Zeros of the partition function and pseudospinodals in long-range Ising models

Natali Gulbahce
Department of Physics, Clark University, Worcester, Massachusetts 01610, USA
and Los Alamos National Laboratory, CCS-3, MS-B256, Los Alamos, New Mexico 87545, USA

Harvey Gould
Department of Physics, Clark University, Worcester, Massachusetts 01610, USA

W. Klein
Los Alamos National Laboratory, X-7 Material Science, Los Alamos, New Mexico 87545, USA
and Department of Physics, Boston University, Boston, Massachusetts 02215, USA
(Received 2 September 2003; published 31 March 2004)

The relation between the zeros of the partition function and spinodal critical points in Ising models with long-range interactions is investigated. We find that the spinodal is associated with the zeros of the partition function in four-dimensional complex temperature/magnetic field space. The zeros approach the real temperature/magnetic field plane as the range of interaction increases.

DOI: 10.1103/PhysRevE.69.036119 PACS number(s): 64.60.Fr, 05.50.+q, 05.70.Fh, 75.10.Hk

I. INTRODUCTION

Mean-field treatments of fluids and Ising models yield metastable and unstable regions, separated by a well-defined line known as the spinodal [1]. As the spinodal is approached, the system shows phenomena similar to that at mean-field critical points. In particular, the isothermal susceptibility χ in an lsing model diverges as a power law as the spinodal value of the magnetic field h_s is approached from the metastable state [2],

$$\chi \propto (h_s - h)^{-1/2}, \tag{1}$$

where h is the (dimensionless) magnetic field. A mean-field Ising system can be realized in a well-defined way by assuming an infinite-range interaction between the spins [1].

If the interaction range is long but finite, the system is no longer mean field, but can be described as near mean field, and the spinodal singularity is replaced by a pseudospinodal, which still has physical effects. As with apparent critical points in finite-size systems, the susceptibility for a finite interaction range can be fit to a power law over a limited range of the scaling field $(h_s - h)$. For example, the susceptibility in the metastable state of a long but finite-range interaction Ising model appears to diverge over several decades in $(h_s - h)$ as the pseudospinodal is approached [3]. However, the divergence is suppressed if the pseudospinodal is approached too closely, indicating that the spinodal singularity has been smeared out [3]. It is also found that the properties of the pseudospinodal converge rapidly with increasing interaction range to those predicted for the spinodal in mean field theory [4].

Because the spinodal is a line of critical points, we expect that the Ising spinodal has properties similar to those of the Ising critical point. In particular, we expect that the spinodal is related to the zeros of the partition function. Lee and Yang [5] showed that the singularity in the free energy for T less than T_c, the critical temperature, arises from the presence of a real positive zero of the partition function in the thermodynamic limit. In finite systems there is no real positive zero for $T < T_c$.

The zeros of the partition function for real temperature T lie on the imaginary axis of the complex magnetic-field plane [6]. For finite systems there is a gap in the distribution of the zeros around $h = 0$. This gap shrinks to zero for $T < T_c$ as $N \to \infty$. The Lee-Yang relation between the zeros of the partition function and critical points is valid for all interaction ranges at the Ising critical point. These ideas were extended to complex temperature by Fisher and collaborators [7].

In order to generalize these ideas to spinodals in Ising models, we consider an Ising model in a magnetic field h. We will consider the "infinite-range" Ising model in which each spin interacts with all other spins [8], and the Domb-Dalton [9] version of the Ising model in which each spin interacts with its neighbors within a given interaction range R with a constant interaction. These models can be described by mean-field theory in the limits $N \to \infty$ and $R \to \infty$ (for N infinite), respectively. Our main result is that the pseudospinodal is related to the zeros of the partition function in four-dimensional complex temperature/magnetic field space. In addition, the zeros approach the real temperature/magnetic field plane as the system becomes more mean field.

The structure of the paper is as follows. In Sec. II we consider the infinite-range Ising model and show both analytically and numerically that the zeros of the partition function approach the real β and h plane as N increases. We find a similar result in Sec. III by estimating the partition function in the metastable state by using the Metropolis algorithm and the single histogram method. In Sec. IV we consider the Domb-Dalton version of the Ising model and estimate the partition function in the metastable state using the same numerical techniques.

II. THE INFINITE-RANGE ISING MODEL: ANALYTICAL APPROACH

We first consider an Ising model in which every spin interacts with every other spin. We will refer to this model as

the infinite-range Ising model [8], although the interaction range becomes infinite only in the limit $N\to\infty$. The Hamiltonian is

$$H=-J_N\sum_{i\neq j=1}^{N}\sigma_i\sigma_j-h\sum_i\sigma_i. \tag{2}$$

We need to rescale the interaction so that the total interaction energy seen by a given spin remains the same as N is increased [1]. We will take

$$J_N=\frac{4J}{N-1}. \tag{3}$$

This choice of J_N yields the Ising mean-field critical temperature $T_c=4$ when $N\to\infty$ [9], where we have chosen units such that $J/k=1$.

