions, which change at the tricritical point from second to first order.

Models of this kind were first introduced in 1966 by Blume [1] and Capel [2], and since then have been investigated by methods like the mean-field approximation [1–4], series expansion [5], renormalization [6], and Monte Carlo simulation [7–9], to name but a few. An introduction to tricriticality was given in Ref. [10].

The aim of this paper is a determination of the coordinates of the tricritical point in the plane of coupling ratio and temperature for a three-dimensional ferromagnetic Blume-Capel model on a simple cubic (sc) lattice. Although $\alpha^{(t)}$ and $T^{(t)}$ are not universal quantities (i.e., they also depend on details of the lattice topology), their knowledge is helpful in the process of determining tricritical exponents. A method of localizing the tricritical point to a fairly high accuracy is described, which basically relies on conventional Monte Carlo techniques, and combines the advantages of working in the microcanonical ensemble, reweighting two-dimensional histograms and investigating the precursors of a phase transition in finite systems as a function of α. Lattices with periodic boundaries and $N=L^3$ spins with $L\in\{8,10,12,14,18\}$ were studied.

MICROCANONICAL FORMALISM

The starting point for the microcanonical treatment of finite systems will be the microcanonical partition function

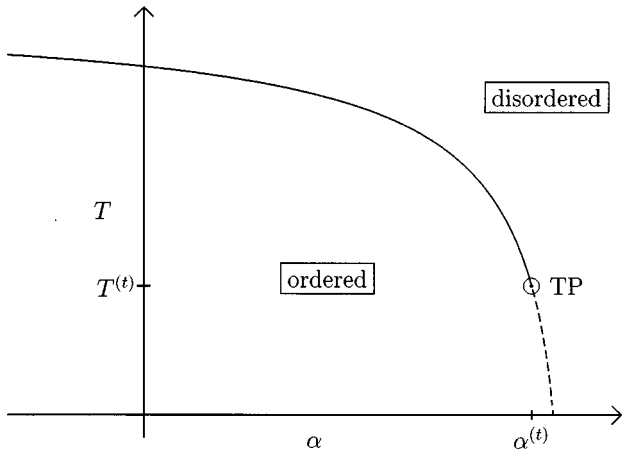

FIG. 1. Schematic phase diagram of the Blume-Capel model in the plane of coupling ratio and temperature. The solid curve is a line of second-order, the dashed curve of first-order phase transitions. They separate the spin-ordered from the disordered phase, and meet at a tricritical point (TP).

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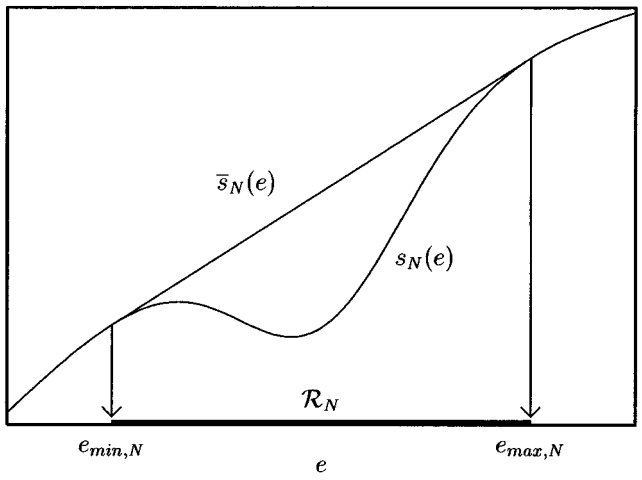

FIG. 2. Qualitative picture of an entropy $s_N(e)$, which differs on a range $\mathcal{R}_N$ from its concave envelope $\overline{s_N}(e)$, the latter being just a straight line on $\mathcal{R}_N$. For clarity, this feature has been vastly exaggerated.

and its logarithm, the specific entropy as a function of the specific energy. If we suppress the coupling α in a first step, these functions are defined as

$$\Omega_N(E) := \sum_{x \in \Gamma_N} \delta_{E,H(x)}, \tag{3}$$

$$s_N(e) := \frac{k_B}{N} \ln[\Omega_N(Ne)]. \tag{4}$$

Dependencies on further observables (like, e.g., the magnetization) are — at least for the moment — ignored. As usual, *small* letters represent *intensive* quantities. Whereas in the thermodynamic limit (which is assumed to exist) the specific entropy is a concave function of the energy, this need not be the case in *finite* systems. First, single-spin excitations may be visible in $s_N(e)$ as rapid (small scale) oscillations. However, conditions for their appearance and typical properties will not be discussed in this paper. Second, on a large scale $s_N(e)$ can be convex in a certain range of energies, and this in turn is related to the possibility of phase transitions occurring in the corresponding infinite system. The following discussion will be restricted to temperature-driven first-order phase transitions.

