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Analytic Continuation at First-Order Phase Transitions

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We study the analytic structure of thermodynamic functions at first-order phase transitions in systems with short-range interactions and in particular in the two-dimensional Ising model. We analyze the nature of the approximation of the $d = 2$ system by an $N \times \infty$ strip. Investigation of the structure of the eigenvalues of the transfer matrix in the vicinity of $H = 0$ in the complex H plane allows us to define a new function which provides rapidly convergent approximations to the stable free energy f and its derivatives for all $H \geqslant 0$. This new function is used for numerical calculation of the coefficients C_n in the power series expansions of the magnetization m in the form $m(H) = 1 + \sum C_n(H - H_0)^n$ for various $H_0 \geqslant 0$. The resulting series are studied by conventional methods. We confirm recent series analysis results on the existence of the droplet model type essential singularity at $H = 0$. Evidence is found for a spinodal at $H = H_{sp}(T) < 0$.

KEY WORDS: First-order phase transitions; analytic continuation; metastable states; Ising model; essential singularity; spinodal.

1. INTRODUCTION

The problem of analytic continuation of thermodynamic functions arises when metastable phases are described. The theory of metastability at first-order phase transitions is a challenging subject for which a complete understanding is still lacking. Several rigorous results are available[1–3] in the simplest models (see Ref. 1 for a review), as well as negative results in more general situations.[4] Most of the known methods are approximate or phenomenological. Historically, the simplest approach to metastability is obtained with the mean-field type models: van der Waals (liquid–gas) and

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Currie–Weiss (ferromagnet), from which much of our intuition on metastability comes.

The droplet model,[5,6] which accounts for the nucleation processes phenomenologically by considering the most probable compact dropletlike configurations, predicts an essential singularity[8] of thermodynamic functions at the coexistence curve. Therefore an analytic continuation to the metastable region, if possible, must be performed by going to complex field values. The nature of this singularity is of considerable theoretical interest and was studied recently by several methods in the two-dimensional Ising model. Lattice models with the ferromagnetic transition are usually the simplest to be investigated because the nature of the transition is well understood, the position of the coexistence line is known ($H = 0$, where H is the magnetic field), and also because the spontaneous symmetry breaking (of the $H \leftrightarrow -H$ symmetry), which is associated with this first order phase transition, is easily recognized and visualized.

The method of Ref. 8 is based on the analysis of renormalization group flows in the vicinity of the $T = 0$, $H = 0$ fixed point (see also Ref. 9 for a discussion of such flows) and predicts a singularity at $H = 0$. There is some controversy[10] over whether this method gives the form of the singularity consistent with different variants of the droplet model.

Another approach is based on series analysis methods.[11–13] Recently, a long low-temperature series was derived[13] at two specific temperatures. This series was used in Ref. 11 to calculate the coefficients of the power series expansion of the magnetization $m(H)$ in powers of H. The resulting series is apparently divergent and the nature of the divergence is consistent with the predictions of the field theoretic droplet model type calculations.[14] The presence of the singularity at $H = 0$ was confirmed by the analysis[12] of the high-field series at two specific temperatures.

These recent series analysis[11–13] did not find an indication of another possible singularity: the spinodal line at $H = H_{sp}(T) < 0$ (we consider the case when the $H \geqslant 0$ stable branch is continued to the $H < 0$ metastable region), which is conjectured on the basis of mean-field and other phenomenological models.[15,16] It was apparently observed for $T \simeq T_c^-$ in high-temperature series analysis.[17,18] In fact the spinodal cannot be a physically sharp singularity [such that the susceptibility χ diverges as $(H - H_{sp})^{-\sigma}$] because when the correlation length ξ within the metastable phase exceeds the radius R of the critical droplet this phase is destroyed by fluctuations.[19] However, it may well be the case that there is a behavior characteristic of a smoothed second-order phase transition (as if the system were in a finite volume $\sim R^d_{H = H_{sp}(T)}$). It has been noted[20,21] that for $H \simeq H_{sp}(T)$, the description of metastable phase using an analytic continuation of equilibrium thermodynamic functions is not applicable and the dynamical nature of metastability becomes important. These observations were made on the basis of detailed dynamical considerations.[20,21] By contrast in the analysis of *finite* power series the spinodal may manifest itself as a sharp singularity.[18,22]

A method of analytic continuation that uses the eigenvalues of the transfer matrix (TM) was suggested in Ref. 23 and was further developed in Ref. 24. The TM is defined for a finite $N \times \infty$ strip with periodic boundary conditions. For $N \leqslant 11$ satisfactory agreement was found between the "metastable" magnetization calculated by this method and by Monte Carlo simulation. Information on the positions of "crossings" (regions of near degeneracy between different TM eigenvalues) suggested an essential singularity at $H = 0$. However, the low N intuition of the TM model probably breaks down for higher N values (as was found in a quantum mechanical model[25] with similar analytic properties).

In the present work we develop in detail a new scheme of extrapolation of finite N results to the $N \to \infty$ limit, a short account of which was presented in Ref. 19. In Section 2 a preliminary discussion is combined with an introduction of the necessary notation and with a summary of the relevant results on the properties of the TM eigenvalues (from the TM model[23,24] and from the exact solution[26,27] at $H = 0$). In Section 3 we complete the derivation of the formalism.

In Section 4, we apply the method to calculate numerically the first ten coefficients in the expansion of the magnetization in powers of H. We work with N's up to $N = 9$. For such N values the calculation converges in the low-temperature range $u \leqslant 0.3u_c$ (where $u \equiv e^{-4\beta}$ and $u_c = 3 - 8^{1/2}$) and we confirm the result of Ref. 11 on the divergence of the power series and thus the existence of the singularity of the droplet model type at $H = 0$.

In Section 5, we calculate the first ten coefficients in the expansion of the magnetization in powers of a variable $x \equiv H - H_0$, for various $H_0 > 0$ (on the stable side). In the low-temperature range, we analyze the series for χ'/χ by the Padé method and find evidence for a spinodal. Its temperature dependence is studied. Our calculation is apparently the first study of the spinodal line in the low-temperature range.

Our method relies heavily on the fact that the "mathematical mechanism" of the phase transition (long-range order) when $N \to \infty$ in the $d = 2$ Ising model is due to the asymptotic degeneracy between the two largest eigenvalues of the TM. This point was emphasized in Ref. 28, where a class of $d = 1$ and 2 models was studied. Our method is applicable to models with such an asymptotic eigenvalue degeneracy. In particular, it can be generalized to d-dimensional ferromagnetic spin systems with short-range interactions, which will be approximated by $N_1 \times N_2 \times \cdots \times N_{d-1} \times \infty$ "strips."

Section 6 is a short summary.

2. MIXING THE EIGENVALUES

We consider the two-dimensional Ising model. The energy of the configuration $\{\sigma\}$ of the "spins" $\sigma_{ij} = \pm 1$ on an $N \times M$ lattice (with periodic boundary conditions $i + N \equiv i$ and $j + M \equiv j$) is

$$E\{\sigma\} = -\sum_{i=1}^{N}\sum_{j=1}^{M} \sigma_{ij}(\sigma_{i,j+1} + \sigma_{i+1,j} + H) \tag{2.1}$$

The $2^N \times 2^N$ TM is defined between two column configurations $\sigma \equiv (\sigma_1, \ldots, \sigma_N)$ and $\sigma' \equiv (\sigma_1', \ldots, \sigma_N')$

$$(\mathrm{TM})_{\sigma\sigma'} = (\mathrm{TM})_{\sigma'\sigma} = \exp\left[\frac{\beta}{2}\sum_{i=1}^{N}(\sigma_i\sigma_{i+1} + \sigma_i'\sigma_{i+1}' + 2\sigma_i\sigma_i' + H\sigma_i + H\sigma_i')\right] \tag{2.2}$$

where $\beta = 1/T$ is the inverse temperature [note that $\sigma_{N+1} \equiv \sigma_1$ and $\sigma_{N+1}' \equiv \sigma_1'$ in Eq. (2.2)]. The partition function Z of the $N \times M$ system and the free energy per spin f are

$$Z = \sum_{\{\sigma\}} e^{-\beta E\{\sigma\}} = \mathrm{Tr}\left[(\mathrm{TM})^M\right] = \sum_{j=1}^{2^N} \lambda_j^{(N)M} \tag{2.3}$$

$$f_{N\times M} = -(1/\beta MN)\log Z = -(1/\beta MN)\log\left[\sum_{j=1}^{2^N}\lambda_j^{(N)M}\right] \tag{2.4}$$

where $\lambda_j^{(N)}$ are the eigenvalues of TM in nonincreasing order ($\lambda_1^{(N)} > \lambda_2^{(N)} \geqslant \lambda_3^{(N)} \geqslant \cdots$). The free energy of the $N \times \infty$ strip is obtained as a limit ($M \to \infty$) of Eq. (2.4):

$$f_1^{(N)} = -(1/\beta N)\log\lambda_1^{(N)} \tag{2.5}$$

We will now consider briefly the analytic properties of $f_1^{(N)}(H)$ for a fixed temperature in the range $0 < T < T_c$. $\lambda_1^{(N)}(H)$ is a branch of the analytic function whose other branches are some of the lower $\lambda_j^{(N)}$'s. The choice of the relevant $\lambda_j^{(N)}$'s is simplified by the observation that they (and $\lambda_1^{(N)}$) have eigenvectors which belong to the completely symmetric representation of the group of symmetry operations of the TM. The TM is invariant under translations along the columns (due to periodic boundary conditions); this symmetry is discussed in Ref. 24. An additional symmetry is that of changing the order of spins in a column; $(\sigma_1, \ldots, \sigma_N) \to$

