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An Exact Solution of the Renormalization-Group Equations for the Mean Field Theory of Stable and Metastable States

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An exact solution of the renormalization-group equations corresponding to the mean field theory of stable and metastable states is given which yields the correct free energies for these states. An unusual feature of this solution is that the renormalized Hamiltonian in the two-phase region becomes a multivalued function of the order parameter for all values of the length rescaling parameter beyond a certain critical value. This is closely related to the multivaluedness of the free energy as a function of magnetic field which characterizes the classical theory of metastable and unstable states. As a consequence of this multivaluedness, the trajectory flow in the space of coupling constants exhibits unusual "bifurcation." This leads to difficulties in evaluating the metastable and unstable free energies by a trajectory integral of the spin-independent term, which can be resolved by an extension of the standard formalism.

KEY WORDS: Renormalization group; mean field theory; metastable states; bifurcation.

1. INTRODUCTION

In recent years there have been several renormalization-group studies of mean-field or long-range force models of phase transitions.[1-3] Two of these were analyses of the recursion equations for stable thermodynamic states, with particular stress on the critical region. The first emphasized the existence of a so-called "van der Waals" fixed point in terms of which the

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classical values of the critical exponents could be obtained for all dimensionality by a standard linearization of the renormalization-group equations. This analysis involved a steepest descent evaluation of the smooth-cutoff renormalization equations[4,5] for the usual Landau–Ginzburg field theory, in the long-range force limit in which the coefficient of the gradient term in the Ginzburg–Landau Hamiltonian is taken to be infinite. The second[2] was a study of the closely related Kac long-range force model of spins on a lattice. Here an exact formal solution of the equations was obtained for a rather general class of renormalization transformations above the critical point ($T > T_c$). The emphasis in this paper was on the breakdown of hyperscaling relations for critical exponents. Neither paper dealt with the properties of the long-range force model below the critical point, nor, except for the special case of the zero-magnetic-field, $T > T_c$ situation, with the actual evaluation of the free energy by the usual renormalization trajectory methods.[6] Finally, in the third paper[3] an extension of Green's procedure[1] was used to obtain a renormalization-group description of the classical theory of metastability. A novel feature of this work was the discovery of a so-called "spinodal fixed point" associated with the classical spinodal curve. A linearization of the renormalization-group equations about this fixed point yielded the exponents which correctly characterize the singularity in the free energy at any point on the spinodal curve. In addition to this fixed point, a hierarchy of multicritical fixed points (such as a tricritical fixed point) corresponding to the Landau theory of multicritical phenomena was obtained. A corresponding set of multicritical "spinodal" fixed points was also found.

In this paper we complete the description of the stable and metastable states for the long-range force limit of the Ginzburg–Landau model by presenting an exact solution of the renormalization-group equations in the entire thermodynamic domain which yields the free energies of the stable, metastable, and unstable states. In particular, we find a renormalization-group analog of the classical theory of metastable and unstable states in the intensive thermodynamic representation of temperature and magnetic field. According to this theory, there are two branches of the Gibbs free energy for a fixed temperature below T_c, which as a function of magnetic field cross each other at zero field. The analytic continuation of each of these branches represents each metastable state and these two branches are connected (at spinodal points) by the unstable branch. We find that the renormalized Hamiltonian (for a finite value of the length rescaling parameter) exhibits a similar behavior. On the other hand, if one attempts to study this multivalued renormalized Hamiltonian by a standard Ginzburg–Landau power series expansion, one encounters quite unusual flow, as, for example, multiple values of the renormalized magnetic field and higher order expansion coefficients. This is presumably a manifestation of the fact that a power series expansion is not always a useful description of these states in this metastable domain.

Before outlining the structure of the paper, it is appropriate to make two additional remarks. The first concerns the nature of the renormalization group for the long-range force limit of the Ginzburg–Landau model. In one sense there is little physical significance associated with this renormalization, since this is a case in which the Landau assumption concerning the analyticity of the expansion coefficients as a function of temperature remains valid for any value of the cutoff in wavenumber space. That is, the effect of fluctuations is, by definition of the model, negligible. A related fact is that in the steepest descent evaluation for this model, only the zero-wavenumber Fourier component of the order parameter (the spatially uniform mode) is retained, the other components being statistically negligible in the infinite-range force limit. Thus the renormalized Hamiltonian has only one degree of freedom, so that in a sense only a remnant of the usual fluctuation effects described by the renormalization equations is present in our equations. On the other hand, the relative simplicity of these equations allows us to give an exact solution for this model, in contrast to the usual situation with renormalization-group problems. Thus the model is of some mathematical interest. Furthermore, it seems useful to understand a simple example of metastability in the one case where a metastable state can be unambiguously defined in an equilibrium description in renormalization-group language, before attempting to attack the much more interesting problem of metastability for real systems. It is perhaps appropriate to note here that the renormalization group provides a natural tool for the description of first-order phase transitions, including metastability, in addition to its well-known usefulness in describing second-order phase transitions. The point is that in both cases the microscopic details are not crucial to obtaining a basic understanding of the physics of the transition. The second remark is that we have not yet provided a rigorous renormalization-group description of the mean field theory of metastability. To do this would presumably involve a renormalization appropriate to the constrained partition function used by Penrose and Lebowitz[7] in their rigorous statistical description of the classical theory of metastability. Our point of view has been to follow the approach taken by Langer[8] and others in which the metastable state is considered to correspond to a local (but not absolute) minimum in the Hamiltonian in the two-phase region below the critical point, or, correspondingly, to the smaller of the two peaks in the Boltzmann probability function.

The outline of this paper is the following. In Section 2 we briefly review the classical theory of stable and metastable states, primarily to introduce notation useful in our subsequent analysis. We also summarize the renormalization-group equations of Ref. 3. We then effectively "unscale" these equations by a suitable transformation of variables, which yields a partial differential equation. In Section 3 we present an exact solution of this renormalization-group equation and examine the solution in three different cases: (a) the one-phase, stable region in the presence of an external magnetic field H; (b) the two-phase coexistence region ($T < T_c, H = 0$); (c) the metastable and unstable region (with $T < T_c, H = 0$). We show how the exact classical free energy can be obtained for each of these cases from our renormalization-group solution. In Section 4 we study a power series solution (of the usual Ginzburg–Landau form) of the renormalization-group equation in the two-phase region. We find interesting and unusual flow both in the case of equilibrium, two-phase coexistence, and, particularly, in the metastable domain. It is shown that in the latter case a calculation of the metastable free energy by a trajectory integral of the spin-independent piece involves what appears to be "unphysical" flow.