The exact density of states is easily calculated for this model and is given by

$$g(M)=\frac{N!}{n!(N-n)!}, \tag{4}$$

where n is the number of up spins. We have $M=2n-N$ and the total energy $E=J_N(N-M^2)/2$, where M is the magnetization. [In general, the density of states depends on both E and M, but because E is a unique function of M in the infinite-range Ising model, we need to only write $g(M)$.] Hence the partition function Z can be expressed analytically for arbitrary complex inverse temperatures β and magnetic fields h:

$$Z(\beta,\beta h)=\sum_{\text{all M}}g(M)e^{-\beta E}e^{\beta hM}. \tag{5}$$

To understand the nature of Z in the metastable state, imagine a simulation of an Ising model in equilibrium with a heat bath at inverse temperature β in the magnetic field $h=h_0>0$. Because $h_0>0$, the magnetization values will be positive. Then we let $h\to-h_0$. If h_0 is not too large, the system will remain in the metastable state for a reasonable amount of time and sample positive values of M. Hence, to determine the zeros of Z associated with the pseudospinodal, we need to restrict the sum in Eq. (5) to magnetization values M that are representative of the metastable state. The following examples will illustrate the need for this restriction and the procedure for determining the zeros of Z.

The notion of using a restricted partition function sum to describe the metastable state has a long history. Penrose and Lebowitz [10,11] review such restricted partition functions and their properties. A more physical approach can be found in the discussion of the noninteracting droplet model by Langer [12]. In this model fluctuations are restricted to noninteracting compact droplets of the stable phase occurring in the metastable phase. The partition function sum is restricted to droplets less than the critical size. This approximation is reasonable for low temperatures close to the coexistence curve. Langer showed that this restriction gives the same metastable state free energy as the analytic continuation of the stable state free energy in the same model. However, there are additional properties of the analytic continuation that do not appear in the restricted sum which are related to the decay of the metastable state rather than the description of the metastable state itself.

We first consider $N=4$ and retain only the terms in the partition function sum that correspond to the two positive values of M. From Eqs. (4) and (5), we have

$$Z_r(\beta,\beta h)=\sum_{M=2,4}g(M)e^{-\beta E}e^{\beta hM}=e^{8\beta}e^{-4\beta h}+4e^{-2\beta h}. \tag{6}$$

The subscript r denotes that the sum over M is restricted. If we let $x=e^{-2\beta h}$, the equation $Z_r=0$ is equivalent to

$$e^{8\beta}x+4=0, \tag{7}$$

and has the solution

$$\beta h=-\ln 2-i\frac{\pi}{2}+4\beta. \tag{8}$$

In general, we have four unknowns (the real and imaginary parts of β and h); Eq. (8) yields two conditions. In the following we will fix

$$\mathrm{Re}\,\beta=9/16, \tag{9}$$

which is equivalent to a temperature of $T=\frac{4}{9}T_c$. For this value of T, the value of the spinodal magnetic field is known to be $h_s\approx 1.2704$ [13]. Equation (7) then gives a line of zeros in complex $(\beta,\beta h)$ space. However, if we are interested only in the zero closest to the real β, βh plane, we need a fourth condition. This condition is found by requiring that the quantity,

$$D^2=(\mathrm{Im}\,\beta)^2+(\mathrm{Im}\,\beta h)^2, \tag{10}$$

be a minimum, which is equivalent to requiring that the leading zero of Z_r, the zero closest to the real β and βh plane, be as close to this plane as possible. If we let $y=\mathrm{Im}\,\beta$ and use Eq. (8), we can rewrite D^2 as

$$D^2=y^2+\left(-\frac{\pi}{2}+4y\right)^2. \tag{11}$$

Because we want D^2 to be a minimum, we require

$$\frac{dD^2}{dy}=2y+2\left(-\frac{\pi}{2}+4y\right)(4)=0. \tag{12}$$

The solution is

$$y=\mathrm{Im}\,\beta=\frac{2\pi}{17}\approx 0.3696, \tag{13}$$

and $D=0.380\,97$. Note that $\mathrm{Re}\,T=\mathrm{Re}\,\beta/(\mathrm{Re}\,\beta^2+\mathrm{Im}\,\beta^2)=1.2417$. We finally use Eq. (8) to obtain the value of complex h. The result is summarized in the first row of Table I.

TABLE I. Results for the infinite-range Ising model if all positive values of M are retained in Z. For larger N, $|\mathrm{Re}\, h|$ overshoots $h_s = 1.27$ and goes to zero as N is increased still further.

N	$\mathrm{Im}\,\beta$	$\lvert\mathrm{Re}\, h\rvert$	$\mathrm{Im}\, h$	D
4	0.3696	1.8577	1.3849	0.3810
9	0.1704	1.1987	0.4782	0.1823
16	0.1070	1.1359	0.2926	0.1153
100	0.0145	0.8854	0.0366	0.0164
1000	0.0014	0.8335	0.0035	0.0016

The solutions for $N=9$, 16, 100, and 1000, keeping all the positive M contributions to the partition function, also are shown in Table I. We see that although D becomes smaller as N is increased, $|\mathrm{Re}\, h|$ overshoots the mean-field value of $h_s \approx 1.27$ (for $\beta = 9/16$). Hence, retaining all the positive M terms in the partition function allows the system to explore more than the metastable state, and we need to further restrict the sum over values of M. Physically we want to exclude values of M that would drive the system to the stable phase.