$(\sigma_N, \ldots, \sigma_1)$. We employed both symmetries in our numerical work; this restricts the number of the eigenstates that must be considered to 3, 4, 6, 8, 13, 18, 30, 46 for $N = 2, \ldots, 9$, respectively. In the following discussion we mean by TM the restriction to the invariant subspace, and

$$\lambda_1^{(N)} > \lambda_2^{(N)} > \lambda_3^{(N)} > \cdots \tag{2.6}$$

denote the eigenvalues in that subspace in decreasing order. The corresponding branches of the free energy analytic function are

$$f_j^{(N)} = -(1/\beta N)\log\lambda_j^{(N)} \tag{2.7}$$

Consider first the $T \to 0$ limit of the $f_i^{(N)}$'s. It easy to see from Eq. (2.2) that the $f_j^{(N)}$'s at $T = 0$ are straight lines of the form

$$2a_j/N + Hb_j/N \tag{2.8}$$

where a_j and b_j are integers satisfying

$$-N \leqslant a_j \leqslant N - \left[1 - (-1)^N\right]/2, \qquad -N \leqslant b_j \leqslant N \tag{2.9}$$

[not all (a_j, b_j) pairs are realized].

The situation is illustrated in Fig. 1a, where the eigenvalues are plotted in the $N = 3$ case. The "stable" free energy $f_1^{(N)}$ is (for any N)

$$f_1^{(N)}(T \to 0) = -2 - |H| \tag{2.10}$$

and corresponds to the lower of the branches $-2 \pm H$. The eigenvalue which gives $f_+^{(N)} = -2 - H$ describes the stable branch for $H \geqslant 0$ and its continuation to the $H < 0$ region. In both regions the corresponding eigenvector consists purely of the $(+ + \cdots +)$ state.

For small finite temperatures the situation changes appreciably only in the crossing regions (see Fig. 1b for $N = 3$ case). The degeneracies are broken and to each near degeneracy there corresponds an exact degeneracy in the complex H plane at a pair of the complex conjugate branch points close to the real axis. For $H \gtrsim \Delta^{(N)}$ (where $\Delta^{(N)}$ is the size of the "central" near crossing between $f_1^{(N)}$ and $f_2^{(N)}$ at $H = 0$; we discuss $\Delta^{(N)}$ in detail later) the stable $f_1^{(N)}$ is the branch with the largest positive magnetization ($m_j^{(N)} \equiv -f_j^{(N)}$), part a of $f_1^{(N)}$ in Fig. 1b, and the corresponding eigenvector is close to a pure $(+ \cdots +)$ state. On the negative side $H \lesssim -\Delta^{(N)}$ and between the relevant near crossings such an eigenvector is still associated with the branch of the largest positive magnetization, parts b, c, d of $f_2^{(N)}, f_3^{(N)}, f_4^{(N)}$ in Fig. 1b. The path $a \to b \to c \to d$ of Fig. 1b, for example, may be followed continuously in the complex H plane and is presumably related to the metastable continuation. References 23 and 24 may be consulted for further exploration of this program, numerical work, and a discussion of more complicated cases (e.g., the near crossing between

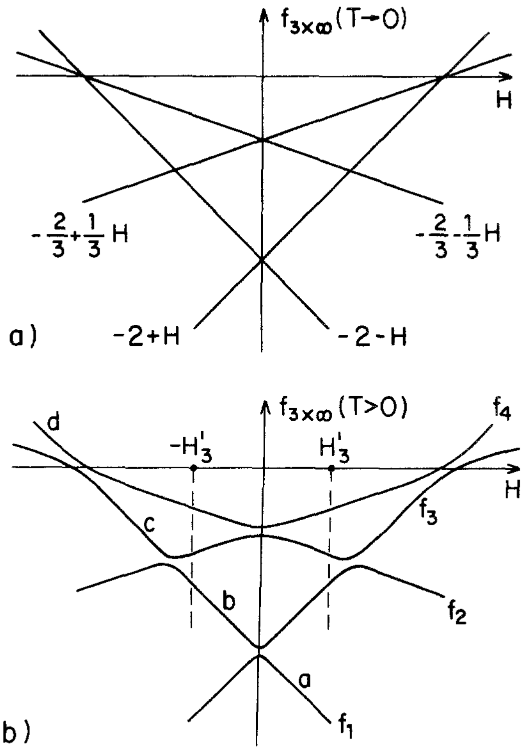

Fig. 1. (a) The free energy branches for $N = 3$ in the $T \to 0$ limit; (b) the free energy branches for $N = 3$ for a small $T > 0$ (the notation is explained in Section 2; superscript N is suppressed).

more than two free energy curves). The single near-crossing picture breaks down (for fixed $T > 0$) at higher N values[25] (for Ising model we found by explicit calculation of the first noncentral near degeneracy that the correct condition is $N \gg u^{-1}$, note that $u_c^{-1} \simeq 6$). The branch points in the complex H plane do not approach the negative H axis.[25] Therefore the identification of the metastable continuation along the real $H < 0$ axis runs into difficulties. Analytic continuation can still be performed using a dispersion relation but the domain of analyticity obtained in this way probably does not include the negative H axis.

In order to perform analytic continuation to the metastable region $H < 0$ we must go directly through the complex plane. To perform such a continuation efficiently we first consider the following question: is $f_1^{(N)}$ the best object to be used even on the stable side $H \geqslant 0$? The answer is negative.[19] The reason for this is in that the derivatives $D^k f_1^{(N)}$ (where $D \equiv \partial/\partial H$) behave badly at $H = 0$, and there is a region of nonuniformity of size $\sim\Delta^{(N)}$ at $H=0$. In order to clarify this property, let us consider the following qualitative picture.

In the infinite N system the $H \leftrightarrow -H$ symmetry is spontaneously broken: the free energy f consists of two branches f_+ and f_- (Fig. 2a):

$$f_+(H) = f_-(-H) \tag{2.11}$$

each one presumably has a metastable continuation (see Fig. 2a). Let us consider, however, the stable f as one symmetric function with a cusp at

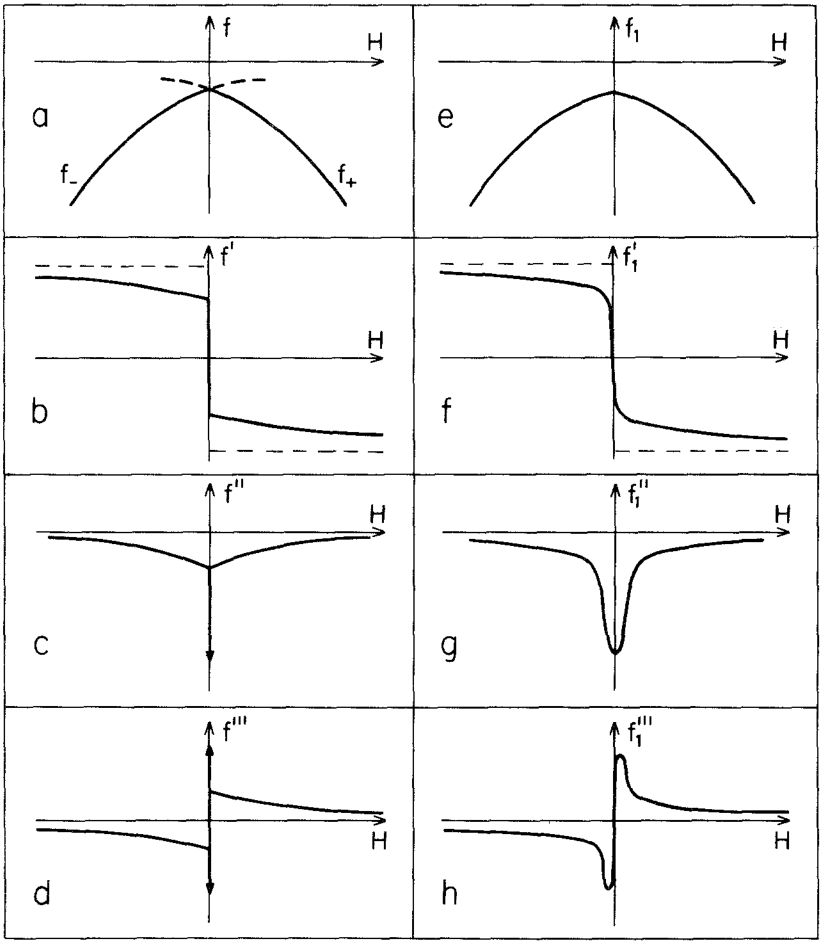

Fig. 2. (a–d) The free energy f of the $N=\infty$ system and its derivatives f', f'', f''', respectively (f consists of two branches $f_\pm$); (e–h) the free energy $f_1^{(N)}$ of a finite N system and its corresponding derivatives f_1', f_1'', f_1''' (superscript N is suppressed).