If $s_N(e)$ is not a concave function of the specific energy, then it will differ from its *concave envelope* $\overline{s_N}(e)$ in a certain range $\mathcal{R}_N := [e_{\min,N}; e_{\max,N}]$ of energies, and without loss of generality there shall be only one such range. $\overline{s_N}(e)$ is just a straight line on $\mathcal{R}_N$ (see Fig. 2). Now one can define three quantities related to $\mathcal{R}_N$:

$$e_N^{(\mathrm{lat})} := |\mathcal{R}_N| := e_{\max,N} - e_{\min,N}, \tag{5}$$

$$T_N^{(d)} := [d\,\overline{s}_N(e)/de]^{-1} \quad \text{for any } e \in \mathcal{R}_N, \tag{6}$$

$$\Delta s_N := \max_{e \in \mathcal{R}_N} [\overline{s}_N(e) - s_N(e)]. \tag{7}$$

They will be called FS latent heat, FS transition temperature, and FS entropy barrier, respectively, where ''FS'' stands for ''finite system'' and the label ''d'' in Eq. (6) for ''discontinuous.'' Despite its clumsiness, this choice of names is used because it alludes to the meaning of the objects, and it reminds one at the same time that a connection to a possible phase transition of the infinite system still has to be established.

The importance of these definitions relies on the following fact: The entropy of an infinite system cannot show partially convex behavior, because the system could increase its entropy inside the convex range by transferring energy from one region of the system to another, i.e., spontaneously developing local inhomogeneities and splitting up into two phases [11]. This happens without a change in energy, since the (intensive) surface energy between these phases vanishes in the thermodynamic limit (suitable short-range interactions are presupposed). The process continues, until the entropy of the system coincides with its concave envelope, which then qualitatively resembles $\overline{s_N}(e)$. However, such an entropy, with a linear part over a certain energy range, is known to describe a system with a temperature-driven first-order phase transition, and values of latent heat and transition temperature as given in Eqs. (5) and (6) (with $\mathcal{R}$ being the linear range). In a *finite* system such a phase separation cannot render a partly convex entropy completely concave, because the surface effects are not negligible. Hence a FS entropy barrier Δs_N exists, which vanishes in the thermodynamic limit and, according to its origin, it should scale like $N^{-1/d}$ (compare Ref. [12]).

Carrying out this limit does of course not reduce to merely replacing $s_N(e)$ for some arbitrary (perhaps quite small) N by its concave envelope, i.e., $\overline{s_N}(e)$ is evidently still a function of N, but the easily measurable FS quantities (5), (6) and (7) can be investigated as functions of N. In particular, if the limits

$$e^{(\mathrm{lat})} := \lim_{N \to \infty} e_N^{(\mathrm{lat})}, \tag{8}$$

$$T^{(d)} := \lim_{N \to \infty} T_N^{(d)} \tag{9}$$

exist, and $e^{(\mathrm{lat})}$ is larger than zero, then the infinite system undergoes a first-order phase transition with latent heat $e^{(\mathrm{lat})}$ at the transition temperature $T^{(d)}$. This can be seen by looking at the *canonical* partition function

$$Z_N(T) := \sum_{e \in H(\Gamma_N)/N} \exp\left\{ \frac{N}{k_B} [s_N(e) - e/T] \right\}. \tag{10}$$

For large N a Laplace evaluation of the sum becomes appropriate. If T is chosen to be $T_N^{(d)}$ from Eq. (6), the exponent $s_N(e) - e/T$ has a double-hump structure with two maxima of equal height, and small variations to higher or lower temperature give preference to the maximum at higher or lower energy. In the thermodynamic limit this results in the characteristic jump of $e(T)$ at $T = T^{(d)}$ which is equal in size to the latent heat $e^{(\mathrm{lat})}$.