What are the appropriate values of the magnetization that will keep the system in the metastable state? One way to determine these values is to look at $P(M)$, the probability that the system has magnetization M for a particular value of β and h:

$$P(M) = g(M) e^{-\beta E} e^{\beta h M}. \tag{14}$$

Figure 1 shows $P(M)$ for a system of $N=400$ spins for $h = -1.0$ and $\beta = 9/16$. The negative magnetization values have a relatively high probability (because $h<0$) and correspond to the stable phase. The positive values of magnetization have a much lower probability, and the peak at $M = 360$ corresponds to the most probable value of M in the metastable state. In between the peak at $M=-400$ and the peak at $M=360$, $P(M)$ has a minimum at $M_{\min}=192$ for this value of h and an inflection point at $M_I = 298$. We will only include values of the magnetization in the partition function sum that are greater than M_I.

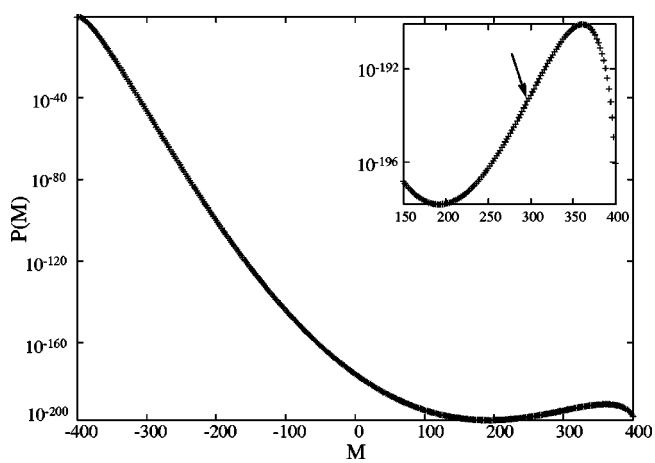

FIG. 1. The probability of the magnetization, $P(M)$, obtained from Eq. (14) for the infinite-range Ising model with $N=400$, $h = -1.0$, and $\beta = 9/16$. The values of $P(M)$ are plotted on a log-linear scale because of the dominance of the negative values of M. We include terms in the partition function sum over M from the inflection point of $P(M)$ at $M_I = 298$ to $M=400$ in the partition function. The inset shows the region where the inflection point is (see arrow).

The reason for this choice of the cutoff has to do with the nature of metastability. We expect that $P(M) \propto \exp(-\beta F(M))$, where $F(M)$ is the metastable state free energy. We want to exclude from the partition function values of M that correspond to states which are not characteristic of equilibrium. In the infinite-range model the configurations with $M_{\min} < M < M_I$ are unstable in that the initial evolution of a fluctuation does not monotonically decay to the metastable well. This behavior translates into an initial growth of fluctuations rather than the monotonic decay expected in equilibrium.

This behavior is a consequence of the fact that the free energy, which is proportional to $\log(P(M))$, is not convex for these values of M. Obviously, this behavior holds for a range of values of $M < M_{\min}$ as well. However, we can exclude all configurations with $M < M_{\min}$ because they are in the stable free energy well and do not occur in the metastable state. Our particular choice of the cutoff is well defined, but is arbitrary to some extent as long as M is greater than M_I.

To determine M_I, we calculate the second derivative of $P(M)$ as given in Eq. (14). We find the value of M that satisfies

$$\frac{\partial^2 P(M)}{\partial M^2} = \frac{-N}{(N-M)(N+M)} + \beta J = 0. \tag{15}$$

Clearly there will be two inflection points (see Fig. 1). We choose the one closest to the metastable state maximum of $P(M)$. We find that the value of M_I is independent of h, which is consistent with the idea that the free energy for this system can be written in the Landau-Ginzburg form where the magnetic field appears only in a term linear in M.

We now write the restricted partition function $Z_r(\beta, \beta h)$ as

$$Z_r(\beta, \beta h) = \sum_{M=M_I}^{N} C_M x^{M/2}. \tag{16}$$

The coefficients C_M extend over a wide range of values and are as large as 10^{200} for the values of N that we considered. For this reason we computed C_M to arbitrary precision so as not to lose accuracy. The zeros of Z_r, which is a polynomial in x, were found using MPSOLVE [14,15].

For a given value of $\mathrm{Im}\,\beta$, we solve for the zeros of Z_r in Eq. (16) and find the value of x that corresponds to the leading zero, the zero that minimizes D in Eq. (10). We repeat this step for a range of values of $\mathrm{Im}\,\beta$ and determine numerically the value of $\mathrm{Im}\,\beta$ that yields the minimum value of D. The typical dependence of D on $\mathrm{Im}\,\beta$ is shown in Fig. 2. From Fig. 2 we see that for $N=400$, D is a minimum for $\mathrm{Im}\,\beta \approx 0.035$. Once we know this value of $\mathrm{Im}\,\beta$, we solve

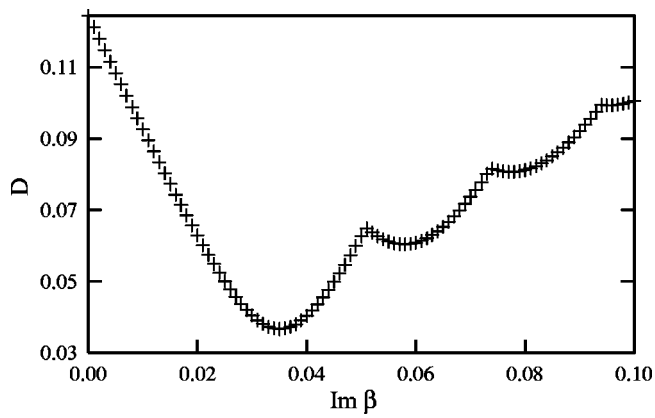

FIG. 2. The value of D, a measure of the distance of the leading zero to the real β and βh plane, vs $\mathrm{Im}\,\beta$ for the infinite-range Ising model for $N=400$. The minimum distance to the real axes occurs at $\mathrm{Im}\,\beta \approx 0.035$ for this value of N.

for h from the relation $h=\log x/(-2\beta)$. (The value of x was determined from the solution of $Z_r=0$.)