$H = 0$. In Figs. 2b–d we plot schematically the first three derivatives of f. $f' = -m$ has a discontinuity (twice the spontaneous magnetization) at $H = 0$. $f'', f''', \ldots$ have contributions proportional to a δ function and its successively higher derivatives (represented by arrows in Figs. 2c, d). For finite N the symmetric $f_1^{(N)}$ approximates this behavior, see Figs. 2e–h. $f_1^{(N)''}, f_1^{(N)'''}, \ldots$ perform rapid fluctuations in the vicinity of $H = 0$. In order to study this behavior quantitatively we note first that $f_1^{(N)}$ and $f_2^{(N)}$ are asymptotically degenerate at $H = 0$ in the $N \to \infty$ limit. The gap size $\Delta^{(N)}$ is[26]

$$\Delta^{(N)} = \left[f_2^{(N)}(0) - f_1^{(N)}(0) \right]/2 \propto e^{-C(T)N}/N \tag{2.12}$$

(for fixed $T < T_c$) and vanishes much faster than other relevant "sizes" of the problem. In particular, we expect

$$H_N' \propto \text{const}/N \tag{2.13}$$

where $\pm H_N'$ are H values at which $f_2^{(N)}$ encounters higher branches (Fig. 1b). For large N this encounter of $f_2^{(N)}$ with $f_3^{(N)}, \ldots$ may not be a separate near degeneracy. Let us stress that Eq. (2.13) is not rigorously established, but is an assumption supported by the observation that the encounter of $f_2^{(N)}$ with higher branches is typical fluctuation ($\sim 1/N$) effect, and by the known fact[26] that $f_3^{(N)}(0) - f_2^{(N)}(0) \propto 1/N$ plus the expectation that the $f_i^{(N)}$'s have finite derivatives (magnetizations) outside the "mixing" region $|H| = O(\Delta^{(N)})$. Note also that for fixed N the $T \to 0$ limit of H_N' is $2/(N-1)$.

The behavior of $f_1^{(N)}$ and $f_2^{(N)}$ for $|H| < H_N'$ is governed by the central near degeneracy. In this region $f_{1,2}^{(N)}$ are effectively a two-level system and may be phenomenologically parameterized by the two eigenvalues of the matrix

$$M^{(N)} = \begin{pmatrix} f_+^{(N)} & \Delta^{(N)} \\ \Delta^{(N)} & f_-^{(N)} \end{pmatrix} \tag{2.14}$$

where the functions $f_+^{(N)}(H) = f_-^{(N)}(-H)$ break the $H \leftrightarrow -H$ system in a way similar to that of the branches $f_\pm$ of $f^{(N=\infty)}$. $f_\pm^{(N)}$ were introduced in Ref. 19 and on the real H axis are given by

$$f_\pm^{(N)} = (f_2^{(N)} + f_1^{(N)})/2 \mp \text{sign}(H) \left| \left[(f_2^{(N)} - f_1^{(N)})^2/4 - \Delta^{(N)2} \right]^{1/2} \right| \tag{2.15}$$

We will discuss their properties in the complex H plane in detail in the next section. Here we consider the parametrization of $f_{1,2}^{(N)}$:

$$f_{1,2}^{(N)} = (f_+^{(N)} + f_-^{(N)})/2 \mp \left| \left[(f_+^{(N)} - f_-^{(N)})^2/4 + \Delta^{(N)2} \right]^{1/2} \right| \tag{2.16}$$

In terms of the symmetric functions

$$F^{(N)} = (f_+^{(N)} + f_-^{(N)})/2 \tag{2.17}$$

$$G^{(N)} = (f_+^{(N)} - f_-^{(N)})/2H \tag{2.18}$$

where $G^{(N)}(0)$ is finite, we have

$$f_{1,2}^{(N)} = F^{(N)}(H) \mp \left| \left[H^2 G^{(N)2}(H) + \Delta^{(N)2} \right]^{1/2} \right| \tag{2.19}$$

All the rapid N dependence is represented by $\Delta^{(N)} \sim e^{-CN}/N$. The derivatives of $f_1^{(N)}$ (and $f_2^{(N)}$) have terms with increasing powers of the square root in the denominator. The functions $G^{(N)}$ and $F^{(N)}$ are of the order of unity as functions of N, and are finite when $H \to 0$. Therefore for $|H| = O(\Delta^{(N)})$ the square root is proportional to $\Delta^{(N)}$, and the kth derivative $D^k f_1^{(N)}$ has a leading contribution of magnitude $\Delta^{(N)(1-k)}$. These terms are responsible for violent changes of $D^k f_1^{(N)}$ (Figs. 2e, f, g, h) at $|H| = O(\Delta^{(N)})$. Such behavior is easily visualized if we replace for small H the functions $F^{(N)}$ and $G^{(N)}$ by the first terms in their power series expansions (the notation for the coefficients will become clear in Section 3),

$$F^{(N)}(H) \to f_+^{(N)}(0) - \chi_+^{(N)}(0) H^2/2, \qquad G^{(N)}(H) \to -m_+^{(N)}(0) \tag{2.20}$$

$$f_1^{(N)} \to f_+^{(N)}(0) - \chi_+^{(N)}(0) H^2/2 - \left[H^2 m_+^{(N)2}(0) + \Delta^{(N)2} \right]^{1/2} \tag{2.21}$$

and plot the first few derivatives of this function.

In summary, we observe that the near degeneracy at $H = 0$ provides a mechanism for the fluctuations of $D^k f_1^{(N)}$ in the region $O(\Delta^{(N)})$ and of amplitudes ($k \geqslant 2$) $\Delta^{(N)(1-k)} \propto e^{(k-1)CN} \cdot N^{k-1}$. These fluctuations of $D^k f_1^{(N)}$ approximate the $-2|m_+(0)| D^{k-2}\delta(H)$ term of $D^k f^{(N=\infty)}$. In fact $f_{1,2}^{(N)}$ have actual crossings at a pair of branch points at $H_{\mathrm{BP}} \simeq \pm i\Delta^{(N)}/|m_+^{(N)}(0)|$. The above behavior causes a nonuniformity in the convergence of $D^k f_1^{(N)}$ to the $N \to \infty$ limit $D^k f_+$ for $H > 0$. At $H \equiv 0$ $D^k f_1^{(N)} \nrightarrow D^k f_+$ [in fact, $D^{2p+1} f_1^{(N)}(0) = 0$, $|D^{2p} f_1^{(N)}(0)| \to \infty$].