2. BRIEF REVIEW

We begin by noting that the classical theory of stable and metastable states can be obtained from an evaluation of the partition function

$$Z = \int_{\sigma(\mathbf{r})} \exp\left(-\overline{\mathcal{H}}\{\sigma\}\right) \tag{2.1}$$

where $\sigma(\mathbf{r})$ is the local magnetization and $\overline{\mathcal{H}}(\sigma)$ is the Landau–Ginsburg Hamiltonian, given by

$$\overline{\mathcal{H}}\{\sigma(\mathbf{r})\} = \int d\mathbf{r}\left[\frac{1}{2}\frac{T_c}{T}R^2(\nabla\sigma)^2 + \frac{1}{2}u_2\sigma(\mathbf{r})^2 + \frac{1}{4}u_4\sigma(\mathbf{r})^4 + u_1\sigma(\mathbf{r}) + \cdots\right] \tag{2.2}$$

where T_c is the mean field critical temperature, R^2 is the second moment of the interaction potential, $u_1 = -H/kT$, and $u_2 = T/T_c - 1$. In the weak long-range force limit when $R \to \infty$ the usual mean field theory can be obtained by steepest descent evaluation of (2.1). In this case, states which are spatially uniform are statistically favored. These states are given by the solution of the Euler–Lagrange equation,

$$\left.\frac{\delta\overline{\mathcal{H}}}{\delta\sigma(\mathbf{r})}\right|_{\sigma=\bar{\sigma}} = \psi(\bar{\sigma}) = 0 \tag{2.3}$$

where $\psi(\sigma)$ has the form

$$\psi(\sigma) \equiv u_1 + u_2\sigma + u_4\sigma^3 \tag{2.4}$$

[The function $\psi(x)$ will play a central role in our subsequent renormalization-group analysis.] Above the critical point there is one real solution of (2.3), with $\exp[-\overline{\mathcal{H}}(\sigma)]$ being a singly peaked function around $\bar{\sigma}$, and the free energy per unit volume is given by

$$W(u_1, u_2, u_4) = -(1/V)\ln Z = \overline{\mathcal{H}}(\bar{\sigma})/V \tag{2.5}$$

Below the critical point, there are three real solutions of (2.3) (which define the spatially uniform solutions) and have the standard form

$$\begin{aligned}\bar{\sigma}_1 &= 2\left(\frac{|u_2|}{3u_4}\right)^{1/2}\cos\phi \\ \bar{\sigma}_2 &= -\left(\frac{|u_2|}{3u_4}\right)^{1/2}\cos\phi + \left(\frac{|u_2|}{u_4}\right)^{1/2}\sin\phi \\ \bar{\sigma}_3 &= -\left(\frac{|u_2|}{3u_4}\right)^{1/2}\cos\phi - \left(\frac{|u_2|}{u_4}\right)^{1/2}\sin\phi\end{aligned} \tag{2.6}$$

and

$$\phi = \frac{1}{3}\cos^{-1}\frac{-u_1}{2u_4(|u_2|/3u_4)^{3/2}}$$

In this case the function $\exp[-\overline{\mathcal{H}}(\sigma)]$ is a two-peaked function whose extrema occur at the values $\bar{\sigma}_i$ given by (2.6). For positive u_1 (negative H) and large system size, the stable state, being the absolute minimum, gives the dominant contribution to (2.1). On the other hand, we can calculate the metastable free energy by evaluating (2.1) only in the neighborhood of the metastable extrema. We also note that the two extrema (associated with the metastable and unstable states) coincide as u_1 moves toward its spinodal value. Knowing the $\bar{\sigma}$'s as functions of u_1, we can obtain the free energy density function,

$$W(u_1) \equiv \mathcal{H}(\bar{\sigma}_i(u_1))/V \tag{2.7}$$

(which is a multivalued function of u_1 for $T < T_c$), where

$$\mathcal{H}(\sigma) = u_1\sigma + \tfrac{1}{2}u_2\sigma^2 + \tfrac{1}{4}u_4\sigma^4 \tag{2.8}$$

This function is shown for illustrative purposes in Fig. 1 for the values $|u_2| = 2.0$ and $u_4 = 0.1$.

We now turn to a discussion of the renormalization-group equations for this model, which are given by[3]

$$\frac{\partial}{\partial l}\mathcal{H}(\sigma, l) = d\mathcal{H}(\sigma, l) - \frac{\alpha}{2}\left(\frac{\partial\mathcal{H}(\sigma, l)}{\partial\sigma}\right)^2 - \left(\frac{d}{2} - \beta\right)\sigma\frac{\partial\mathcal{H}(\sigma, l)}{\partial\sigma} \tag{2.9}$$

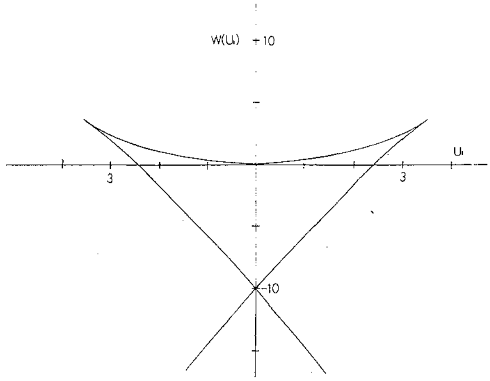

Fig. 1. A plot of $W(u_1)$ with $|u_2| = 2.0$ and $u_4 = 0.1$.