One might object that the (microcanonical) FS quantities defined by Eqs. (5) and (6) correspond to a Laplace evalua-

tion of Eq. (10) for *arbitrary* N, since they rely on finding the maximum in the exponent $s_N(e)-e/T$, and hence estimate corresponding quantities derived from the (canonical) partition function $Z_N(T)$ rather poorly for *small* N. Of course that is true. Generally, microcanonical and canonical ensemble are *not* equivalent with respect to the description of finite systems. On the other hand, if the microcanonical specific entropy shows no substantial system size dependencies, the FS quantities thus defined are excellent approximations to the respective *infinite* system properties [13,14].

''SKEW SUMMING''

In the last section $s_N(e)$ was presented as the quantity encoding in a convenient way all necessary information needed for the study of phase transitions. However, the behavior of the Blume-Capel model also depends on the ratio $\alpha:=D/J$ of the coupling constants in Hamiltonian (1). This can be taken into account by defining the slightly more general microcanonical partition function

$$\Omega_{\alpha,N}(E,S_D):=\sum_{x\in\Gamma_N}\delta_{E,H(x)}\delta_{S_D,\Sigma_D(x)}, \tag{11}$$

which classifies the degree of degeneracy according to the energy *and* the value S_D of the second spin sum Σ_D in the Hamiltonian [Eqs. (1) and (2)]. The subscript α should remind one of the coupling ratio, and from now on it will be added as an index or argument, where it is needed. Note the connection

$$\sum_{S_D\in\Sigma_D(\Gamma_N)}\Omega_{\alpha,N}(E,S_D)=\Omega_{\alpha,N}(E) \tag{12}$$

between the partition functions defined in Eqs. (3) and (11).

Given a different Hamiltonian

$$H':=-J\Sigma_J+D'\Sigma_D=:H+\mathcal{D}\Sigma_D, \tag{13}$$

with H being defined in Eqs. (1) and (2) and $\mathcal{D}:=D'-D$ denoting the shift in the second coupling constant, it is possible to calculate its microcanonical partition function as a function of energy by a transformation of $\Omega_{\alpha,N}(E,S_D)$:

$$\Omega_{\alpha',N}(E'):=\sum_{\substack{E\in H(\Gamma_N)\\ S_D\in\Sigma_D(\Gamma_N)}}\delta_{E+\mathcal{D}S_D,E'}\Omega_{\alpha,N}(E,S_D). \tag{14}$$

By a suitable choice of $\mathcal{D}$, which depends on α, every new coupling ratio α' can be reached. The Kronecker δ in Eq. (14) defines a set of straight lines in the (E,S_D) plane with a constant *new* energy E'. For $\mathcal{D}\neq 0$ these summing lines are tilted against the ones for $\mathcal{D}=0$, the latter case corresponding to Eq. (12). This suggests the name ''*skew summing*'' for the procedure.

Transformations of this kind found widespread applications soon after the work of Ferrenberg and Swendsen [15,16], but have ever since usually been combined with a change to the canonical ensemble (essentially by using the exponential function instead of the Kronecker δ), which will be avoided here. [If it comes to that, the Laplace transformation from $\Omega_{\alpha,N}(E)$ to $Z_{\alpha,N}(T)$ can always be done in a second step.]

Taking the logarithm of Eq. (14) and multiplying by k_B/N one ends up with the microcanonical specific entropy of the Blume-Capel model as a function of specific energy *for any desired value of* α:

$$s_{\alpha,N}(e):=\frac{k_B}{N}\ln[\Omega_{\alpha,N}(Ne)]. \tag{15}$$

TRICRITICALITY

Localizing the tricritical point of the Blume-Capel model means finding the tricritical ratio $\alpha^{(t)}$ at which the phase transition changes between first and second order, and the corresponding tricritical transition temperature $T^{(t)}$. In order to track down these objects it is useful to define two further FS quantities, which — like the ones introduced before — are finite-system counterparts of infinite-system properties: the ''FS tricritical ratio'' $\alpha_N^{(t)}$ and the ''FS tricritical transition temperature'' $T_N^{(t)}$. For values of α larger than the tricritical ratio $\alpha^{(t)}$ (and smaller than half the coordination number of the lattice) the Blume-Capel model shows a nonzero latent heat $e^{(\mathrm{lat})}$. Similary, in the *finite* system there is a FS tricritical ratio above which a FS latent heat exists. This motivates the following definitions:

$$\alpha_N^{(t)}:=\inf\{\alpha:e_N^{(\mathrm{lat})}(\alpha)>0\}, \tag{16}$$

$$T_N^{(t)}:=\lim_{\alpha\downarrow\alpha_N^{(t)}}T_N^{(d)}(\alpha). \tag{17}$$

The construction of the latter indirectly via the limit $\alpha\downarrow\alpha_N^{(t)}$ is necessary, since the FS transition temperature from Eq. (6) is not defined for $\alpha\leqslant\alpha_N^{(t)}$. The tricritical point of the Blume-Capel model may now be obtained by *scaling the FS quantities* (16) *and* (17) *to the infinite system*.

At this point a word of caution seems appropriate. It is not too difficult to construct entropies $s_{\alpha,N}(e)$ such that $\alpha_N^{(t)}$ is a well-defined quantity and $\lim_{N\to\infty}\alpha_N^{(t)}=:\alpha^{(t)}$ exists, *although* the corresponding system does *not* show a tricritical point. [One might think of entropies, which yield a FS latent heat $e_N^{(\mathrm{lat})}(\alpha)=(\alpha-\alpha^{(t)})/N$ for $\alpha>\alpha^{(t)}$ and $e_N^{(\mathrm{lat})}(\alpha)=0$ otherwise.] The method just presented, which in the end just uses $\alpha_N^{(t)}$, only works the other way around: If one knows — for whatever reason — that a tricritical point occurs, it can be localized (apart from possible difficulties which the scaling $N\to\infty$ can impose). In other words, questions concerning the *existence* of such a point have to be treated differently. One could for instance show that in the thermodynamic limit the FS latent heat indeed remains finite on the presumed first-order side or investigate scaling properties of the FS entropy barrier [12,17]. However, in consideration of today's knowledge of the Blume-Capel model, this paper will not dwell upon this point.

MONTE CARLO SIMULATION

The remaining problem is the determination of the partition function (11). From the numerous methods devised for dealing with this perpetual task of statistical physics, this paper chooses the Monte Carlo (MC) way. Generally, if w is a probability distribution and f a function on a phase space Γ_N, one often wants to know the expectation value $\langle f\rangle_w := \mathrm{Tr}_{\Gamma_N}(wf)$ of the observable f in the state w. With $\{x\}_{M,w}$ being a collection of M elements drawn from Γ_N *according to the distribution* w, one can define

$$\mathcal{E}(f,\{x\}_{M,w}) := \frac{1}{M}\sum_{x\in\{x\}_{M,w}} f(x). \tag{18}$$

Since this has expectation value $\langle f\rangle_w$ [with respect to all possible $\{x\}_{M,w}$ samples and probability $P(\{x\}_{M,w}) = \Pi_{x\in\{x\}_{M,w}} w(x)$] and variance $(\langle f^2\rangle_w - \langle f\rangle_w^2)/M$, it can serve as an *estimate* for $\langle f\rangle_w$, because the $\{x\}_{M,w}$ sample entering on the right-hand side of (18) can be simulated on a computer by means of an ergodic Markov process with a stationary distribution w.

Many different Monte Carlo methods can be classified according to the choice of w and f. Taking, e.g., $w \propto \exp(-\beta H)$ and $f = H^n$ $(n\in\mathbb{N})$, one ''simulates'' the nth moment of the energy in the canonical ensemble. With the introduction of observables like $\delta_{E,H(x)}$ the door to histogram techniques was opened [15,16]. If, additionally, w satisfies $w(x) = \tilde{w}[H(x)]$, the microcanonical partition function (3) can be written as

$$\Omega_{\alpha,N}(E) = \frac{\langle \delta_{E,H(x)}\rangle_w}{\tilde{w}(E)} \overset{M\gg 1}{\simeq} \frac{1}{M\tilde{w}(E)}\sum_{x\in\{x\}_{M,w}} \delta_{E,H(x)}. \tag{19}$$