We repeat the above steps for a range of values of N and obtain D, $\mathrm{Im}\,\beta$, $\mathrm{Re}\,h$, and $\mathrm{Im}\,h$. Our results are summarized in Table II. Note that $\mathrm{Im}\,h$, $\mathrm{Im}\,\beta$, and D decrease as N increases and $|\mathrm{Re}\,h|$ approaches $h_s=1.27$. A plot of the zeros of Z for the infinite-range Ising model in the $\mathrm{Im}\,x$, $\mathrm{Re}\,x$ plane is shown in Fig. 3. The values of D listed in Table II are plotted as a function of N in Fig. 4. Because this log-log plot indicates a power-law dependence, we write

$$D \propto N^{-a}. \tag{17}$$

A least-squares fit gives $a=0.659\pm0.003$. The estimate of the error is only statistical.

Our numerical result for the exponent a can be understood by a simple scaling argument. In order for a mean-field approach, including the idea of a spinodal, to be a reasonable approximation, the system must satisfy the Ginzburg criterion, that is, the Ginzburg parameter G must be much greater than unity. For the infinite-range Ising model, the Ginzburg criterion can be written as [16]

TABLE II. Values of M_I/N, $|\mathrm{Re}\,h|$, $\mathrm{Im}\,h$, $\mathrm{Im}\,\beta$, and the distance D for increasing values of N for the infinite-range Ising model. As explained in the text, the inflection point of $P(M)$ determines M_I, the cutoff for M. Note that $|\mathrm{Re}\,h|$ approaches $h_s=1.27$ and M_I/N approaches $m_s=0.745\,356$. For $N=4\,000\,000$, $M_I/N=0.745\,356$.

N	M_I/N	$\mathrm{Im}\,\beta$	$\lvert\mathrm{Re}\,h\rvert$	$\mathrm{Im}\,h$	D
100	0.7400	0.086	1.1601	0.2257	0.0902
400	0.7450	0.035	1.2125	0.0949	0.0367
800	0.7450	0.022	1.2322	0.0603	0.0230
1200	0.7450	0.017	1.2407	0.0453	0.0176
1600	0.7450	0.014	1.2456	0.0375	0.0145
2400	0.7458	0.011	1.2508	0.0280	0.0112

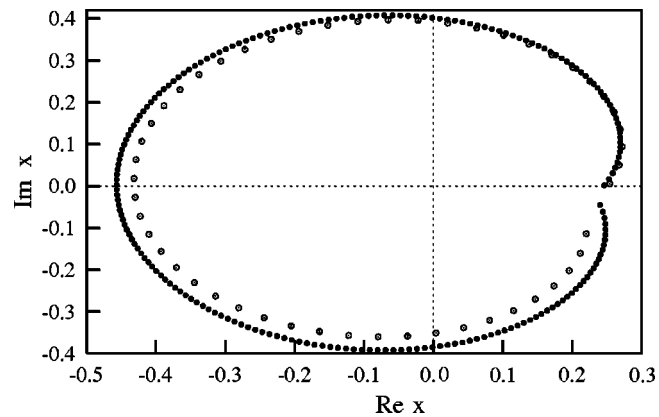

FIG. 3. The imaginary vs the real part of the zeros of the partition function plotted in terms of the variable $x=e^{-2\beta h}$ for $N=400$ (empty circles) and 1600 (filled circles) for the infinite-range Ising model. The zeros were obtained by the analytical method described in Sec. II using $\mathrm{Im}\,\beta$ listed in Table II.

$$\frac{\xi^d \chi}{\xi^{2d}\phi^2} \ll 1, \tag{18}$$

where ξ is the correlation length, ϕ is the order parameter, and d is the spatial dimension. We have $\chi \sim \Delta h^{-1/2}$ and $\phi \sim \Delta h^{1/2}$ [2], where $\Delta h = h_s - h$, and obtain

$$G=\xi^d \Delta h^{3/2} \gg 1. \tag{19}$$

For the infinite-range model, $N \sim \xi^d$. Hence,

$$G=N\Delta h^{3/2}, \tag{20}$$

up to a constant of order unity. The Ginzburg parameter G is a measure of how mean field the system is for finite N; the larger the value of G, the more mean field the system is. If we keep G constant as we approach the spinodal, we see that

$$\Delta h \propto N^{-2/3}. \tag{21}$$

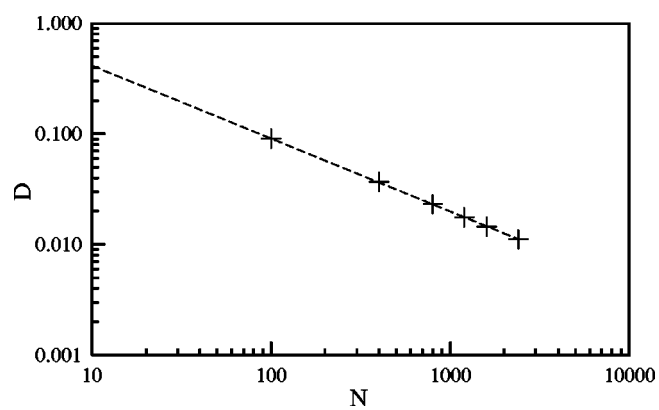

FIG. 4. Log-log (base 10) plot of D, the distance of the leading zero of the partition function to the real β-βh axes [see Eq. (10)], vs the system size N, using the analytical approach described in Sec. II. The slope is -0.659 ± 0.003. The data are from Table II.

