Zeros of the Partition Function and Pseudospinodals in Long-Range Ising Models

Natali Gulbahce
Clark University, Department of Physics, Worcester, MA 01610 and
Los Alamos National Laboratory, CCS-3, MS-B256, Los Alamos, NM 87545

Harvey Gould
Clark University, Department of Physics, Worcester, MA 01610

W. Klein
Los Alamos National Laboratory, X-7 Material Science, Los Alamos NM 87545 and
Boston University, Department of Physics, Boston, MA 02215

The relation between the zeros of the partition function and spinodal critical points in Ising models with long-range interactions is investigated. We find 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.

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 $\chi$ diverges as a power law as the spinodal value of the magnetic field $h_s$ is approached from the metastable state [2],

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

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 also is 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 \(T < T_c\), 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. This ideas were extended to complex temperature by 
Fisher \([7]\).

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 limit \(N \to \infty\) 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. \([1]\) we consider the infinite-range Ising 
model and show both analytically and numerically that the zeros of the partition function
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

\[
H = -J_N \sum_{i \neq j = 1}^{N} \sigma_i \sigma_j - h \sum_i \sigma_i.
\]

(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

\[
J_N = \frac{4J}{N - 1}.
\]

(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

\[
g(M) = \frac{N!}{n!(N - n)!},
\]

(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 only write \(g(M)\).) Hence the partition function \(Z\) can be expressed analytically for arbitrary complex inverse temperatures \(\beta\) and magnetic fields \(h\):

\[
Z(\beta, \beta h) = \sum_{\text{all } M} g(M) e^{-\beta E} e^{\beta h M}.
\]

(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 \(\beta\) 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
non-interacting droplet model by Langer [12]. In this model fluctuations are restricted to
non-interacting 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

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

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,

$$e^{8\beta} x + 4 = 0, \quad (7)$$

and has the solution

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

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

$$\text{Re} \beta = 9/16, \quad (9)$$

which is equivalent to a temperature of $T = \frac{4}{15}T_c$. 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 $\beta$, $\beta h$ plane, we need a fourth condition. This condition is found by requiring that the quantity,

$$D^2 = (\text{Im} \, \beta)^2 + (\text{Im} \beta h)^2,$$

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

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

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

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

The solution is

$$y = \text{Im} \, \beta = \frac{2\pi}{17} \approx 0.3696,$$

and $D = 0.38097$. Note that $\text{Re} \, T = \text{Re} \, \beta / (\text{Re} \, \beta^2 + \text{Im} \, \beta^2) = 1.2417$. We finally use Eq. (8) to obtain the value of complex $h$. The result is summarized in the first row of Table I.

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, $|\text{Re} \, h|$ 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 $\beta$ and $h$:

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

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
$M_{\text{min}} = 192$ 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 $M_I$.

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 $M_{\text{min}} < M < M_I$ 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 $M < M_{\text{min}}$ as well. However, we can exclude all configurations with $M < M_{\text{min}}$ 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

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

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

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

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 $\text{Im} \beta$, 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 $\text{Im} \beta$ and determine numerically the value of $\text{Im} \beta$ that yields the minimum value of $D$. The typical dependence of $D$ on $\text{Im} \beta$ is shown in Fig. 2. From Fig. 2 we see that for $N = 400$, $D$ is a minimum for $\text{Im} \beta \approx 0.035$. Once we know this value of $\text{Im} \beta$, we solve 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 $D$, $\text{Im} \beta$, $\text{Re} h$, and $\text{Im} h$. Our results are summarized in Table II. Note that $\text{Im} h$, $\text{Im} \beta$, and $D$ decrease as $N$ increases and $|\text{Re} h|$ approaches $h_s = 1.27$. A plot of the zeros of $Z$ for the infinite-range Ising model in the $\text{Im} x$, $\text{Re} x$ 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

$$D \propto N^{-a}. \quad (17)$$

A least squares fit gives $a = 0.659 \pm 0.003$. 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

$$\frac{\xi^d \chi}{\xi^{2d} \phi^2} << 1, \quad (18)$$

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

$$G = \xi^d \Delta h^{3/2} >> 1. \quad (19)$$

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

$$G = N \Delta h^{3/2}, \quad (20)$$

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

$$\Delta h \propto N^{-2/3}. \quad (21)$$

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

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 $\nu$ 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 equilibrates 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 $\beta$ 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 approximately 5000 runs for each value of $h_0$ for a total of approximately $1.5 \times 10^7$ MC steps per spin for a given value of $h$ and $N$. Our results for the susceptibility $\chi$ are given in Fig. 3.
As mentioned in Sec. I, $\chi$ shows an apparent divergence with an 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) $\beta$ and $h$ as:

$$Z_m(\beta, \beta h) = \sum_{E, M} H(E, M) e^{(\beta_0-\beta)E} e^{-(\beta_0 h_0-\beta h)M}.$$  \hspace{1cm} (22)

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 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. \[xx note change xx\]

Table III shows our results for $h$, Im $\beta$, and $D$ for a range of values of $N$ at the values of $h_0$ that minimize the distance $D$. A log-log plot of $D$ versus $N$ for the data in Table III is shown in Fig. 6. A least squares fit gives $a = 0.60 \pm 0.03$, which is consistent with the result obtained using the exact density of states (with a cutoff). Note that $\tau$, 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. II 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.