The special choice

$$\tilde{w}(E) \propto 1/\Omega_{\alpha,N}(E) = \exp\{-N s_{\alpha,N}(E/N)/k_B\} \tag{20}$$

obviously leads to equipartition in the sampled histogram [18,19]. (Note also the early work of Torrie and Valleau [20] on non-Boltzmann sampling distributions.) The paradox situation that the *final result* of the simulation — the microcanonical partition function — is needed in the implemented algorithm from the *very beginning* is surmounted by an iteration procedure in the starting phase and constitutes no real problem. The complete method might be called *entropic sampling with respect to the energy*.

The *two-dimensional* partition function (11) is related to the observable $\delta_{E,H(x)}\delta_{S_D,\Sigma_D(x)}$, i.e.,

$$\Omega_{\alpha,N}(E,S_D) \overset{M\gg 1}{\simeq} \frac{1}{M\tilde{w}(E)}\sum_{x\in\{x\}_{M,w}} \delta_{E,H(x)}\delta_{S_D,\Sigma_D(x)}. \tag{21}$$

Concerning the appropriate state, one might have the idea to extend Eq. (20) by performing something like entropic sampling with respect to E *and* S_D by introducing a likewise two-dimensional stationary distribution $\tilde{w}(E,S_D) \propto 1/\Omega_{\alpha,N}(E,S_D)$. This would make sure that a predeterminable range $[E_{\min};E_{\max}]\times[S_{D,\min};S_{D,\max}]$ is surveyed with a constant statistical quality. However, since $\Omega_{\alpha,N}(E,S_D)$ varies over many orders of magnitude, there would be a large number of terms in Eq. (14), which were calculated most accurately but are completely insignificant for the value of the sum. Since only the close neighborhood of the FS tricritical point is of actual interest, one can restrict oneself to small shift parameters $\mathcal{D}$ when doing the skew summing, if the simulation is performed close to $\alpha_N^{(t)}$. Then the contributing terms in Eq. (14) are almost the same as in the case $\mathcal{D}=0$. Hence it suffices to concentrate the sampling on a small range around the maxima of $\Omega_{\alpha,N}(E,S_D)$ as a function of S_D for every value of E. This is exactly what happens if the conventional one-dimensional stationary distribution is applied.

The confinement to a small region in the phase diagram and the need for a sound prior knowledge of $\alpha_N^{(t)}$ should not be regarded as a drawback, since the method is designed exactly for the purpose of enhancing ones knowledge of this small region. In addition it is in accord with the idea of *importance sampling*, for the statistical quality of the histograms is large where it is actually needed.

ESTIMATION OF ERRORS

In order to obtain quantities like the latent heat (5), the entropy derived from the MC estimate (21) and Eqs. (14) and (15) first has to be smoothed, which was done by fitting a polynomial of sufficiently high degree (typically 20–40) to the scattered data. Thereafter the necessary double tangent construction is a simple numerical business.

The attachment of error bars to the values of $e_N^{(\mathrm{lat})}$, e.g., was done by a procedure described in Ref. [21]: Since the data points scatter around the ''true'' entropy in a known way, which in this case is approximately Gaussian, it is easy to generate a large number of fictitious entropies (i.e., ones that were not the result of the MC simulation but *could have been*) from the actual entropy by adding a Gaussian noise with proper variance. The fictitious values of, say, $e_N^{(\mathrm{lat})}$ derived from this set of entropies can now be used to determine the deviations.

SIMULATION, SCALING, AND RESULTS

The Blume-Capel model was simulated on three-dimensional simple cubic lattices with periodic boundary conditions and $L\in\{8,10,12,14,18\}$. Some preliminary MC runs showed that the coupling ratio $\alpha = 2.85$ lies sufficiently close to the expected FS tricritical points, so $J=20$ and $D=57$ were selected for the Hamiltonian during the simulation. The chosen range of the energy and the number of lattice sweeps is shown in Table I.