where β is the spin rescaling parameter, α is a constant which parametrizes the group, l is the length rescaling parameter, and d is the dimensionality. (Note that in the usual notation $2\beta = 2 - \eta$, where η is the correlation length exponent.) Exact solutions for the fixed points, eigenfunctions, and eigenvalues of (2.9) were found earlier.[3] This form of the renormalization-group equation is a useful one if one wishes to discuss a scale-invariant theory such as characterizes a critical point. However, if one wishes to calculate the free energy, as is our purpose, or obtain a solution of (2.9), it is more useful to introduce transformations which remove the spin and length rescaling that is one part of the usual renormalization-group operation. Thus we introduce new variables

$$x = (2\beta/\alpha)^{1/2} \exp\left[-(d/2 - \beta)l\right]\sigma \tag{2.10}$$

and

$$t = \exp(2\beta l) - 1 \tag{2.11}$$

in terms of which (2.9) becomes

$$\frac{\partial}{\partial t}\hat{\mathcal{H}}(x,t) = -\frac{1}{2}\left(\frac{\partial\hat{\mathcal{H}}(x,t)}{\partial x}\right)^2 \tag{2.12}$$

where

$$\hat{\mathcal{H}}(x,t) = \exp(-dl)\,\mathcal{H}(\sigma,l) \tag{2.13}$$

This equation is nothing but the Hamilton–Jacobi equation of a free particle with unit mass. Finally, we note that certain invariance properties of $\mathcal{H}(\sigma,l)$ also hold for $\hat{\mathcal{H}}(x,t)$. For example, in the previous paper we showed that the values for the extrema $\bar{\sigma}_l$ of the renormalized Hamiltonian

$\mathcal{H}(\bar{\sigma}, l)$ satisfy the equation

$$d\bar{\sigma}_l/dl = (d/2 - \beta)\bar{\sigma}_l \tag{2.14}$$

This effect was shown to be related to a redundant variable and was eliminated by a simple shift of variables. In the present case, it is even simpler, since it follows immediately from (2.10) that

$$\bar{x}(t) = (2\beta/\alpha)^{1/2}\exp[-(d/2 - \beta)l]\,\bar{\sigma} \tag{2.15}$$

and hence from (2.14) and (2.15),

$$d\bar{x}(t)/dt = 0 \tag{2.16}$$

That is, the extrema of $\hat{\mathcal{H}}(x,t)$ remain invariant. (In the mechanical analog this corresponds to the particle at rest with zero momentum.) Similarly, it can be shown that

$$\mathcal{H}(\bar{x}(t),t) = \mathcal{H}(\bar{x}(0),0) \tag{2.17}$$

i.e., that the free energy is invariant.

The results (2.16) and (2.17) reflect the simple fact that the renormalization does not affect thermodynamic properties.

3. EXACT SOLUTIONS OF THE RENORMALIZATION GROUP EQUATIONS

In this section we discuss the main result of this paper, namely the exact solution of the unscaled renormalization equation [see (2.12)]

$$\frac{\partial\mathcal{H}(x,t)}{\partial t} = -\frac{1}{2}\left(\frac{\partial\mathcal{H}(x,t)}{\partial x}\right)^2$$

where from now on we drop the "hat" on $\mathcal{H}$. The solution of Eq. (2.12) can be shown to be

$$\mathcal{H}(x,t) = \tfrac{1}{2}th^2(x,t) + \mathcal{H}(x - th(x,t),0) \tag{3.1}$$

where

$$h(x,t) \equiv \partial\mathcal{H}(x,t)/\partial x \tag{3.2}$$

satisfies

$$h(x,t) = \psi(x - th(x,t)) \tag{3.3}$$

The function ψ depends only on the initial Hamiltonian, with

$$\psi(x) = h(x,0) = \partial\mathcal{H}(x,0)/\partial x \tag{3.4}$$

The details of solving (2.12) are given in the Appendix. It is easy to show that (3.1) is a solution of (2.12), however, since the derivative with respect to t of (3.1) yields, using (3.2) and (3.3),

$$\frac{\partial}{\partial t}\mathcal{H}(x,t)=\frac{1}{2}h^2(x,t)+th(x,t)\frac{\partial h(x,t)}{\partial t}$$
$$+\psi(x-th(x,t))\left[-h(x,t)-t\frac{\partial h}{\partial t}\right]$$
$$=-\frac{1}{2}h^2(x,t)$$

which is the original differential equation (2.12). In order to actually construct the explicit solution from (3.1) one must, of course, first solve (3.3) for $h(x,t)$. The results of this are given later in this section. However, it is useful to first discuss the qualitative features which we find.

To simplify the discussion we consider an initial Hamiltonian[3]

$$\mathcal{H}(x,0)=u_1(0)x+\tfrac{1}{2}u_2(0)x^2+\tfrac{1}{4}u_4(0)x^4 \tag{3.5}$$

which is normally used in the mean field theory of critical phenomena. The coefficient $u_2(0)$ is positive or negative, depending on whether the temperature is greater or less than the critical temperature. From (3.4) and (3.5) we have

$$\psi(x)=u_1(0)+u_2(0)x+u_4(0)x^3 \tag{3.6}$$

which is shown in Fig. 2. In order to discuss the solution of (3.3) [and hence (3.1)] corresponding to (3.6), it is useful to make a change of variables

$$y(x,t)=x-th(x,t) \tag{3.7}$$

[3] More complicated cases, such as tricritical behavior, can be included in our general solution by choosing, for example, a polynomial of degree six for $\mathcal{H}(x,0)$, where a tricritical point would correspond to both $u_2(0)$ and $u_4(0)$ vanishing.

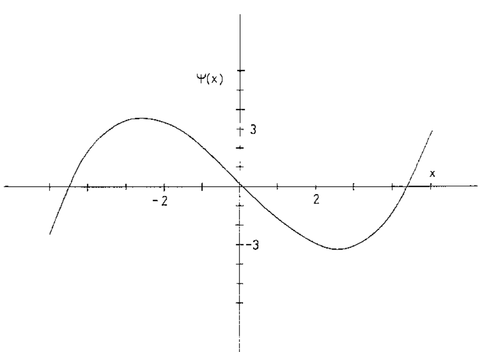

Fig. 2. A plot of $\psi(x)$ with $u_1(0)=0.175$, $u_2(0)=-2.0$, and $u_4(0)=0.1$.