3. CONVERGENCE OF THE EIGENVALUE COMBINATIONS AT $H = 0$

From the discussion of the preceding section it follows that for $H > 0$ there are two contributions to the difference $|D^k f_1^{(N)} - D^k f_+|$. The first is the result of finite size effects. For periodic boundary conditions those are expected[29] to vanish like $e^{-N/\xi}$. The second contribution arises from "mixing" effects, which are appreciable in the range $\sim\Delta^{(N)}$ at $H = 0$. The origin of this contribution is a mixing between two branches $f_\pm^{(N)}$, which are

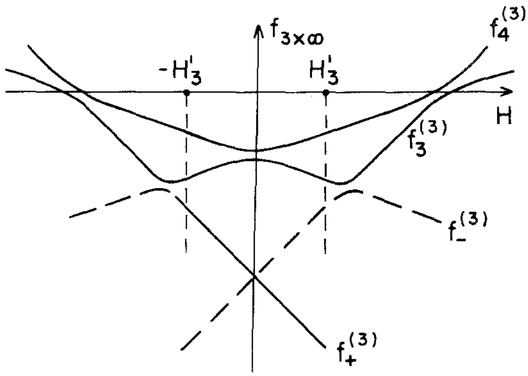

Fig. 3. Modified free energy branches $f_\pm^{(N)}$ for $N = 3$. Solid section of $f_+^{(N)}$ approximates f_+ (details in Section 3).

determined by the requirement that $f_{1,2}^{(N)}$ are the eigenvalues of $M^{(N)}$ of Eq. (2.14). In the complex H plane

$$f_\pm^{(N)} = \left(f_2^{(N)} + f_1^{(N)}\right)/2 \pm \left[\left(f_2^{(N)} - f_1^{(N)}\right)^2/4 - \Delta^{(N)2}\right]^{1/2} \tag{3.1}$$

where the argument of the square root is proportional to H^2 at $H \simeq 0$ and thus $f_\pm^{(N)}$ are analytic at the origin; the branch of the square root which is proportional to $-H$ is chosen in Eq. (3.1). On the real axis, $f_\pm^{(N)}$ [Eq. (2.15)] are two intersecting branches (Fig. 3). $f_\pm^{(N)}$ are free of the mixing effects, and $f_+^{(N)}$ provides a better approximation to f_+ for $H \geqslant 0$ than $f_1^{(N)}$ does. Indeed, if for $\Delta^{(N)} \ll |H| \ll 1$, $f_1^{(N)} \sim f_1(0) - m_+^{(N)}(0)|H| + O(H^2)$, then for $|H| \ll 1$, $f_+^{(N)} \sim f_+(0) - m_+^{(N)}(0)H + O(H^2)$, and $f_+^{(N)}$ reproduces correctly the cusp with the second branch $f_-^{(N)}$.

For $H > 0$, $f_1^{(N)}$ is analytic (as is f_+) and $D^k f_1^{(N)}$ converges to $D^k f_+$. It is a straightforward exercise to show that $D^k f_+^{(N)}$ also converges to $D^k f_+$ for $H > 0$. For $H = 0$ the situation is more complicated because the $D^k f_1^{(N)}$ behave nonuniformly at $H \sim 0$ (see Section 2). We will now show that with several reasonable assumptions on the properties of $f_1^{(N)}$ the following is true:

$$\lim_{N\to\infty} D^k f_+^{(N)}(0) = D^k f_+(0) = \lim_{H\downarrow 0} D^k f(H) \tag{3.2}$$

This is the principal result of this section. First note that $f_+^{(N)}$ is analytic at $H \equiv 0$ and it does not have the branch points associated with the central near degeneracy (at $H_{\mathrm{BP}} \simeq \pm i\Delta^{(N)}/|m_+^{(N)}(0)|$); this property follows directly from Eq. (3.1). The singularities of $f_+^{(N)}$ which are closest to the origin are expected to be at $|H| \sim H_N'$ when $f_2^{(N)}$ encounters higher branches $f_3^{(N)}, f_4^{(N)}, \ldots$. Therefore we assume that we can find a constant P such that $f_+^{(N)}$ is analytic in a circle $|H| < P/N$ in the complex H plane (arguments in favor of this assumption are the same as those given for $H'_N \propto 1/N$ and are not rigorous; see Section 2). Denote $\sup_{|H|<P/N}(|f_+^{(N)}(H)|) = S$. Let us define a new function (for fixed H)

$$F(Z) = f_+^{(N)}(Z+H) - f_+^{(N)}(H) \tag{3.3}$$

and consider it for $|H| < P/2N$ and $|Z| < P/2N$. We observe that both $|H+Z| < P/N$ and $|H| < P/N$, thus $|F(Z)| \leqslant 2S$ and $F(Z)$ is analytic (for $|Z| < P/2N$) and $F(0) = 0$. By Schwarz's lemma[30] we obtain ($|H|$, $|Z| < P/2N$)

$$|f_+^{(N)}(Z+H) - f_+^{(N)}(H)| \leqslant \frac{4S}{P} N|Z| \tag{3.4}$$

and ($Z \to 0$)

$$|Df_+^{(N)}(H)| \leqslant (4S/P)N \tag{3.5}$$

Thus we have found a bound on $Df_+^{(N)}$ in the circle $|H| < P/2N$. Repeat the same construction for $Df_+^{(N)}, D^2f_+^{(N)}, \ldots$ and obtain by induction that for $|H|, |Z| < P/2^kN$

$$|D^{k-1}f_+^{(N)}(Z+H) - D^{k-1}f_+^{(N)}(H)| \leqslant \frac{2^{k(k+3)/2}S}{P^k} N^k|Z| \tag{3.6}$$

and[2]

$$|D^kf_+^{(N)}(H)| \leqslant \frac{2^{k(k+3)/2}S}{P^k} N^k \tag{3.7}$$

In order to prove the convergence of $D^kf_+^{(N)}(0)$ to $D^kf_+(0)$ we choose some sequence that approaches the origin from the $H > 0$ side faster than $1/N^{k+1}$ but slower than $\Delta^{(N)} \propto e^{-CN}/N$. We choose $1/N^{k+2}$:

$$\begin{aligned} |D^kf_+^{(N)}(0) - D^kf_+(0)| \leqslant\ & |D^kf_+^{(N)}(0) - D^kf_+^{(N)}(1/N^{k+2})| \\ & + |D^kf_+(1/N^{k+2}) - D^kf_+(0)| \\ & + |D^kf_+^{(N)}(1/N^{k+2}) - D^kf_+(1/N^{k+2})| \end{aligned} \tag{3.8}$$

When $N \to \infty$, $1/N^{k+2}$ is inside the circle $|H| < P/2^kN$ and thus the first term on the right-hand side is bounded by $\text{const} \cdot (1/N^{k+2})N^{k+1} = O(1/N)$ [we used Eq. (3.6)]. The second term is $O(1/N^{k+2})$ because $f_+(H)$ is infinitely differentiable[31] at $H = 0^+$. The last term in Eq. (3.8)

[2] The referee has pointed out that Eq. (3.7) can be improved by using Cauchy's inequalities: $|D^kf_+^{(N)}(H)| \leqslant (2^kk!\,S/P^k)N^k$, for $|H| < P/2N$. The improved Eq. (3.6) now reads (again using Schwarz's lemma) $|D^kf_+^{(N)}(Z+H) - D^kf_+^{(N)}(H)| \leqslant (2^{k+3}k!\,S/P^{k+1})N^{k+1}|Z|$, for $|Z|, |H| < P/4N$.

may be simplified if we note that from the definition of $f_+^{(N)}$ it follows that $|D^k f_+^{(N)}(H) - D^k f_1^{(N)}(H)| \propto \Delta^{(N)2}$ for $H \gg \Delta^{(N)}$. Therefore

$$\begin{aligned}|D^k f_+^{(N)}&(1/N^{k+2}) - D^k f_+(1/N^{k+2})| \\ &= |D^k f_1^{(N)}(1/N^{k+2}) - D^k f_+(1/N^{k+2})| + O(\Delta^{(N)2}) \end{aligned} \tag{3.9}$$

and finally

$$|D^k f_+^{(N)}(0) - D^k f_+(0)| = |D^k f_1^{(N)}(1/N^{k+2}) - D^k f_+(1/N^{k+2})| + O(1/N) \tag{3.10}$$

Thus a sufficient condition for $D^k f_+^{(N)}(0) \to D^k f_+(0)$ is

$$\lim_{N\to\infty} \left[D^k f_1^{(N)}(1/N^{k+2}) - D^k f_+(1/N^{k+2}) \right] = 0 \tag{3.11}$$

or equivalently

$$\lim_{N\to\infty} D^k f_1^{(N)}(1/N^{k+2}) = D^k f_+(0) \tag{3.12}$$

The conditions given in Eqs. (3.11) and (3.12) have the simple physical interpretation that typical sizes of mixing effects in $D^k f_1$'s ($\propto e^{-CN}/N$) are asymptotically smaller than any power of a typical fluctuation effect ($\propto 1/N$). This property is the last assumption that we make on the basis of our qualitative understanding of the mechanism of the building up of a phase transition in the $N \to \infty$ limit.

To show that $D^k f_+^{(N)}(0) \to D^k f_+(0)$ we needed several physically plausible assumptions on the properties of $f_1^{(N)}$. We added only one point $H = 0$ to the domain of convergence. In practical calculations with finite N's the removal of the nonuniformity at $H = 0$ improves the rate of convergence for small positive H's as well, so that only finite size effects ($\propto e^{-N/\xi}$) contribute to $|D^k f_+^{(N)}(H \geqslant 0) - D^k f_+(H \geqslant 0)|$.