Both the FS latent heat $e_N^{(\mathrm{lat})}(\alpha)$ and the FS entropy barrier $\Delta s_N(\alpha)$ become smaller when approaching the FS tricritical point from above. Since a clear identification of the convex part in $s_{\alpha,N}(e)$ is impossible, if $\Delta s_N(\alpha)$ gets considerably smaller than the unavoidable scatter of the measured entropy, the functions $e_N^{(\mathrm{lat})}(\alpha)$ and $T_N^{(d)}(\alpha)$ are not known

TABLE I. Chosen energy range and MC steps per spin for the five simulated Blume-Capel models. (Note that the implemented coupling constants were $J=20$ and $D=57$.)

L	$E_{\min}$	$E_{\max}$	Lattice sweeps
8	4846	6016	1.47×10^8
10	10 000	12 200	4.51×10^8
12	17 712	21 384	3.84×10^8
14	28 812	34 300	1.08×10^8
18	62 700	73 700	5.35×10^7

down to the FS tricritical point. Hence one needs extrapolations before Eqs. (16) and (17) can be used.

It was found that near the FS tricritical point the behavior of the FS latent heat is excellently described by a power law, so that the following functional form was assumed:

$$e_N^{(\mathrm{lat})}(\alpha)\propto(\alpha-\alpha_N^{(t)})^{1/\theta_N},\quad \alpha>\alpha_N^{(t)}. \tag{22}$$

Figure 3 demonstrates this for the system with $L=10$. Since Landau theory also predicts a power law for the latent heat close to the tricritical point, Eq. (22) is expected to be of general validity for tricritical behavior and not a specialty of the Blume-Capel model, although further studies on different models are certainly needed to confirm this. In any case, the fact that a nonanalytic function can be successfully fitted to *finite system* data is a typical feature of the microcanonical approach [22].

The investigated values of α were between $\frac{131}{46}\approx2.8478$ (only for $L=18$) and $\frac{20}{7}\approx2.8571$. Over this small interval the FS transition temperature appears almost as a straight line, but a functional form $T_N^{(d)}(\alpha)\propto(\alpha_N^{(0)}-\alpha)^{1/\kappa_N}$ was assumed in order to allow for a small curvature, which increases with increasing α, cf. Fig. 1.

The final task is the scaling of the FS quantities $\alpha_N^{(t)}$ and $T_N^{(t)}$ to the thermodynamic limit. For lack of a well-established scaling theory this was done empirically. The assumed functional forms were

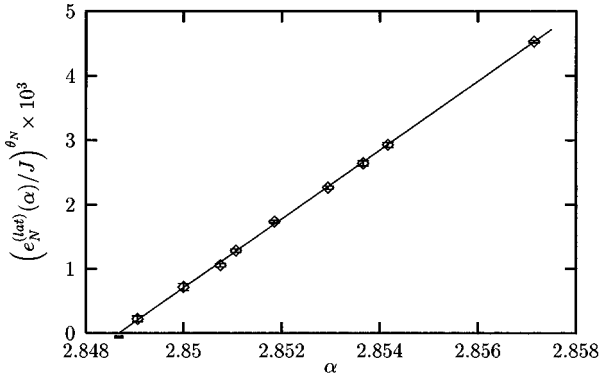

FIG. 3. Plot of the FS latent heat $e_N^{(\mathrm{lat})}$ raised to a power $\theta_N=1.982$ as a function of the coupling ratio α for the Blume-Capel system with $N=10^3$ spins. With this value of θ_N the measured values of $e_N^{(\mathrm{lat})}(\alpha)$ collapse nicely onto a straight line, confirming the functional form proposed in Eq. (22). The intersection of this line with the abscissa gives the FS tricritical point $\alpha_N^{(t)}$. The error in the latter is indicated as a horizontal bar.

TABLE II. Measured values of the FS tricritical transition temperature and the FS tricritical coupling ratio, as well as their extrapolations to the infinite system. The numbers in brackets give the error in the last digits.