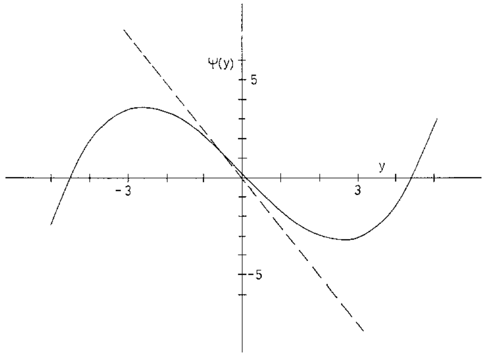

Fig. 3. A plot of $\psi(y)$ with $u_2(0) = 2.0$, $u_4(0) = 0.1$, and $u_1(0) = 0.175$. Also shown is the line $-y/t$ for $t < \bar{t}$.

in terms of which (3.3) becomes

$$-(y-x)/t = \psi(y) \tag{3.8}$$

We show the graphical solution of (3.8) in Fig. 3 for the special case $x = 0$. Note that in general the renormalization parameter now occurs in a very simple way in (3.8). From Fig. 3 it is clear that there are two qualitatively different situations to consider in the solution of (3.8). In one case there is only one real solution for y [and hence $h(x,t)$], but in the second case there are three possible real solutions for $y(x,t)$ and $h(x,t)$. It is the latter case which is unusual insofar as normal renormalization-group results are concerned, since it can yield a multivalued $\mathcal{H}(x,t)$ through (3.1), (3.7), and (3.8). This requires a somewhat careful discussion, which we give below. However, at this stage it is useful to note that the multivaluedness of $h(x,t)$ and $\mathcal{H}(x,t)$ which we find originates from the simple fact that we must solve the cubic equation (3.8) which involves the function $\psi(x)$. However, this same function determines the Gibbs free energy $W(u_1)$ through the identity

$$W(u_1) = \int_0^{\bar{x}_i} \psi(x)\, dx \tag{3.9}$$

where the $\bar{x}_i$ are the solutions of $\psi(x) = 0$ [i.e., the extrema of $\mathcal{H}(x,0)$]. Therefore the multivaluedness which we find in $\mathcal{H}(x,t)$ is intimately linked to the multivaluedness of $W(u_1)$, as shown in Fig. 1 for $T < T_c$. Thus in a loose sense one can say that our solution for $\mathcal{H}(x,t)$ is "slaved" by the function $\psi(x)$ through (3.1) and (3.3). We now turn to a more quantitative discussion of our results.

3.1. Stable One-Phase Region

We first consider a solution of (3.3) using the substitution (3.7) in the one-phase region, i.e., $u_2(0) > 0$, and in the presence of a magnetic field. That is, we consider solutions of Eq. (3.8), which reduces to

$$y^3 + \frac{1}{u_4(0)}\left[u_2(0) + \frac{1}{t}\right]y + \frac{1}{u_4(0)}\left[u_1(0) - \frac{x}{t}\right] = 0. \qquad (3.10)$$

The coefficient of the linear term is always positive, which implies that there is only one real solution of this equation for all positive t. The real solution for $h(x,t)$ has the form

$$h(x,t) = \frac{x}{t} - \frac{1}{t}\left[\left(\frac{x/t - u_1(0)}{2u_4(0)} + D\right)^{1/3} + \left(\frac{x/t - u_1(0)}{2u_4(0)} - D\right)^{1/3}\right] \qquad (3.10a)$$

where

$$D = \left\{\frac{[u_1(0) - x/t]^2}{4u_4^2(0)} + \frac{[u_2(0) + 1/t]^3}{27u_4^3(0)}\right\}^{1/2}$$

Then, using the expression for $\mathcal{H}(x,t)$ given in Eq. (3.1), we can calculate $\mathcal{H}(x,t)$ and $h(x,t)$ for any values of x and t. A plot of $h(x,t)$ as a function of x for $t = 2$ is shown in Fig. 4a. The corresponding function $\mathcal{H}(x, t = 2)$ is shown in Fig. 4b. $\mathcal{H}(x,t)$ has one minimum as a function of x at $\bar{x}_1(0)$, which remains fixed, i.e., $\bar{x}(t) = \bar{x}(0)$. We also have that $\mathcal{H}(\bar{x},t) = \mathcal{H}(\bar{x},0)$. In addition, as expected, $h(x,t)$ has one zero as a function of x for all t.

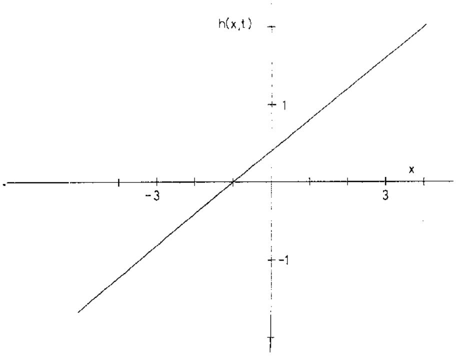

Fig. 4a. A plot of $h(x,t)$ for $t = 2$, $u_1(0) = 2.0$, $u_2(0) = +2.0$, and $u_4(0) = 0.1$.

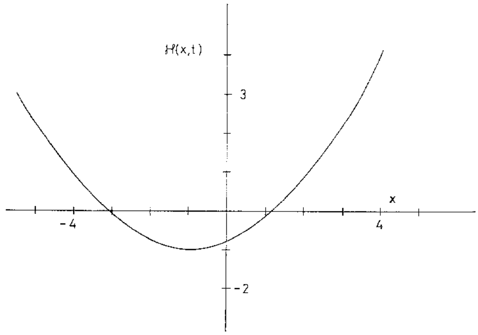

Fig. 4b. A plot of $\mathcal{H}(x,t)$ for $t=2$, $u_1(0)=2.0$, $u_2(0)=+2.0$, and $u_4(0)=0.1$.

Finally we note that in the limit as $t\to\infty$ one should obtain the equilibrium free energy from $\mathcal{H}(x,t)$. That this is indeed the case can be seen from (3.8), which implies that, in general,

$$\lim_{t\to\infty} th(x,t) = x - \bar{x}_i \tag{3.11}$$

where $\bar{x}_i$ are the zeros of $h(x,t)$. In the stable one-phase region there is only one zero, as noted above. Thus from (3.1) and (3.11) we have

$$\begin{aligned}\lim_{t\to\infty} \mathcal{H}(x,t) &= \lim_{t\to\infty} \tfrac{1}{2}th^2(x,t) + \lim_{t\to\infty} \mathcal{H}(x - th(x,t), 0)\\ &= \mathcal{H}(\bar{x}_i, 0)\end{aligned} \tag{3.12}$$

which is the correct free energy for the stable state.