Note that use of $f_+^{(N)}$ does not give a direct method of analytic continuation to the $H < 0$ region. However, the analytic continuation may be done indirectly. $f_+^{(N)}$ provides rapidly convergent (with N) approximations to f_+ and its derivatives on the stable side $H \geqslant 0$. Calculating a finite number of derivatives at some $H_0 \geqslant 0$ we obtain a truncated power series which may be used for approximate analytic continuation by conventional series analysis methods. We follow this program in the following sections.

Let us add a number of comments. First, the choice of $f_\pm^{(N)}$ is not unique; we may replace $\Delta^{(N)}$ in Eqs. (2.14) and (3.1) by $D^{(N)}(H)$ such that $D^{(N)}(0) = \Delta^{(N)}$ and $D^{(N)}(H)/\Delta^{(N)}$ is of the order of unity for all H and N. Second, we considered the free energy branches $f_j^{(N)}$ for which the derivatives have an intuitive association with magnetization and the size estimates (e.g., $\Delta^{(N)} \sim e^{-CN}/N$) are easy to visualize. However, it is possible to express the entire formalism in terms of other functions, for example the $\lambda_j^{(N)}$'s. Both of these modifications introduce negligible ($\sim\Delta^{(N)2}$) corrections. With regard to using $\lambda_+^{(N)}$ instead of $f_+^{(N)}$ we checked numerically that the results of the following sections are not affected.

4. BEHAVIOR OF THE POWER SERIES AT $H = 0$

We consider the following power series:

$$m_+(H) = 1 + \sum_{n=0}^{\infty} c_n H^n \tag{4.1}$$

where m_+ is the magnetization of the branch f_+ (Fig. 2a) of the infinite system free energy, f ($m \equiv -f'$). Characteristic temperature ranges of the problem are defined in terms of the low-temperature variable $u = e^{-4\beta}$. For fixed $u < u_c$ the coefficients c_n, which are defined by

$$c_n(u) = \left[(-1/n!)D^{n+1}f_+(H,u)\right]_{H\to 0^+} - \delta_{n0} \tag{4.2}$$

are approximated by

$$c_n^{(N)}(u) = \left[(-1/n!)D^{n+1}f_+^{(N)}(H,u)\right]_{H=0} - \delta_{n0} \tag{4.3}$$

The value of $f_+^{(N)}(H=0)$ is also of interest (it approximates $f_+(0)$); both $f_+(0)$ and c_0 are known from the exact solution.[26,27]

Let us describe briefly our PL/1 computer program which performs the following calculations:

1. Classification of the elements of the TM for the $N \times \infty$ system;
2. Construction of the subspace of states which are invariant under the symmetry operations discussed in Section 2;
3. Calculation of the restriction of the TM to the invariant subspace and calculation of the eigenvalues $f_1^{(N)}$ and $f_2^{(N)}$ to about 30-figure accuracy;
4. Step 3 is performed at several H values near $H = 0$, and the polynomial that interpolates the values of $f_+^{(N)}$ is used to calculate the first ten derivatives of $f_+^{(N)}$ at $H = 0$.

The large accuracy (step 3) in the $f_{1,2}^{(N)}$ values is needed to avoid roundoff errors when we use a limited number of interpolation points (15) which are closely spaced ($\sim 10^{-2}$); the number of times that step 3 is performed is further decreased owing to the symmetry of $f_1^{(N)}$ and $f_2^{(N)}$. We discuss the accuracy of the derivative values later. We calculated up to $N = 9$ with reasonable computing times. For a given temperature it takes about $1\frac{1}{2}$ hours on the IBM/370 Technion–IIT computer to calculate for $N = 3, \ldots, 9$.

Before considering in detail the results for some representative temperatures let us summarize the convergence properties. We found that for $N \leqslant 9$ sufficiently accurate $c_0, \ldots, c_9$ values are obtained in the temperature range

$$0 < u \lesssim 0.3 u_c \tag{4.4}$$

The convergence is faster for lower temperatures. This is connected with the fact that when T increases from zero toward T_c finite size effects decay more slowly. The convergence is better for lower derivatives. This is not a special property of our procedure, but a general feature of the numerical approximation of derivatives using approximate values of a function.

Let us discuss the results for some representative temperatures. The case $u = 0.1 u_c$ is interesting because for this temperature the first 24 coefficients $c_1, \ldots, c_{24}$ were obtained in Ref. 11 using a numerical resummation of the long low-temperature series of Ref. 13. Our values of $c_n^{(N)}$ for $N = 7, 8, 9$ were listed in Ref. 19, and good agreement with the values of Ref. 11 was found. In Table I we list some results for $u = 0.05 u_c$. Here the rate of convergence is better than for $0.1 u_c$ (Ref. 19). The coincidence between the first figures of $c_n^{(8)}$ and $c_n^{(9)}$ is already close to best possible before the roundoff errors manifest themselves, thus demonstrating the limits of the accuracy of our computational method.

In Table II we list estimates of the c_n's for $u/u_c = 0.09, 0.15, 0.21, 0.27$; one can follow the decrease in accuracy as u increases. For $u/u_c = 0.06$, 0.12, 0.18, 0.24 we plot in Fig. 4 the ratios c_n/c_{n-1} as functions of n (see Ref. 19 for similar plot for several other u values). The asymptotically linear divergence of c_n/c_{n-1} (see Ref. 11 and 19 and Fig. 4) implies that the radius of convergence of the power series [Eq. (4.1)] is zero. The nature of the essential singularity at $H = 0$, as implied by such linear behavior of c_n/c_{n-1}, was discussed in detail in Ref. 11. In Ref. 14 it was shown to be consistent with field theoretic droplet model predictions.

We consider now how such a singularity arises when $N \to \infty$. There are two types of singularities in the problem. Intrinsic ones, which are the real singularities of the branches $f_\pm$ of f of the infinite system, and the cusp in f at $H = 0$. In the finite N system the cusp is approximated by the mixing of $f_1^{(N)}$ and $f_2^{(N)}$, which is associated with the pair of branch points in the complex H plane at $H \sim \pm i\Delta^{(N)}/|m_+^{(N)}(0)|$ (notation of Section 2). Using $f_+^{(N)}$ eliminates this pair of branch points. The next singularities of $f_+^{(N)}$ are close to the real H axis and at $|H| \sim H_N'$ where $f_2^{(N)}$ encounters higher $f_j^{(N)}$'s. For lower N these are single near crossings, and a "condensation" of the corresponding branch points to produce an essential singularity at $H = 0$ may be followed.[24] For larger N, however, the picture is more complicated[25]; no general information on the distribution of branch

Table I. The Coefficients $c_n^{(N)}$ and the Values of $f_+^{(N)}(0) + 2$ for $u = 0.05u_c$ $(N = 8, 9)$; Exact Values of $f(0) + 2$ and c_0 Also Listed (Notation of Section 4)

	$N = 8$	$N = 9$	$N \to \infty$ estimates	
$f(0) + 2$	− 6.294509222865217 . . .	− 6.294509222865890 . . .	− 6.2945092228659(±7)	$\times 10^{-5}$
Exact $f(0) + 2$			− 6.294509222865897 . . .	$\times 10^{-5}$
c_0	− 1.524283928837645 . . .	− 1.524283928838331 . . .	− 1.524283928838(±1)	$\times 10^{-4}$
Exact c_0			− 1.524283928838339 . . .	$\times 10^{-4}$
c_1	3.758686096239 . . .	3.758686096250 . . .	3.75868609625(±1)	$\times 10^{-4}$
c_2	− 4.80706592297 . . .	− 4.8070659309 . . .	− 4.807065931(±1)	$\times 10^{-4}$
c_3	4.4071550708 . . .	4.4071550718 . . .	4.407155072(±1)	$\times 10^{-4}$
c_4	− 3.471945321 . . .	− 3.471945328 . . .	− 3.471945328(±7)	$\times 10^{-4}$
c_5	2.74114101 . . .	2.74114106 . . .	2.74114106(±5)	$\times 10^{-4}$
c_6	− 2.44365288 . . .	− 2.44365318 . . .	− 2.4436532(±3)	$\times 10^{-4}$
c_7	2.5733021 . . .	2.5733038 . . .	2.573304(±2)	$\times 10^{-4}$
c_8	− 3.141802 . . .	− 3.141811 . . .	− 3.14181(±1)	$\times 10^{-4}$
c_9	4.30435 . . .	4.30440 . . .	4.30440(±5)	$\times 10^{-4}$