L	$k_BT_N^{(t)}/J$	$\alpha_N^{(t)}$
8	1.3422(36)	2.8493(13)
10	1.362 99(31)	2.848 674(93)
12	1.375 97(35)	2.847 970(95)
14	1.384 02(69)	2.847 62(17)
18	1.394 07(58)	2.846 94(14)
∞	1.4182(55)	2.844 79(30)

$$\alpha_{L^3}^{(t)}=\alpha^{(t)}+\frac{c_1}{L}, \tag{23}$$

$$T_{L^3}^{(t)}=T^{(t)}+\frac{c_2}{L}+\frac{c_3}{L^2}. \tag{24}$$

Table II summarizes the coordinates found for the (FS) tricritical point in finite systems and the scaled values for the infinite system. Thus the best estimates for the thermodynamic limit are $\alpha^{(t)}=2.844\,79\pm0.000\,30$ and $k_BT^{(t)}/J=1.4182\pm0.0055$. (The deviations were calculated via standard error propagation in the linear fit.) The results as well as the assumed scaling functions are also plotted in Figs. 4 and 5.

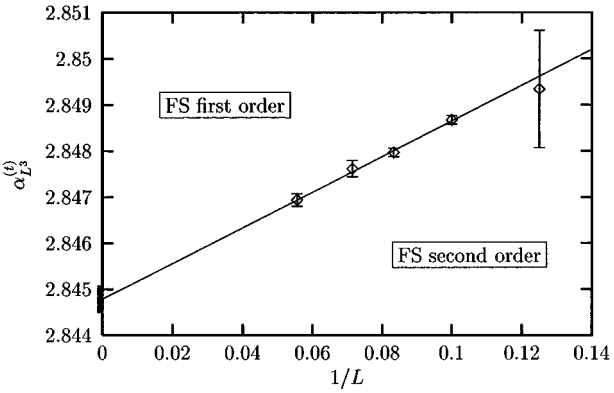

FIG. 4. Extrapolation of the FS tricritical coupling ratio $\alpha_{L^3}^{(t)}$ to the infinite system via Eq. (23). The error in $\alpha^{(t)}$ is indicated as a vertical bar on the ordinate. The comparatively large error for the system with $L=8$ has its origin in single-spin excitations, which are more pronounced in smaller systems and reduce the accuracy with which a double-hump structure in the entropy can be detected. Note that the function $\alpha_{L^3}^{(t)}$ can also be seen as a borderline between finite systems which show FS first-order transitions (above) and systems which do not (below).

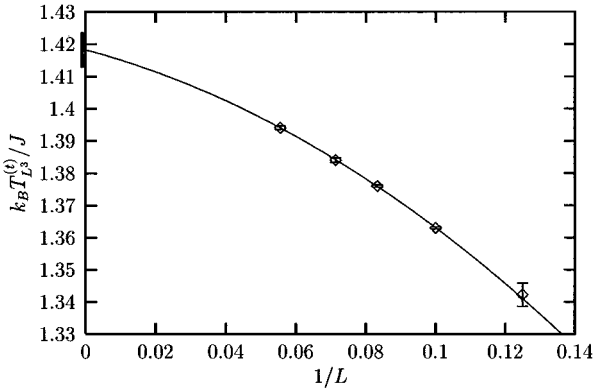

FIG. 5. Extrapolation of the FS tricritical transition temperature $T_{L^3}^{(t)}$ to the infinite system via Eq. (24). The error in $T^{(t)}$ is indicated as a vertical bar on the ordinate.

DISCUSSION

To the author's knowledge no prior studies with the aim of precisely localizing the tricritical point of the Blume-Capel model on a *simple cubic* lattice exist, so the results will be compared with those obtained on fcc lattices. Saul, Wortis, and Stauffer [5] investigated the fcc system by means of high- as well as low-temperature series expansions and found $k_B T^{(t)}/J = 3.138(84)$ for the tricritical transition temperature and $\alpha^{(t)} = 5.659(12)$ for the tricritical coupling ratio. Later Jain and Landau [7] found $k_B T^{(t)}/J = 3.072(24)$ and $\alpha^{(t)} = 5.652(48)$ within a MC study.

In a fcc lattice each spin has twice as many nearest neighbors as in a sc lattice, and mean-field theory predicts a trivial scaling of $T^{(t)}$ and $\alpha^{(t)}$ with the coordination number. However, both quantities are not universal (unlike critical exponents), and the tricritical transition temperature of the fcc lattice — reduced by a factor $\frac{1}{2}$ — is still 11% [5] or 8% [7] *higher* than its value obtained in this work with sc topology. This can be made plausible by considering that (i) for the system with larger coordination number mean-field theory might be regarded as a better approximation, and (ii) it always overestimates the transition temperature. Note that for the three-dimensional Ising model the value for $T^{(c)}$ scaled with the coordination number is about 9% larger in the fcc case compared with the sc one. (see, e.g., Ref. [23]).