3.2. Stable Two-Phase Coexistence

We next consider the region below the critical point. Consider first the simplest case, in which $u_1(0)=0$, so that there are two stable, coexisting phases, with the Gibbs free energy being the same for the two phases. In spite of this single-valuedness of the free energy, however, we will see that there is a region of t for which $\mathcal{H}(x,t)$ becomes multivalued. We begin with (3.8), which for $T<T_c$ and $u_1=0$ yields

$$y^3 + \frac{1}{u_4(0)}\left[\frac{1}{t} - |u_2(0)|\right]y - \frac{x}{tu_4(0)} = 0 \tag{3.13}$$

We note that for $t < t^* = |u_2|^{-1}$, there is only one real solution for y, but for $t > t^*$ there are three real solutions for y. That is, for $t>t^*$, $h(x,t)$ is a multivalued function of x. These three real solutions have the form

$$h^{(1)}(x,t) = -\frac{2}{t}\left[\frac{|u_2| - 1/t}{3u_4}\right]^{1/2}\cos\phi + \frac{x}{t}$$

$$h^{(2)}(x,t) = \frac{1}{t}\left[\frac{|u_2| - 1/t}{3u_4}\right]^{1/2}\cos\phi - \frac{1}{t}\left[\frac{|u_2| - 1/t}{u_4}\right]^{1/2}\sin\phi + \frac{x}{t}$$

$$h^{(3)}(x,t) = \frac{1}{t}\left[\frac{|u_2| - 1/t}{3u_4}\right]^{1/2}\cos\phi + \frac{1}{t}\left[\frac{|u_2| - 1/t}{u_4}\right]^{1/2}\sin\phi + \frac{x}{t} \tag{3.14}$$

where

$$\phi = \frac{1}{3}\cos^{-1}\frac{x/t}{2u_4\left[(|u_2| - 1/t)/3u_4\right]^{3/2}} \tag{3.15}$$

where, for the remainder of this section, we will use the notation u_1, u_2, and u_4 to denote the initial values of $u_1(t)$, $u_2(t)$, and $u_4(t)$.

Thus we find that for $t > t^*$ and for certain values of x, $h(x,t)$ is a multivalued function, as shown in Fig. 5a. The corresponding plot of $\mathcal{H}(x,t)$ for $t > t^*$ is shown in Fig. 5b. As can be seen, there are three separate branches of $\mathcal{H}(x,t)$ in this region, similar to the situation for the Gibbs free energy $W(u_1)$ for $T < T_c$, Fig. 1. Furthermore, each of these branches of $\mathcal{H}(x,t)$ has one (and only one) of the extrema $\bar{x}_i(t) = \bar{x}_i(0)$, so that in a certain sense one could associate each of these branches with the one unstable and two stable phases, respectively. For $t < t^*$ there is only one branch of $\mathcal{H}(x,t)$, which has all three extrema associated with it. As $t = t^*$, $\mathcal{H}(x,t^*)$ has a "cusp-like" structure.

In view of the multivalued nature of $h(x,t)$ and $\mathcal{H}(x,t)$ it is of some

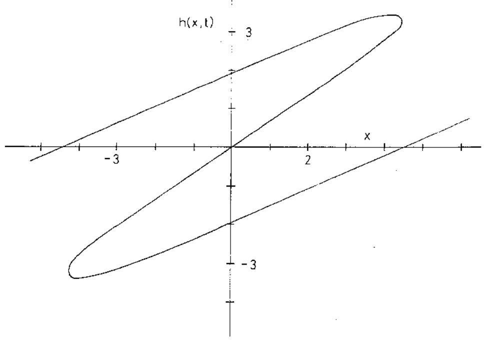

Fig. 5a. A plot of $h(x,t)$ for $t = 2$, $u_1(0) = 0$, $u_2(0) = -2.0$, and $u_4(0) = 0.1$.

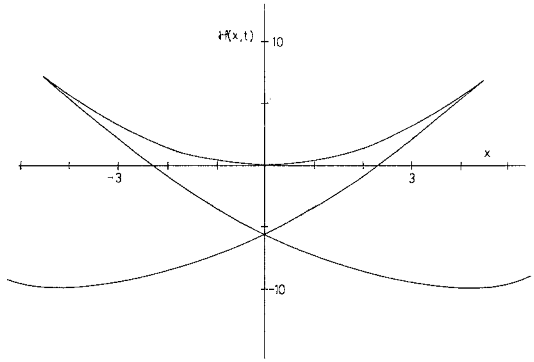

Fig. 5b. A plot of $\mathcal{H}(x,t)$ for $t=2$, $u_1(0)=0$, $u_2(0)=-2.0$, and $u_4(0)=0.1$.

mathematical interest to note that if one uses the relation

$$\mathcal{H}(x,t)=\int_0^x h(x',t)\,dx' \tag{3.16}$$

to compute $\mathcal{H}$, then one is faced with a choice of contours in the multivalued region. For instance, if one considers Fig. 6, evaluating $\int_0^x h(x',t)\,dx'$ at the point labeled 3 on the diagram, we can integrate along the contours (1-2-3), (4-3), or (5-4-3). It can be shown that no matter which contour one uses to evaluate $\mathcal{H}(x,t)$, $\mathcal{H}(x,t)$ is uniquely determined at each point of the contour. Finally, we note that the free energies of the two stable and one unstable phases can be obtained from the $t\to\infty$ limit of $\mathcal{H}(x,t)$, using the same argument as at the end of the previous paragraph. The only difference is that there are now three real extrema $\bar{x}_i$, so that one gets three free energies.