We present an argument for why G should be held constant in Sec. V.

From Eq. (21) we see that Δh and the distance D approach zero with an exponent $a=2/3$, in good agreement with our numerical result. Because Δh in Eq. (21) could be associated with $\mathrm{Im}\,h$, $(h_s-|\mathrm{Re}\,h|)$, or D, we note that $\mathrm{Im}\,h$ in Table II goes to zero with the same exponent as in Eq. (17). We also find that $(h_s-|\mathrm{Re}\,h|)\propto N^{-0.61}$.

III. THE INFINITE-RANGE ISING MODEL: MONTE CARLO APPROACH

In general, the partition function is not known analytically. However, we can use a Monte Carlo (MC) method to determine the density of states from which we can determine an estimate of the partition function. Such an approach has been used to find the density of states for the nearest-neighbor Ising model [17,18]. In this way the leading partition function zeros at the critical point have been computed, and the critical exponent ν and corrections to scaling have been found with high precision [18]. Our goal is not to obtain precise estimates of the critical exponents near the pseudospinodal, but to show that the same simulations that show an apparent divergence in the susceptibility also yield an estimate for the leading zero of the partition function which behaves as expected as the system becomes more mean field.

To this end we use the Metropolis algorithm to equilibrate the system at temperature $T=16/9$ and applied magnetic field $h=h_0$ for about 100 MC steps per spin. (The system equilibriates as quickly as 10 MC steps per spin depending on the strength of the field.) Then we flip the magnetic field and compute the histogram $H(E,M)$ from which we determine the density of states $g(E,M)$ and the partition function for complex β and h. We save the values of M after $h\rightarrow -h_0$ and run until M changes sign or for 5000 MC steps per spin, whichever comes first. We then throw away the first 20% of the data to ensure that the system is in metastable equilibrium and the last 20% of the data to ensure that we do not retain values of M that are too close to the stable state. The remaining 60% of the run is used to obtain $H(E,M)$. We also omit any run whose lifetime in the metastable state is less than 100 MC steps per spin. Our results for $H(E,M)$ are not sensitive to the choice of the minimum lifetime nor the percentage of each run that we use to estimate $H(E,M)$. [Because E is a function of M for the infinite-range Ising model, we need only to compute $H(M)$. However, we need to compute $H(E,M)$ in Sec. IV.] We averaged $H(E,M)$ over ≈ 5000 runs for each value of h_0 for a total of $\approx 1.5\times 10^7$ MC steps per spin for a given value of h and N. Our results for the susceptibility χ are given in Fig. 5. As mentioned in Sec. I, χ shows an apparent divergence with a mean-field exponent of 1/2 until the pseudospinodal is approached too closely.

Given the histogram $H(E,M)$ at $\beta_0=9/16$ and $h=-h_0$, we use the usual single histogram method [19] and express the partition function for arbitrary (complex) β and h as

$$Z_m(\beta,\beta h)=\sum_{E,M} H(E,M)e^{(\beta_0-\beta)E}e^{-(\beta_0 h_0-\beta h)M}. \quad (22)$$

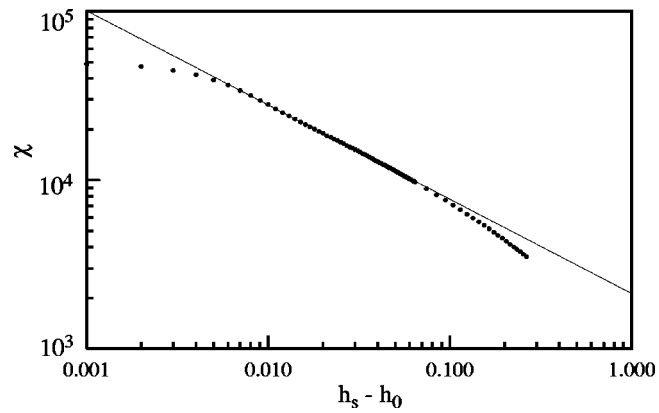

FIG. 5. Log-log (base 10) plot of the isothermal susceptibility χ as a function of (h_s-h_0) for the infinite-range Ising model with $N=10\,000$. The system was equilibrated using the Metropolis algorithm at a temperature $T=16/9$ and applied field $h=h_0$. Then the field was flipped and the values of the magnetization were sampled in the metastable state. Note that χ exhibits mean-field behavior over about two decades and the apparent divergence of χ at the spinodal field $h_s=1.27$ is rounded off when (h_s-h_0) becomes too small. This behavior is an example of the influence of a pseudospinodal. The straight line with a slope of 1/2 is drawn as a guide to the eye.