Table II. Estimates of c_n' s for $u/u_c = 0.09, 0.15, 0.21, 0.27$ using $N \leqslant 9$ Values (Exact Values of f_0 and c_0 Also Listed)

	$u = 0.09u_c$	$u = 0.15u_c$	$u = 0.21u_c$	$u = 0.27u_c$
$f(0) + 2$	− 0.236001536921 (±1)	− 0.7634719268 (±3)	− 1.68518834 (±1)	− 0.30839343 (±2)
Exact $f(0) + 2$	− 0.2360015369216 . . .	− 0.76347192686 . . .	− 1.685188340 . . .	− 0.308393431 . . .
c_0	− 0.50841573414 (±2)	− 1.477912318 (±4)	− 3.0389820 (±1)	− 0.5285375 (±3)
Exact c_0	− 0.508415734144 . . .	− 1.4779123182 . . .	− 3.03898206 . . .	− 0.52853752 . . .
c_1	1.1332423184 (±3)	3.04024585 (±7)	6.004490 (±3)	1.027866 (±5)
c_2	− 1.353608853 (±4)	− 3.5404485 (±9)	− 7.14665 (±4)	− 1.29122 (±6)
c_3	1.23353816 (±4)	3.465439 (±8)	7.8799 (±4)	1.6518 (±6)
c_4	− 1.0657383 (±3)	− 3.62620 (±6)	− 10.143 (±2)	− 2.625 (±4)
c_5	1.024955 (±2)	4.5659 (±4)	16.21 (±2)	5.24 (±4)
c_6	− 1.17523 (±1)	− 6.934 (±2)	− 31.15 (±11)	− 12.5 (±2)
c_7	1.58656 (±6)	12.27 (±2)	69.5 (±7)	34.5 (±12)
c_8	− 2.4411 (±4)	− 24.64 (±9)	176. (±4)	− 107. (±8)
c_9	4.191 (±3)	55.3 (±5)	495. (±20)	365. (±40)
All values	$\times 10^{-3}$	$\times 10^{-3}$	$\times 10^{-3}$	$\times 10^{-2}$

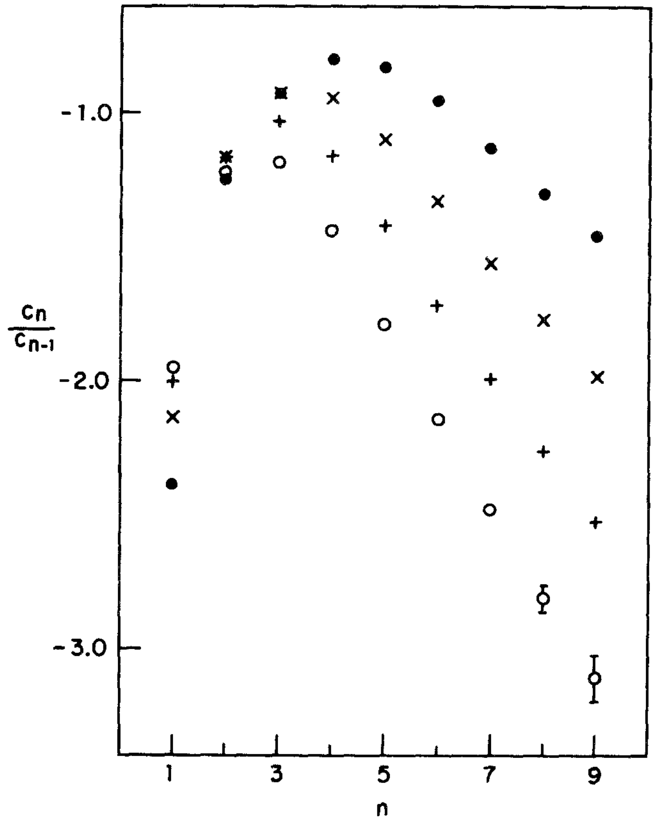

Fig. 4. Plot of c_n/c_{n-1} as a function of n for $u/u_c = 0.06$ (points), 0.12 (crosses), 0.18 (plus symbols) and 0.24 (open circles); only in the last case and for $n = 8, 9$ are error bars comparable to the size of the symbols (and are drawn).

points in the complex plane is available. The only (nonrigorous) information is that the closest branch points lie at a distance $\sim H_N' \sim 1/N$ from the origin. The radius of convergence of the power series for $f_+^{(N)}$ vanishes like $1/N$. The behavior of the ratios $c_n^{(N)}/c_{n-1}^{(N)}$ when N increases may be followed visually for u close to $0.3u_c$ where the convergence is relatively slow. For $u = 0.3u_c$ the approach of the ratios $c_n^{(N)}/c_{n-1}^{(N)}$ to linear behavior was plotted in Ref. 19.

The range $u \lesssim 0.3u_c$ corresponds to $T \lesssim 0.6T_c$. For higher temperatures $N \leqslant 9$ calculations provide accurate values for the first few derivatives. For example, when $u = 0.5u_c$ ($T \simeq 0.72T_c$) only the first 4 c_n's are reasonably accurate. For $u = 0.9u_c$ ($T \simeq 0.94T_c$) only $f(0)$, c_0 and c_1 are obtained. Note that for $0.9u_c$ $c_1, \ldots, c_{12}$ were obtained in Ref. 11 by a different method. As we already mentioned the slower convergence when $T \to T_c^-$ is due to larger finite size effects.

5. SPINODAL

Mean-field theories predict that the susceptibility diverges at some $H = H_{sp}(T) < 0$ in the metastable phase according to $(H - H_{sp})^{-1/2}$. As for the usual second-order phase transitions such divergent susceptibility ought to be associated with a divergent ξ when $H \to H_{sp}^+$. In real systems with short-range interactions the existence of the spinodal is questionable. In Section 1 we mentioned arguments in favor of the expectation that the spinodal (if it exists) is a smoothed singularity. However, in the analysis of short power series an apparently sharp singularity may be observed.[18,22] Explicitly, we try to fit (for $H \to H_{sp}^+$)

$$m_+(H) \simeq \text{const}(H - H_{sp})^{1-\sigma} + \text{(less singular terms)} \tag{5.1}$$

where $0 < \sigma < 1$ on the basis of mean-field intuition that m is finite at H_{sp} and the susceptibility diverges $[\chi \sim 1/(H - H_{sp})^\sigma]$.

Singularities of the form of Eq. (5.1) are usually studied by the Padé method. The origin of the difficulties in observing the spinodal by series analysis methods in the $d = 2$ Ising model is that even if we neglect the smoothing it is a weak singularity (we will find later that σ is small). In the power series in H the coefficients c_n are dominated by the factorially growing dropletlike contribution, and the spinodal is difficult to detect. Let us consider a more general power series

$$m = 1 + \sum_{n=0}^{\infty} C_n (H - H_0)^n, \qquad H_0 \geqslant 0 \tag{5.2}$$

We may hope to observe the spinodal if it is possible to choose H_0 sufficiently small, such that the $H < 0$ behavior can be detected in a short power series, but still sufficiently far from $H = 0$, such that the power series is not dominated by the singularity at $H = 0$. The function that is studied by the Padé method is

$$\frac{\chi'}{\chi} = \frac{m''}{m'} \sim \frac{-\sigma}{H - H_{sp}} + \text{(less singular terms)} \tag{5.3}$$

The $[L, M]$ Padé approximant is

$$[L, M] = \frac{\sum_{l=0}^{L} a_l (H - H_0)^l}{1 + \sum_{m=1}^{M} b_m (H - H_0)^m} \tag{5.4}$$

where a_l's and b_m's are calculated using the condition that the first

$L + M + 1$ coefficients in the expansion of $[L, M]$ in powers of $(H - H_0)$ coincide with those of m''/m'. We consider $L + M = 5, 6, 7$.