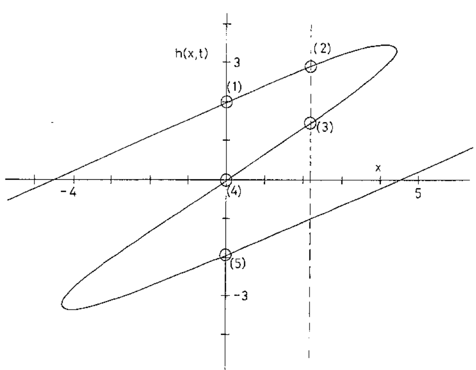

Fig. 6. A plot of $h(x,t)$ for $t=2$, $u_1(0)=0$, $u_2(0)=-2.0$, and $u_4(0)=0.1$, showing the possible contours.

3.3. The Metastable and Unstable Free Energies

We conclude our discussion of the solution of the RG equations by considering the $T < T_c$ and $u_1 \neq 0$ case. This is of most interest for our discussion since it includes the metastable and unstable states in addition to the stable state; our primary concern is to obtain a renormalization-group description of the metastable state. The mathematical details are very similar to Section 3.2. The equation for $y(x,t)$ is

$$y^3 + \frac{1}{u_4}\left(\frac{1}{t} - |u_2|\right)y + \frac{1}{u_4}\left(u_1 - \frac{x}{t}\right) = 0 \tag{3.17}$$

and the solutions are of the same form as (3.14) but with

$$\phi = \frac{1}{3}\cos^{-1}\frac{x/t - u_1}{2u_4\left[\left(|u_2| - 1/t\right)/3u_4\right]^{3/2}} \tag{3.18}$$

Again we find that $h(x,t)$ and $\mathcal{H}(x,t)$ become multivalued for $t > t^*$, where

$$t^* = 1/|u_2| \tag{3.19}$$

The behavior of $h(x,t)$ and $\mathcal{H}(x,t)$ for $t > t^*$ is shown in Figs. 7a and 7b. As in the two-phase coexistence region, each of the branches of $\mathcal{H}(x,t)$ is associated with one of the three invariant extrema corresponding to the stable, metastable, and unstable phases. For each branch one also has $\mathcal{H}^{(i)}(\bar{x}_i, t) = \mathcal{H}(\bar{x}_i, 0)$, expressing the invariance of each of the three "free energies." Finally we note that we obtain these free energies from the $t \to \infty$ limit of each of these branches; i.e.,

$$\begin{aligned}\lim_{t\to\infty} \mathcal{H}^{(i)}(x,t) &= \lim_{t\to\infty} \tfrac{1}{2}t\left[h^{(i)}(x,t)\right]^2 + \lim_{t\to\infty} \mathcal{H}\left(x - th^{(i)}(x,t), 0\right)\\ &= \mathcal{H}(\bar{x}_i, 0)\end{aligned} \tag{3.20}$$

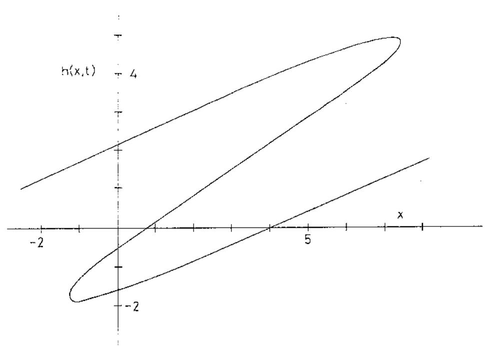

Fig. 7a. A plot of $h(x,t)$ for $t = 2$, $u_1(0) = 1.5$, $u_2(0) = -2.0$, and $u_4(0) = 0.1$.

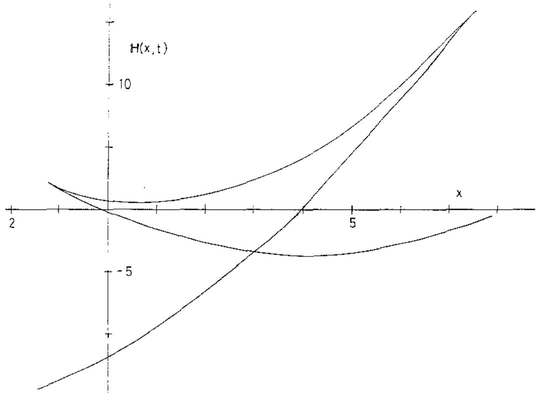

Fig. 7b. A plot of $\mathcal{H}(x,t)$ for $t=2$, $u_1(0)=1.5$, $u_2(0)=-2.0$, and $u_4(0)=0.1$.

In summary, it would seem that the most interesting result of our exact solution is that of the multivaluedness of $\mathcal{H}(x,t)$ for $t>t^*$ which occurs in the renormalization-group description for our system with more than one phase. In the context of this simple mean field theory, the existence of the three invariant extrema $\bar{x}_i$ leads to an initial $\mathcal{H}(x,0)$ with two wells developing into three distinct branches, each characterized by one of the $\bar{x}_i$.

4. EVALUATION OF THE FREE ENERGY BY A TRAJECTORY INTEGRAL

It has become standard in renormalization-group literature both to represent the renormalized Hamiltonian by a functional Taylor series expansion and to evaluate the free energy via an evaluation of the spin-independent piece. In view of the multivalued $\mathcal{H}(x,t)$ encountered in this mean field model (Section 3), it is not obvious that this standard procedure is useful in the two-phase region. In this section we examine the consequences of such an expansion and display the rather unusual trajectories which arise. In particular, we will show that it is possible to obtain the correct values for the metastable and unstable free energies by the trajectory integral formalism. However, this involves considering negative values of t, for which we have at present no convincing physical interpretation. We also find that each branch of $\mathcal{H}(x,t)$ has its own Taylor series expansion.

We begin by seeking a power series solution for the equation

$$\frac{\partial}{\partial t}\mathcal{H}(x,t) = -\frac{1}{2}\left[\frac{\partial}{\partial x}\mathcal{H}(x,t)\right]^2$$

where we write

$$\mathcal{H}(x,t) = u_0(t) + \sum_{n=1}^{\infty} \frac{u_n(t)}{n} x^n \tag{4.1}$$

Then Eq. (4.1) implies a series of coupled differential equations for the coupling constants,

$$\begin{aligned} \partial u_0(t)/\partial t &= -\tfrac{1}{2}u_1^2(t) \\ \partial u_1(t)/\partial t &= -u_1(t)u_2(t), \quad \text{etc.} \end{aligned} \tag{4.2}$$

Thus, if we wish to formulate a typical trajectory integral[6] for the free energy we see that the $u_0(t)$ equation involves knowing $u_1(t)$ only,

$$u_0(t) = -\tfrac{1}{2}\int_0^t u_1^2(t')\,dt' \tag{4.3}$$

where $u_1(t) \to u_1(0)$ as $t \to 0$.