Note that we do not have to determine the lower cutoff for M because the Monte Carlo simulation only samples values of M while the system is in a metastable state [noted by the subscript m in Eq. (22)]. As h_0 is increased for fixed N, the distance D initially decreases, but then begins to increase as h_s is approached too closely, that is, D shows a minimum as a function of h_0. For each of value of N we choose the value of h_0 for which D is a minimum. A comparison of the histogram that was determined analytically in Sec. II and estimated by the Metropolis Monte Carlo algorithm shows a similar qualitative behavior, except that the latter is approximately a Gaussian and extends to lower values of M (see Table III), but with a smaller amplitude.

Table III shows our results for h, $\mathrm{Im}\,\beta$, and D for a range of values of N at the values of h_0 that minimize the distance

TABLE III. Results from Monte Carlo simulations of the infinite-range Ising model. The simulations were done in the applied field $-h_0$ and at the inverse temperature 9/16. The values of h_0 for each value of N were chosen so that the distance D to the real β-βh plane is a minimum. As noted in the text, this criterion for h_0 also yields metastable state lifetimes that are roughly constant for the different values of N. The values of M_{cut} represent the smallest values of M that were sampled in the metastable state.

N	h_0	M_{cut}/N	τ	$\mathrm{Im}\,\beta$	$\lvert\mathrm{Re}\,h\rvert$	$\mathrm{Im}\,h$	D
128	0.9	0.23	4808	0.0144	1.181	0.0165	0.0163
400	1.0	0.44	>5000	0.0070	1.196	0.0095	0.0076
800	1.1	0.56	>5000	0.0050	1.229	0.0063	0.0056
2400	1.205	0.59	4995	0.0026	1.256	0.0043	0.0027
4000	1.226	0.63	4992	0.0021	1.264	0.0033	0.0022
8000	1.246	0.65	4908	0.0016	1.269	0.0024	0.0017

D. A log-log plot of D versus N for the data in Table III is shown in Fig. 6; a least-squares fit gives $a=0.60\pm0.03$, which is consistent with the result obtained using the exact density of states (with a cutoff). Note that τ, the average lifetime of the metastable state, for each value of N is approximately a constant at the value of h_0 that was chosen to minimize D (see Fig. 7). We will use this fact to choose the value of h_0 for the long-range Ising model in Sec. IV.

IV. LONG-RANGE TWO-DIMENSIONAL ISING MODEL

As discussed in Sec. I, the susceptibility of long-range Ising models in the metastable state shows an apparent divergence as the applied magnetic field is increased. In the following we show that this effect of a pseudospinodal in long-range Ising models is reflected in the behavior of the zeros of the partition function as a function of the complex temperature and magnetic field. We will show that as the interaction range R increases, the leading zero moves closer to the real plane.

Following Refs. [1] and [9], we consider an Ising model such that each spin interacts with its neighbors within a given interaction range R with a constant interaction $J=4/q$, where q is the number of interaction neighbors. (The factor 4 is included so that $J=1$ for the usual Ising model on the square lattice.) If the thermodynamic limit is taken first [1], the system is mean field in the $R\rightarrow\infty$ limit, and the system is described by Curie-Weiss theory [11]. In this limit the metastable state ends at a spinodal point. The spinodal is a critical point and the susceptibility χ diverges as in Eq. (1).

We consider the Ising system on a square lattice with linear dimension $L=240$ and $N=57\,600$. The interaction range R is defined such that a given spin interacts with any spin that is within a circle of radius R. The number of neighbors of a given spin is shown in the second column of Table IV. This system is large enough (L is 10 times larger than the maximum value of R) for finite-size effects to be minimal, but the finite size of the system implies that the zeros of the partition function must be complex for any range R.

As in Sec. III, we equilibrate the system at inverse temperature $\beta=9/16$ and applied magnetic field h_0 for 100 MC steps per spin. Then we flip the field and compute the histogram $H(E,M)$ from which we determine the density of states $g(E,M)$ and the partition function for complex β and h. The most time consuming part of our procedure is determining the appropriate value of h_0. Although we could determine h_0 by minimizing D as in Sec. III, we instead determined the mean lifetime τ of the metastable state as a function of h_0. For small h_0 (away from the spinodal), τ is greater than the duration of our runs which are 2×10^4 Monte Carlo steps per spin. As h_0 approaches h_s, the lifetime begins to decrease. As mentioned in Sec. III, we found that the values of h_0 that minimize D are near h_s and also yield approximately constant lifetimes for different values of N. (This behavior was found for both the infinite- and long-range Ising models.) We choose the largest value of h_0 for which the mean lifetime of the metastable state just begins to decrease below 2×10^4 Monte Carlo steps per spin. This criterion for choosing h_0 is not as sensitive as minimizing D, but is much quicker, although some additional error is intro-

TABLE IV. Summary of results for the Ising model with interaction range R on the square lattice with linear dimension $L=240$. The number of neighbors q within an interaction range R is given in the second column. The value of h_0 is determined for each R by choosing the lifetime of the metastable state to be $\approx2\times10^4$ MC steps per spin. The duration of each run was 2×10^4 MC steps per spin and each run was repeated 10^3 times. Because we did not use the first and last 20% of each run, the total number of MC steps per spin for each value of R was 1.2×10^7.