Since mean-field theory underestimates the tricritical coupling ratio (for coordination number 6, $\alpha_{MF}^{(t)} = 4\ln(2) \approx 2.7726$; see, e.g., Ref. [2]), one could expect the properly scaled fcc values for $\alpha^{(t)}$ to be smaller than the sc results obtained in this paper. This is easily seen to be the case, but the difference is surprisingly small, and, in order to determine it more precisely, a reduction of the fcc error bars is needed.

There is another point to be learned from the scaling of the FS tricritical ratio. The function $\alpha_{L^3}^{(t)}(1/L)$ separates the finite systems, which show a FS latent heat, from those which do not (the latter lying under the curve, see Fig. 4). Since this function has a *positive* slope, there exist systems (e.g., $\alpha = 2.847$) which show a first-order phase transition in the thermodynamic limit, but even a microcanonical analysis cannot find a precursor if L is too small. Such a behavior is not obvious in the first place. Indeed, a simulation of the *two-dimensional* Blume-Capel model indicates that the slope of $\alpha_{L^2}^{(t)}$ plotted against $1/L$ is *negative*, i.e., sufficiently small systems show signs of a first-order transition, which do not survive in the thermodynamic limit [24].

TABLE III. FS entropy barrier $\Delta s_N(\alpha)/k_B \times 10^4$ for three coupling ratios near the tricritical point. Note that Δs_N *increases* with increasing system size, although in the limit $N \to \infty$ it must become zero for *all* values of α.

L	$\alpha = \frac{57}{20}$	$\alpha = \frac{77}{27}$	$\alpha = \frac{97}{34}$
8	0.0100(62)	0.0460(67)	0.0754(76)
10	0.0088(19)	0.0479(17)	0.0900(24)
12	0.0199(14)	0.0757(12)	0.128 38(11)
14	0.0258(13)	0.0917(15)	0.1490(18)
18	0.0432(12)	0.1228(11)	0.1905(14)

A final remark concerns the scaling of the FS entropy barrier (7). Kosterlitz and Lee [12] investigated the two-dimensional Potts model with $q \in \{8,10\}$, and found that it takes larger systems to see the expected behavior $\Delta s_N \propto 1/L$ for $q = 8$ than for $q = 10$. They conjectured that small systems obey this scaling relation only, if the transition is *strongly* first order. Since the phase transitions investigated in this paper are only just located on the first-order side of the tricritical point, any feature of a discontinuous transition can be regarded as being very weakly developed. Consequently, the proper scaling of $\Delta s_N(\alpha)$ is not only violated quantitatively but also *qualitatively*: From Table III it can be seen that — at least for the presented values of L — the specific entropy barrier *increases* with increasing system size, if α is chosen closely to $\alpha^{(t)}$. Hence, to judge the order of the phase transition from the *scaling* of $\Delta s_N(\alpha)$, and thus localize the tricritical point, is clearly inferior to the possibility of observing the ''meta order parameter'' FS latent heat as a function of α.

CONCLUSION

Given the two-dimensional microcanonical partition function $\Omega_{\alpha,N}(E,S_D)$ of the Blume-Capel model, its microcanonical entropy as a function of energy can be calculated for arbitrary values of the coupling ratio α. By defining quantities like $e_N^{(\mathrm{lat})}$ or $\alpha_N^{(t)}$, which are finite-system counterparts of infinite-system properties, it is possible to pinpoint the coordinates of the tricritical point $(\alpha^{(t)}, T^{(t)})$ in the thermodynamic limit.

It might be regarded as a drawback that the extrapolation $N \to \infty$ is done *empirically*. Nevertheless the author considers the presented FS quantities to be excellent probes for the investigation of infinite-system thermodynamic behavior (i.e., easily measurable and clearcut). A deeper understanding of their scaling characteristics undoubtly would be of great practical importance.

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