Consider first fixed $u = 0.1u_c$ and varying $H_0 = 0.05$, 0.10, 0.15, 0.20, 0.30, 0.40. The method of calculating $C_0^{(N)}, \ldots, C_9^{(N)}$ is similar to that of Section 4, but $H_0 > 0$ is not a symmetry point, and more computer time is needed. The rate of convergence improves when H_0 moves away from zero. Most of the values of the C_n's used here were obtained with $N \leqslant 8$, some with $N \leqslant 9$ (we will later discuss in detail the convergence of the $C_n^{(N)}$'s at fixed $H_0 = 0.1$). For $H_0 = 0.00$, 0.05, 0.10, 0.15, 0.20 the majority of poles and zeros of the $[L, M]$'s lie on the negative H axis, suggesting a branch cut along the negative H axis. But Padé analysis does not ensure that this branch cut starts at $H = 0$. The ratio method (see Refs. 11 and 19 and Section 4) is preferable in studying the singularity at $H = 0$. For $H_0 = 0.30$ or 0.40 the tendency of poles and zeros to gather on the negative H axis nearly disappears and the short power series becomes insensitive to the weak singularity at $H = 0$. In the case of $H_0 = 0.1$ we clearly observe one stable pole at H values in the range

$$H_{\rm sp} = -0.415 \pm 0.015 \tag{5.5}$$

The corresponding residues (which approximate $-\sigma$) lie in the range

$$\sigma = 0.07 \pm 0.02 \tag{5.6}$$

This pole also appears in some $[L, M]$'s for $H_0 = 0.05; 0.15$. For $H_0 = 0.2$ it appears sporadically in some $[L, M]$'s (but the H values and the residues vary widely). For $H_0 = 0.3; 0.4$ there is no sign of it. In Fig. 5 we summarize the values of $H_{\rm sp}$ and σ as observed in different Padé approximants for $H_0 = 0.10; 0.05; 0.15$. For $u = 0.1u_c$ a long series in powers of $H (H_0 = 0)$ is available.[11] When this series is analyzed by the Padé method, we find that most of the zeros and poles lie on the negative H axis (an indication of the branch cut). The stable pole at $H_{\rm sp}$ of Eq. (5.5) does not appear in the lower (small $L + M$) $[L, M]$'s. However this pole is present in large number of the higher Padé approximants ($L + M = 22, 21, 20, \ldots$). The $H_{\rm sp}$ and σ values fluctuate, but most of them fall in the range of Eqs. (5.5) and (5.6).

It must be stressed that the identification of the stable pole that we observed as the spinodal singularity should be made with great caution. The spinodal, if it exists, is masked by the essential singularity at $H = 0$. The presence of the branch cut makes the applicability of the Padé method rather questionable and opens the door for systematic errors, especially when such a short series is analyzed. Support for the identification of the stable pole which we observed as evidence of a spinodal comes from its reasonable temperature dependence (see below). Attempts to find evidence of some exceptional behavior of the gap sizes between TM eigenvalues at relevant H values give negative results.[19]

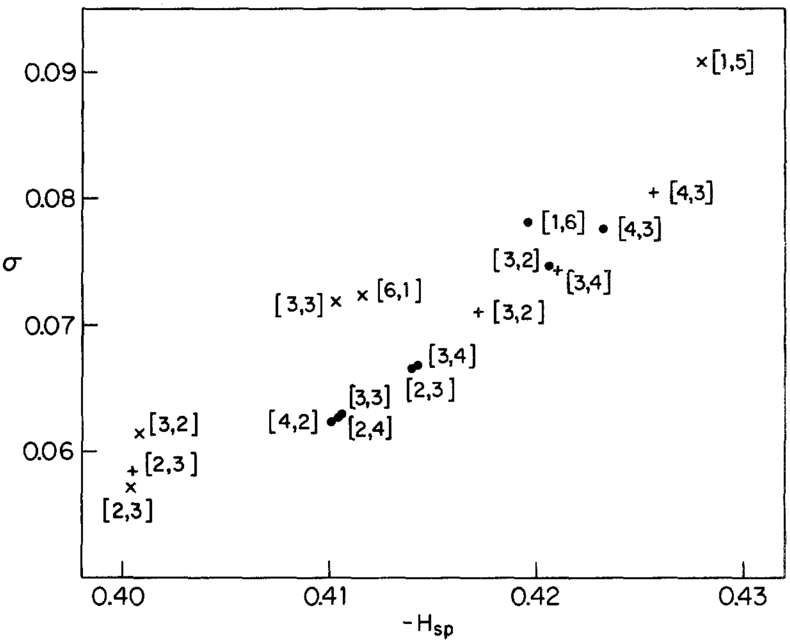

Fig. 5. The values of σ and H_{sp} as obtained with several Padé approximants at $u = 0.1u_c$ for $H_0 = 0.1$ (points), $H_0 = 0.05$ (crosses), $H_0 = 0.15$ (plus symbols).

We now describe the calculation of $H_{sp}(u)$ in the low-temperature range. For all temperatures we use $H_0 = 0.1$ which was the most successful value of H_0 at $u = 0.1u_c$. As was already noted, the convergence of the $C_n^{(N)}$ values (when N is increased) at $H_0 = 0.1$ is better than in $H_0 = 0$ calculations of Section 4, but $H_0 > 0$ calculations require more computer time. When calculating with $N \leqslant 7$ and $N \leqslant 8$ the C_n values are obtained with reasonable accuracy in the temperature ranges $0 < u \lesssim 0.1u_c$ and $0 < u \lesssim 0.3u_c$, respectively. In Tables III, IV, and V we list the coefficients $C_n^{(N)}$ for three representative temperatures $u = 0.02u_c$, $0.1u_c$, $0.3u_c$ for $N = 7$, 8. The $0.1u_c$ values are compared with the estimates obtained by resummation of the (divergent) asymptotic series of Ref. 11 using those first partial sums of the series

$$C_k = \sum_{n=k}^{\infty} \binom{n}{k} c_n H_0^{n-k} \tag{5.7}$$

which stabilize at some C_k value (higher partial sums fluctuate with increasing magnitude because the series is divergent). Owing to the presence of the factor $\binom{n}{k}$ the accuracy of the asymptotic approximation is worse for higher k's (see Table IV).

Table III. The Coefficients $C_n^{(N)}$ of the Expansion $m_+^{(N)}(H) = 1 + \sum_n C_n^{(N)}(H - H_0)^n$ for $H_0 = 0.1$, Calculated with $N = 7$ and 8 at $u = 0.02u_c$

	$N = 7$	$N = 8$	
C_0	− 1.79171187315334 . . .	− 1.79171187315348 . . .	$\times 10^{-5}$
C_1	5.1370861753304 . . .	5.1370861753314 . . .	$\times 10^{-5}$
C_2	− 7.4418834154716 . . .	− 7.4418834154762 . . .	$\times 10^{-5}$
C_3	7.3382860114449 . . .	7.338286011427 . . .	$\times 10^{-5}$
C_4	− 5.65200056326 . . .	− 5.65200056338 . . .	$\times 10^{-5}$
C_5	3.75781505519 . . .	3.75781505576 . . .	$\times 10^{-5}$
C_6	− 2.3745025033 . . .	− 2.3745025054 . . .	$\times 10^{-5}$
C_7	1.567813730 . . .	1.567813724 . . .	$\times 10^{-5}$
C_8	− 1.16007130 . . .	− 1.16007128 . . .	$\times 10^{-5}$
C_9	9.8306057 . . .	9.8306064 . . .	$\times 10^{-6}$

Table IV. The Coefficients $C_n^{(N)}$ in the Case $H_0 = 0.1$, $u = 0.1u_c$ (Estimates Based on the Resummation of the Series of Ref. 11 Also Listed)

	$N = 7$	$N = 8$	Resummed series of Ref. 11	
C_0	− 5.088596269 . . .	− 5.088596275 . . .	− 5.08859 (±1)	$\times 10^{-4}$
C_1	1.097412266 . . .	1.097412272 . . .	1.09741 (±1)	$\times 10^{-3}$
C_2	− 1.2570739 . . .	− 1.2570740 . . .	− 1.25707 (±1)	$\times 10^{-3}$
C_3	1.07807168 . . .	1.07807191 . . .	1.07807 (±1)	$\times 10^{-3}$
C_4	− 8.471638 . . .	− 8.471649 . . .	− 8.47166 (±1)	$\times 10^{-4}$
C_5	7.09025 . . .	7.09030 . . .	7.09028 (±3)	$\times 10^{-4}$
C_6	− 6.81741 . . .	− 6.81760 . . .	− 6.817 (±1)	$\times 10^{-4}$
C_7	7.53401 . . .	7.53470 . . .	7.53 (±2)	$\times 10^{-4}$
C_8	− 9.2978 . . .	− 9.3002 . . .	− 9.4 (±3)	$\times 10^{-4}$
C_9	1.2509 . . .	1.2517 . . .	1.0 (±5)	$\times 10^{-3}$