R	q	h_0	$\mathrm{Im}\,\beta$	$\lvert\mathrm{Re}\,h\rvert$	$\mathrm{Im}\,h$	D
6	112	0.95	0.0036	0.992	0.0084	0.0038
8	196	1.05	0.0035	1.011	0.0071	0.0035
12	440	1.18	0.003	1.199	0.0078	0.0031
15	708	1.215	0.0025	1.230	0.0055	0.0026
18	1008	1.235	0.0013	1.252	0.0039	0.0014
24	1792	1.248	0.00095	1.259	0.0022	0.0010

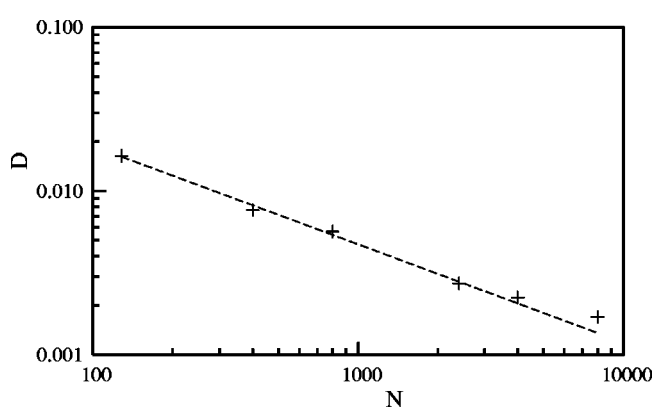

FIG. 6. Log-log (base 10) plot of D, the distance of the leading zero of the partition function to the real axes, vs the system size N for the infinite-range Ising model obtained from Monte Carlo simulations. A least-squares fit gives a slope of -0.60 ± 0.03. The data are from Table III.

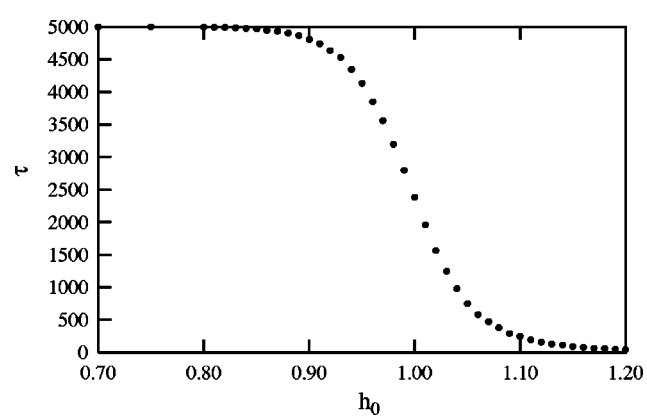

FIG. 7. The lifetime τ of the metastable state in the infinite-range Ising model as a function of the applied field h_0 for $N=128$. The behavior of τ for the long-range Ising model considered in Sec. IV is similar, and for the latter we choose h_0 to be the field at which $\tau(h_0)$ just begins to decrease sharply.

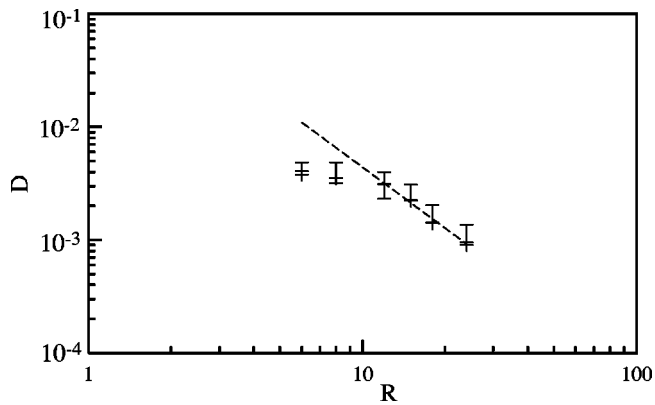

FIG. 8. Log-log (base 10) plot of the distance D to the real β-βh axes vs the interaction range R for the two-dimensional Ising model. Note that the leading zero of the partition function moves closer to the real axes as the system becomes more mean field. A least-squares fit gives a slope of -1.8 ± 0.3. The data are from Table IV.

duced when h_0 is chosen this way. For a given h_0, 10^3 runs of 2×10^4 MC steps per spin were done to determine the histogram $H(E,M)$.

The resulting values of the distance D as a function of the interaction range R are listed in Table IV and are plotted in Fig. 8. We find

$$D\propto R^{-1.8\pm0.3}. \tag{23}$$

The largest contribution to the above error estimate arises from the uncertainty in the values of the applied fields h_0. Similarly, we find that the difference (h_s-h_0) varies with R as (see Fig. 9)

$$h_s-h_0\propto R^{-1.97\pm0.06}. \tag{24}$$

The scaling behavior of $(h_s-|\mathrm{Re}\,h|)$ is similar. The systematic error due to the uncertainty in h_0 is the largest contribution to the error estimates.

The scaling behavior of D and h_s-h_0 can be understood by a scaling argument similar to that given in Sec. II. For a finite-range system, the Ginzburg parameter is [13]

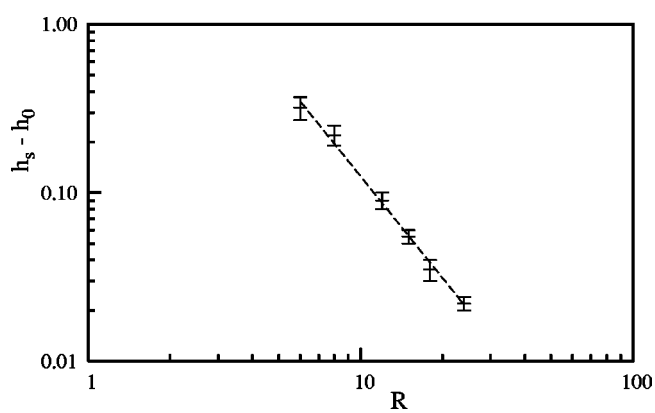

FIG. 9. Log-log (base 10) plot of the difference h_s-h_0 as a function of the interaction range R. A least-squares fit gives a slope of -1.97 ± 0.06. The data are from Table IV.

$$G=R^d\Delta h^{3/2-d/4}. \tag{25}$$

For two dimensions, Eq. (25) becomes

$$G=R^2\Delta h. \tag{26}$$

Hence, if we keep the Ginzburg parameter fixed, we conclude that

$$\Delta h\propto R^{-2}, \tag{27}$$

which is consistent with Eqs. (23) and (24).