FollowingRefs. 1 and 4, 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 $R \to \infty$ 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 $\chi$ diverges as in Eq. (1).

We consider the Ising system on a square lattice with linear dimension $L = 240$ and $N = 57600$. 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 $\beta$ 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 $\tau$ of the metastable state as a function of $h_0$. For small $h_0$ (away from the spinodal), $\tau$ is greater than the duration of our runs which are $2 \times 10^4$ 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 $2 \times 10^4$ 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 introduced when $h_0$ is chosen this way. For a given $h_0$, $10^3$ runs of $2 \times 10^4$ 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

$$D \propto R^{-1.8 \pm 0.3}.$$  \hspace{1cm} (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)

$$h_s - h_0 \propto R^{-1.97\pm0.06}.$$  \hspace{1cm} (24)

The scaling behavior of $(h_s - |\text{Re} h|)$ 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

$$G = R^d \Delta h^{3/2-d/4}.$$  \hspace{1cm} (25)

For two dimensions, Eq. (25) becomes

$$G = R^2 \Delta h.$$  \hspace{1cm} (26)

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

$$\Delta h \propto R^{-2},$$  \hspace{1cm} (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, $\tau$, is given by

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

(28)

where $G$ is defined in Eq. (25). For large $G$ and $R$ as well as small $\Delta h$ (close to the pseudospinodal), it is easily shown that constant $\tau$ implies constant $G$. To see this relation we simply replace $R$ by $R + \delta R$ and $\Delta h$ by $\Delta h + \delta h$ in Eq. (28) and demand that $\tau$ remain constant. For $\delta R$ and $\delta h$ small, constant $\tau$ 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 LDRD-2001501 and was supported in part by the National Science Foundation under grants 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 1979).

[11] O. Penrose and J. Lebowitz, J. Stat. Phys. 3, 211 (1971).

[12] J. Langer, Annals of Phys. 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 polynomial roots – Version 2.0, FRISCO report (1998), <http://www.dm.unipi.it/~bini/papers/mps2.html>.

[15] MPSolve 2.2 is a multi-precision 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, translated by J. B. Sykes and M. J. Kearsley (Pergamon, New York, 1980), Vol. 1, 3rd ed.

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

| $N$ | Im $\beta$ | $|\text{Re } h|$ | 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 |

TABLE II: Values of $M_I/N$, $|\text{Re } h|$, Im $h$, 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 $|\text{Re } h|$ approaches $h_s = 1.27$ and $M_I/N$ approaches $m_s = 0.745356$. For $N = 4000000$, $M_I/N = 0.745356$.

| $N$ | $M_I/N$ | Im $\beta$ | $|\text{Re } h|$ | 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|
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 $\beta$-$\beta h$ 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 $M_{\text{cut}}$ represent the smallest values of $M$ that were sampled in the metastable state.

| $N$ | $h_0$ | $M_{\text{cut}}/N$ | $\tau$ | $\text{Im } \beta$ | $|\text{Re } h|)$ | $\text{Im } h$ | $D$ |
|-----|-------|-------------------|-------|-------------------|-----------------|------------|-----|
| 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 |

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 approximately $2 \times 10^4$ MC steps per spin. The duration of each run was $2 \times 10^4$ 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 $1.2 \times 10^7$.

| $R$ | $q$ | $h_0$ | $\text{Im } \beta$ | $|\text{Re } h|)$ | $\text{Im } h$ | $D$ |
|-----|-----|-------|-------------------|-----------------|------------|-----|
| 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. 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$_{10}$-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).
FIG. 2: The value of $D$, a measure of the distance of the leading zero to the real $\beta$ and $\beta h$ plane, versus $\text{Im}\, \beta$ for the infinite-range Ising model for $N = 400$. The minimum distance to the real axes occurs at $\text{Im}\, \beta \approx 0.035$ for this value of $N$.

FIG. 3: The imaginary versus 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 $\text{Im}\, \beta$ listed in Table II.
FIG. 4: Log-log (base 10) plot of $D$, the distance of the leading zero of the partition function to the real $\beta - \beta h$ axes (see Eq. (10)), versus the system size $N$, using the analytical approach described in Sec. II. The slope is $-0.659 \pm 0.003$. The data is from Table II.

FIG. 5: Log-log (base 10) plot of the isothermal susceptibility $\chi$ as a function of $(h_s - h_0)$ for the infinite-range Ising model with $N = 10000$. 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 $\chi$ exhibits mean-field behavior over about 2 decades and the apparent divergence of $\chi$ 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.
FIG. 6: Log-log (base 10) plot of $D$, the distance of the leading zero of the partition function to the real axes, versus the system size $N$ for the infinite-range Ising model obtained from Monte Carlo simulations. A least squares fit gives a slope of $-0.60 \pm 0.03$. The data is from Table III.

FIG. 7: The lifetime $\tau$ 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 $\tau$ 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 $\beta-\beta h$ axes versus 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 $-1.8 \pm 0.3$. The data is from Table IV.

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 $-2.01 \pm 0.07$. The data is from Table IV.