If we now use the expansion (4.1) for $\mathcal{H}(x,t)$, then we expect that

$$h(x,t) = \frac{\partial \mathcal{H}(x,t)}{\partial x} = \sum_{n=1}^{\infty} u_n(t)x^{n-1} \tag{4.4}$$

Then we get, using (4.4) and (3.3),

$$u_1(t) = h(0,t) = \psi(-th(0,t)) = \psi(-tu_1(t))$$

Thus if we set

$$y = -tu_1(t) \tag{4.5}$$

then we have that

$$-y/t = \psi(y) \tag{4.6}$$

Before we examine the solutions of (4.6), let us look again at the results of Section 3, as well as the mean field theory for $\mathcal{H}(x,0)$ given in Section 2. First, an expression for $u_0(t)$ can be obtained from Eq. (3.1) with x equal to zero,

$$u_0(t) = \tfrac{1}{2}th^2(0,t) + \mathcal{H}(-th(0,t),0) \tag{3.1a}$$

This function becomes multivalued as a function of t at $\bar{t}$ where $h(0,t)$ first becomes multivalued. Thus in using a Taylor series expansion we expect that for $t > \bar{t}$ the coefficients of our expansion for $\mathcal{H}(x,t)$ should become multivalued, corresponding to separate Taylor series for each of the branches of $\mathcal{H}(x,t)$ obtained in Section 3. Second, we found for the particular case where $\psi(x)$ has the form [Eq. (3.6)]

$$\psi(x,0) = u_1(0) - |u_2(0)|x + u_4(0)x^3$$

that in the limit as $t \to \infty$, $u_0(t)$ took on three values, namely $\mathcal{H}(\bar{x}_s,0)$, $\mathcal{H}(\bar{x}_m,0)$, and $\mathcal{H}(\bar{x}_u,0)$, corresponding to the three free energies which are stable, metastable, and unstable, respectively. Thus we expect to find similar behavior for the function (4.3) in the limit as t goes to infinity.

Finally, it follows from (3.4) with the condition $\mathcal{H}(0,0)=0$ [see (3.5)] that the free energies are given by [see (3.9)]

$$\mathcal{H}(\bar{x},0)=\int_0^{\bar{x}}\psi(x)\,dx$$

Thus in the case where $\psi(x)$ has the form above, i.e., Eq. (3.8), then the metastable state involves an integral such that

$$\mathcal{H}(\bar{x}_m,0)=\int_0^{\bar{x}_u}\psi(x)\,dx+\int_{\bar{x}_u}^{\bar{x}_m}\psi(x)\,dx \tag{4.7}$$

Thus, with these three points in mind, let us reexamine Eq. (4.6) in the context of a suggestive graphical solution. Consider Fig. 3, where we exhibit a graphical solution of the equation

$$-y/t=\psi(y)=u_1(0)-|u_2(0)|y+u_4(0)y^3 \tag{4.8}$$

We can see from the diagram that initially there is one real solution, and at a value of $t=\bar{t}$, say, a multivalued solution for $u_1(t)$ develops. These solutions are shown in Fig. 8a for the particular case of $u_1(0)=0.175$. On looking at this diagram, one first notices that although $u_1(t)$ is multivalued for $t>\bar{t}$ we see that only one solution obeys the boundary condition $u_1(t)\to u_1(0)$ as $t\to 0$. We are thus faced with the dilemma as to how to calculate the free energies of the metastable and unstable states in the context of this series solution.

In resolving this problem we first notice that in Fig. 3 there is a section of the curve $\psi(y)$, i.e., for $0<y<\bar{y}_u$, such that the line $-y/t$ does not intersect it for positive t. In mean field theory the unstable free energy is

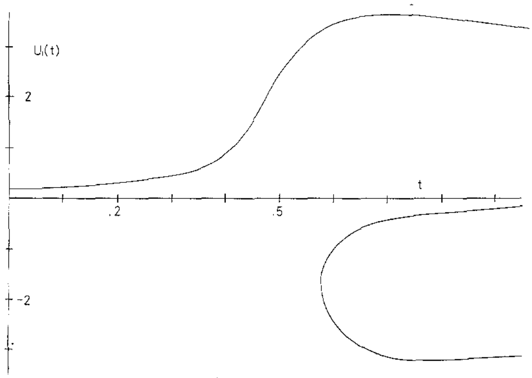

Fig. 8a. A plot of the function $u_1(t)$ for $u_1(0)=0.175$, $u_2(0)=-2.0$, and $u_4(0)=0.1$.

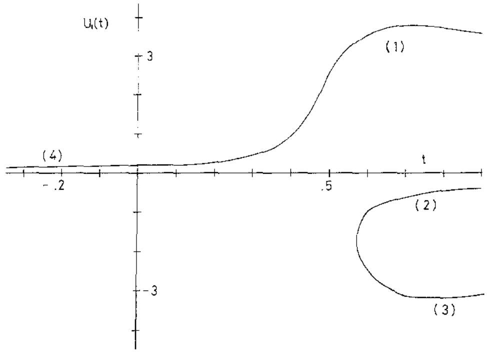

Fig. 8b. A plot of the function $u_1(t)$ for all values of t, where we have labeled the branches of the function (1), (2), (3), and (4).

defined as

$$W_u = \mathcal{H}(\bar{x}_u, 0) = \int_0^{\bar{x}_u} \psi(y)\, dy \tag{4.9}$$

If we make the change of variable such that $y = -tu_1(t)$, then

$$dy = -dt\left[u_1(t) + t\frac{\partial u_1(t)}{\partial t} \right]$$

Then

$$\begin{aligned} \int_0^{\bar{x}_u} \psi(y)\, dy &= -\frac{1}{2}\int_{t(0)}^{t(\bar{x}_u)} u_1^2(t)\, dt - \left[\frac{1}{2} u_1^2(t) \right]_{t(0)}^{t(\bar{x}_u)} \\ &= -\frac{1}{2}\int_0^{t(\bar{x}_u)} u_1^2(t)\, dt \end{aligned} \tag{4.10}$$

But for positive t, and y such that $0 < y < \bar{y}_u$, there is no solution for $u_1(t)$ such that $y = -tu_1(t)$, as can be seen from the graphical solution in Fig. 3.