Table V. The Coefficients $C_n^{(N)}$ in the Case $H_0 = 0.1$, $u = 0.3u_c$

	$N = 7$	$N = 8$	
C_0	− 5.548269 . . .	− 5.548287 . . .	$\times 10^{-3}$
C_1	1.020328 . . .	1.020348 . . .	$\times 10^{-2}$
C_2	− 1.17351 . . .	− 1.17365 . . .	$\times 10^{-2}$
C_3	1.2962 . . .	1.2970 . . .	$\times 10^{-2}$
C_4	− 1.6656 . . .	− 1.6697 . . .	$\times 10^{-2}$
C_5	2.545 . . .	2.563 . . .	$\times 10^{-2}$
C_6	− 4.43 . . .	− 4.51 . . .	$\times 10^{-2}$
C_7	8.51 . . .	8.81 . . .	$\times 10^{-2}$
C_8	− 1.75 . . .	− 1.86 . . .	$\times 10^{-1}$
C_9	3.82 . . .	4.22 . . .	$\times 10^{-1}$

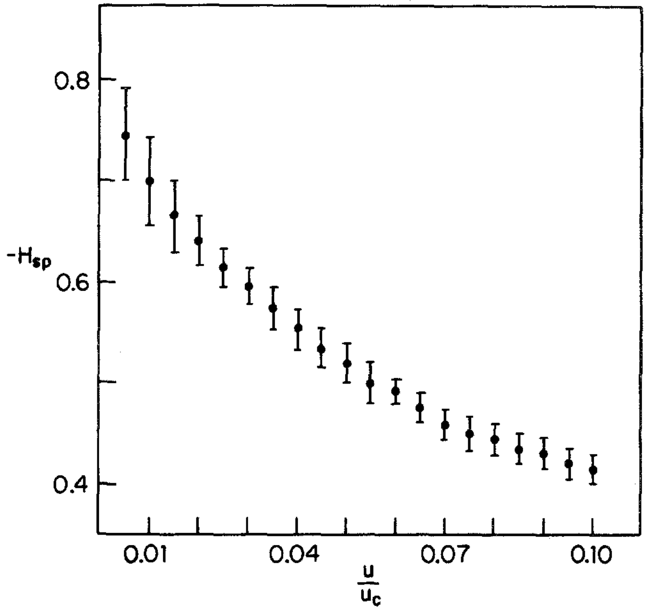

Fig. 6. H_{sp} as a function of u in the temperature range $u \leqslant 0.1u_c$.

In the temperature range $0 < u \leqslant 0.1u_c$ we found that the $N = 7$ C_n values are sufficiently accurate and calculated $H_{sp}(u)$ for 20 temperatures $u/u_c = 0.005, 0.010, \ldots, 0.100$. The results are summarized in Fig. 6. The values of the residues $(-\sigma)$ for all these temperatures fall in the range of Eq. (5.6), σ is apparently constant in this temperature range and is far from the mean-field value $\sigma^{(MF)} = 1/2$. It seems from Fig. 6 that $H_{sp}(u)$ has a finite limit when $u \to 0$,

$$H_{sp}(u = 0^+) = -0.82 \pm 0.07 \tag{5.8}$$

This is also the case in the Curie–Weiss (mean-field) model

$$H_{sp}^{(MF)} = -T_0(1 - T/T_0)^{1/2} + (T/2)\log\left[\left(1 + (1 - T/T_0)^{1/2}\right)/\left(1 - (1 - T/T_0)^{1/2}\right)\right] \tag{5.9}$$

The mean-field transition temperature T_0 may be considered an adjustable parameter which is determined by the position of the second-order phase transition. It may also be fixed in the low-temperature range as the value of $-H_{sp}$ at $T = 0$. In the former case it is well known that the mean-field results do not describe correctly the behavior of the thermodynamic functions of the $d = 2$ Ising model at $T \sim T_c$ both as functions of T and of H. We found that the mean-field result does not describe correctly the H dependence of $m_{\text{metastable}}(H)$ at $H \sim H_{sp}$ $(\sigma \neq \sigma^{(MF)})$. We found also that the points of Fig. 6 cannot be fitted by the curve of the form of Eq. (5.9) with one adjustable parameter T_0. Thus the mean-field model does not describe the functional form of the T dependence of $H_{sp}(T)$ in the low-temperature range.

In the temperature range $0 < u \leqslant 0.3u_c$ we calculated C_n values for 15 temperatures $u/u_c = 0.02, 0.04, \ldots, 0.30$ with $N = 8$. The values of σ are apparently constant in this range of temperatures also and are in the range

$$0.04 \lesssim \sigma \lesssim 0.09 \tag{5.10}$$

[compare Eq. (5.6)]. The estimates of $H_{sp}(u)$ are summarized in Fig. 7 (this figure was included in Ref. 19 and is reproduced for completeness). It is interesting to compare our values with the scaling form of $H_{sp}(T)$ at

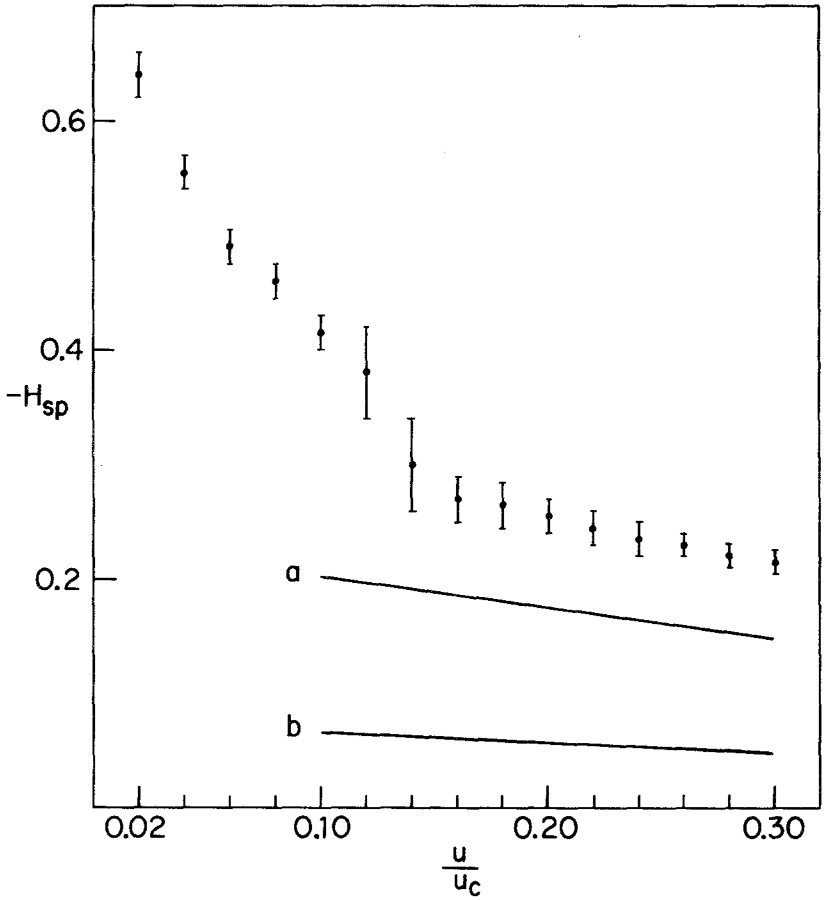

Fig. 7. H_{sp} as a function of u in the temperature range $u \leqslant 0.3u_c$. The scaling from of Ref. 18 defines the range between the curves a and b.

$T \sim T_c^-$ which was studied in Ref. 18 using the high-temperature series. The estimate

$$\tanh(\beta H_{sp}) \simeq -(0.39 \pm 0.20)(1 - T/T_c)^{15/8} \tag{5.11}$$

of Ref. 18 defines the range of H_{sp} values between the curves a and b in Fig. 7. The scaling form [Eq. (5.11)] is valid only in the $T \to T_c^-$ limit. At our $u \lesssim 0.3u_c$ ($T \lesssim 0.6T_c$) temperatures the correction terms cannot be neglected. The behavior of H_{sp} (Fig. 7) that we found is consistent with the statement that it approaches the asymptotic form of Ref. 18 at higher temperatures. Finally, let us stress that the error bars in Fig. 6 and 7 represent the spread of Padé approximant values. Systematic errors may be present owing to the branch cut. Also higher C_n's are obtained for the largest u values ($u \sim 0.3u_c$) with relatively low accuracy when $N = 8$ values are used (see Table V), and H_{sp} estimates may change slightly when more accurate calculation of C_n's at higher u values will be performed.

6. SUMMARY

We studied the problem of optimal approximation of the free energy and its derivatives close to the first-order phase transition in a case when the coexistence of two phases is associated with an asymptotic degeneracy of the two largest eigenvalues of some linear operator. The modified free energies $f_\pm^{(N)}$ approximate the branches $f_\pm$ of the free energy $f^{(N=\infty)}$ and all the derivatives in the stable regions. Analytic continuation is performed using a truncated power series. For the $d = 2$ Ising model we confirmed the existence of the singularity at $H = 0$ and found evidence of a spinodal line of (smoothed) singularities.

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