V. DISCUSSION

We have shown that the pseudospinodal in Ising models has a well-defined thermodynamic interpretation and can be associated with the leading zero of the partition function in complex temperature/magnetic field space in analogy with the behavior of the Ising critical point in finite systems. Our results for the nature of the approach of the leading zero of the partition function to the real temperature and magnetic-field plane are consistent with simple scaling arguments.

An essential ingredient in the scaling arguments was the condition that the Ginzburg parameter G was held constant as the system approached the pseudospinodal. As was seen in Sec. III, choosing the value of h_0 that minimizes the distance of the leading zero to the real temperature/magnetic field plane also leads to a metastable state lifetime that is found numerically to be constant. From nucleation theory near the spinodal, we know that the lifetime of the metastable state, τ, is given by [2]

$$\tau\propto\frac{\Delta h^{1/2}e^G}{R^d\Delta h^{-d/4}}, \tag{28}$$

where G is defined in Eq. (25). For large G and R as well as small Δh (close to the pseudospinodal), it is easily shown that constant τ implies constant G. To see this relation we simply replace R by $R+\delta R$ and Δh by $\Delta h+\delta h$ in Eq. (28) and demand that τ remains constant. For δR and δh small, constant τ implies constant G. Because G is constant, the scaling arguments of Secs. III and IV follow.

The relation between the zeroes of the partition function and the spinodal provides a mathematical foundation for the notion of a pseudospinodal and clarifies the extent to which spinodals act like critical points. It also provides a possible route by which pseudospinodals in supercooled liquids can be characterized [20].

ACKNOWLEDGMENTS

We would like to thank Greg Johnson and Frank Alexander for very useful discussions. This work was carried out in part at Los Alamos National Laboratory (LA-UR 03-5959) under the auspices of the Department of Energy and supported by Grant No. LDRD-2001501 and was supported in part by the National Science Foundation under Grants Nos. PHY99-07949 and PHY98-01878.

[1] M. Kac, G. Uhlenbeck, and P.C. Hemmer, J. Math. Phys. **4**, 216 (1963).
[2] C. Unger and W. Klein, Phys. Rev. B **29**, 2698 (1984).
[3] D.W. Heermann, W. Klein, and D. Stauffer, Phys. Rev. Lett. **49**, 1262 (1982).
[4] M.A. Novotny, W. Klein, and P.A. Rikvold, Phys. Rev. B **33**, 7729 (1986).
[5] C.N. Yang and T.D. Lee, Phys. Rev. **87**, 404 (1952).
[6] T.D. Lee and C.N. Yang, Phys. Rev. **87**, 410 (1952).
[7] M.E. Fisher, in *Lectures in Theoretical Physics*, edited by W.E. Brittin (University of Colorado Press, Boulder, 1965), Vol. 7c, p.1.
[8] E. Milotti, Phys. Rev. E **63**, 026116 (2001).
[9] C. Domb and N.W. Dalton, Proc. Phys. Soc. London **89**, 859 (1966).
[10] O. Penrose and J. Lebowitz, in *Fluctuation Phenomena*, edited by E. Montroll and J. Lebowitz (Elsevier, Amsterdam, 1979).
[11] O. Penrose and J. Lebowitz, J. Stat. Phys. **3**, 211 (1971).
[12] J.S. Langer, Ann. Phys. (N.Y.) **41**, 108 (1967).
[13] L. Monette and W. Klein, Phys. Rev. Lett. **68**, 2336 (1992).
[14] D.A. Bini and G. Fiorentino, "MPSOLVE: Numerical computation of polynomialroots–Version 2.0, FRISCO report (1998), see http://www.dm.unipi.it/~bini/papers/mps2.html.
[15] MPSOLVE 2.2 is a multiprecision polynomial root finder. The software is available at http://fibonacci.dm.unipi.it/~bini/ric.html.
[16] L.D. Landau and E.M. Lifshitz, *Statistical Physics*, 3rd ed., edited by J.B. Sykes and M.J. Kearsley (Pergamon, New York, 1980), Vol. 1.
[17] G. Bhanot, R. Salvador, S. Black, P. Carter, and R. Toral, Phys. Rev. Lett. **59**, 803 (1987).
[18] N.A. Alves, J.R. Drugowich de Felicio, and U.H.E. Hansmann, J. Phys. A **33**, 7489 (2000).
[19] A.M. Ferrenberg and R.H. Swendsen, Phys. Rev. Lett. **61**, 2635 (1988).
[20] N. Grewe and W. Klein, J. Math. Phys. **18**, 1729 (1977); W. Klein, H. Gould, R. Ramos, I. Clejan, and A. Mel'cuk, Physica A **205**, 738 (1994).