Thus to resolve the problem of the unstable free energy and also the interpretation of the two solutions of $u_1(t)$ in Fig. 8a which do not approach $u_1(0)$ as $t \to 0$, we again consider Fig. 3. We see that if we search for a solution for *negative* t, namely a solution of the equation

$$y/|t| = \psi(y) \tag{4.11}$$

then there does indeed exist a solution for which $t = -tu_1(t)$ for $0 < y < y_u$ and which goes over to $u_1(0)$ in the limit as $t \to 0$. Therefore, if we were now to draw in all the solutions of interest to us for $u_1(t)$, we get the diagram in Fig. 8b, where we have labeled the branches as shown. Thus

$$W_u = -\frac{1}{2}\int_0^{-\infty} u_1^2(t)\, dt \tag{4.12}$$

along branch 4, where we have used the result (4.11). Similarly

$$W_s = \left[-\frac{1}{2} \int_0^{\infty} u_1^2(t)\, dt \right]_{①} \tag{4.13}$$

This can be seen by considering the graphical solution of Fig. 3. Similarly we can show that

$$W_n = \left[-\frac{1}{2} \int_0^{-\infty} u_1^2(t)\, dt \right]_{④} + \left[-\frac{1}{2} \int_{\infty}^{\bar{t}} u_1^2(t)\, dt \right]_{②} + \left[-\frac{1}{2} \int_{\bar{t}}^{\infty} u_1^2(t)\, dt \right]_{③} \tag{4.14}$$

where again we have used the graphical solution to choose the correct trajectory. We notice that for each of these trajectories, $u_1(t) \to u_1(0)$ as $t \to 0$, as it must. It can be shown that these interpretations are consistent with the solutions for $u_0(t)$ already obtained in Section 3.

Thus to conclude this section we find that to calculate a free energy associated with a metastable state using a trajectory integral of the function $u_1(t)$, one has to find solutions of Eq. (4.2),

$$\partial u_0 / \partial t = -\tfrac{1}{2} u_1^2(t)$$

such that $u_1(t) \to u_1(0)$ as t goes to zero. Therefore in the case of the metastable and, in particular, the unstable state this involves finding a solution of $u_1(t)$ for negative t.

It should be clear from the above discussion that a single power series expansion is not an appropriate representation for a function such as $\mathcal{H}(x,t)$ which is multivalued in the two-phase region. In particular, the computation of the metastable free energy involves two separate branches of $\mathcal{H}(x,t)$, each of which is represented by its own power series expansion. In order to obtain the expansion coefficients, however, we have had to consider negative t.

APPENDIX

A general solution of the equation [Eq. (2.12)]

$$\partial \mathcal{H}(x,t) / \partial t = -\tfrac{1}{2} (\partial \mathcal{H} / \partial x)^2$$

is of the form

$$\mathcal{H} = a(x,t)x - \tfrac{1}{2} a^2(x,t)t + \phi(a(x,t)) \tag{A1}$$

where ϕ is some arbitrary function of the constant of integration a. The quantity $a(x,t)$ is obtained by solving the equation

$$\phi'(a) = a(x,t)t - x \tag{A2}$$

Thus if we define the function $h(x,t)$ by

$$h(x,t) = \partial\mathcal{H}(x,t)/\partial x \tag{A3}$$

then (A1) and (A3) imply that

$$h(x,t) = a(x,t) + \frac{\partial\mathcal{H}}{\partial a}\frac{\partial a(x,t)}{\partial x} = a(x,t)$$

Therefore we see from this result and (A2) that $h(x,t)$ is the solution of the equation

$$x = th(x,t) - \phi'(h(x,t)) \tag{A4}$$

Further, for $t = 0$ we have

$$h(x,0) = \psi(x,0) = \partial\mathcal{H}(x,0)/\partial x \tag{A5}$$

and

$$x = h(x,0) - \phi'(h(x,0)) \equiv f^{-1}(h) \tag{A6}$$

where $\psi(x)$ is a single-valued function which depends only on the initial Hamiltonian. We therefore see from (A5) and (A6) that $f = \psi$. It immediately follows from (A6) and (A4) that

$$\psi^{-1}(h) = h - \phi'(h) = -ht + x$$

i.e.,

$$h(x,t) = \psi(x - th(x,t)) \tag{A7}$$

Equation (A3) implies

$$\mathcal{H}(x,t) = u_0(t) + \int_0^x h(x',t)\,dx' \tag{A8}$$

If we multiply both sides of (A7) by

$$[1 - t\,\partial h(x,t)/\partial x]$$

and integrate over x, we have that

$$\int_0^x h(x',t)\,dx' - \int_0^x h(x',t)t\frac{\partial h(x',t)}{\partial x}\,dx' = \int_0^x \psi(x' - th(x',t))\left(1 - t\frac{\partial h}{\partial x}\right)dx'$$

Therefore we get that

$$\int_0^x h(x',t)\,dx' = \tfrac{1}{2}t\big[h^2(x,t)\big]\Big|_0^x + \big[\mathcal{H}(x - th(x,t),0)\big]\Big|_0^x \tag{A9}$$

Therefore (A8) implies that

$$\mathcal{H}(x,t) = u_0(t) + \tfrac{1}{2}t\big[h^2(x,t)\big]\Big|_0^x + \big[\mathcal{H}(x - th(x,t),0)\big]\Big|_0^x \tag{A10}$$

This implies that

$$u_0(t) = \tfrac{1}{2}th^2(0,t) + \mathcal{H}(-th(0,t),0) \tag{A11}$$

and hence

$$\mathcal{H}(x,t) = \tfrac{1}{2}th^2(x,t) + \mathcal{H}(x - th(x,t),0) \tag{A12}$$

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