Microcanonical Density Functionals for Critical Systems: An Exact One-Dimensional Example

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Free-energy functionals suitable for describing realistic, nonuniform systems near criticality are discussed with emphasis on the advantages of a local formalism. It is proposed to investigate *micro*canonical functionals in which both the usual order-parameter (or magnetization) density $m(\mathbf{r})$ *and* the local energy density $\varepsilon(\mathbf{r})$, which has independent critical fluctuations, are employed. This approach is tested by an exact calculation of the microcanonical functional $\mathscr{S}[\{m\}, \{\varepsilon\}]$ in the continuum limit for a one-dimensional Ising model. Remarkably, the microcanonical functional is found to be local irrespective of the proximity to the critical point (located at zero temperature and zero field). Furthermore, its form relates closely to the scaling postulate advanced earlier by de Gennes and Fisher and displays features of conformal covariance.

KEY WORDS: Density functionals; energy functionals; Ising model; scaling theory; criticality; surfaces; interfaces; microcanonical; one-dimensional.

1. INTRODUCTION: MICROCANONICAL FUNCTIONALS

One of the advantageous features of the Landau, phenomenological, or mean-field theory of critical phenomena is that the inhomogeneous order parameter profile $m(\mathbf{r})$ induced by an arbitrary external field $h(\mathbf{r})$ (where, for simplicity, we consider only an Ising-like, one-component order parameter) can be obtained by minimization of a simple *local* free energy functional, namely,

$$\Omega[\{m\}] = \int d^d r \left\{ \tfrac{1}{2} c \, |\nabla m|^2 - h(\mathbf{r}) \, m(\mathbf{r}) + \tfrac{1}{2} t_0 m^2(\mathbf{r}) + \tfrac{1}{4} u m^4(\mathbf{r}) + \cdots \right\} \qquad (1.1)$$

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Here the last two terms represent the usual polynomial approximation for the free energy of a homogeneous system (the ellipsis denoting the higher-order terms which may be added if necessary), while $c = \xi^2/\chi$ denotes the order-parameter "stiffness" with ξ the bulk correlation length and χ the susceptibility. Note that $\Omega[\{m\}]$ is similar in form to the standard Landau–Ginzburg–Wilson Hamiltonian $\mathcal{H}_{LGW}[\{s\}]$, where $s(\mathbf{r})$ is the fluctuating spin variable; we regard $m(\mathbf{r}) = \langle s(\mathbf{r})\rangle$ as the thermal *average* of s calculated with the Boltzmann factor $\exp(-\beta\mathcal{H}_{LGW})$. The substitution of the spin variables by their averages yielding $\Omega[\{m\}] \simeq \mathcal{H}_{LGW}[\{s=m\}]$ forms the essence of the mean-field (or, in diagrammatic language, tree) approximation.[1]

A word about the concept "local" is in order. In practice, what one asks for is a functional which is given as a spatial integral over a finite number of locally defined fields or densities $m(\mathbf{r}),...$ and a *finite* number of their simple (i.e., not fractional) derivatives $\nabla m(\mathbf{r})$, $\nabla^2 m(\mathbf{r}),...$, all evaluated at the same point. At the back of one's mind is a more detailed or microscopic functional expression which would involve multipoint integral kernels $\mathcal{K}_2(\mathbf{r}, \mathbf{r}')$, $\mathcal{K}_3(\mathbf{r}, \mathbf{r}', \mathbf{r}'')$, etc. of *finite range* in the sense that all moments with respect to $(\mathbf{r}-\mathbf{r}')$, $(\mathbf{r}-\mathbf{r}''),...$ exist or that the decay of the kernels as $|\mathbf{r}-\mathbf{r}'|$, $|\mathbf{r}-\mathbf{r}''|,...$ increase is "rapid," i.e., exponential or faster. Then a truncated moment expansion, involving a finite number of derivatives, should reproduce all long-wavelength behavior correctly. Conversely, if one allows indefinitely high derivatives *or* infinitely many densities, *any* $\Omega[\{m\}]$ can be made local *formally* by introducing an infinite number of additional densities (entailing all spatial derivatives of m and their combinations, etc.).

The simplicity of (1.1) has provided a basis for many advances in theory. Unfortunately, the basic approximation breaks down in the critical region below the upper critical dimension ($d = 4$, for the specific case of the spin systems under consideration), where the long-range correlations are usually believed to render the exact functional $\Omega[\{m\}]$ nonlocal.

More specifically, starting with a Hamiltonian $\mathcal{H}[\{s\}]$, with the source term

$$- \int h(\mathbf{r})\, s(\mathbf{r})\, d\mathbf{r}$$

added, one obtains the free energy

$$F = -k_B T \ln \left\{ \int \mathcal{D}s \exp[-\beta\mathcal{H}(\{s\})] \right\} \tag{1.2}$$

By definition this is a functional of the external field $h(\mathbf{r})$, say, $F = \mathscr{F}[\{h\}]$. Taking its functional derivatives generates the connected correlation functions of s, the first of which is just

$$m(\mathbf{r}) = \langle s(\mathbf{r}) \rangle = -\delta \mathscr{F} / \delta h(\mathbf{r}) \tag{1.3}$$

If now the relation (1.3) can be inverted to yield $h(\mathbf{r}) = \mathscr{J}[\mathbf{r}, \{m\}]$ as a functional of m, then the Legendre transform

$$\Gamma[\{m\}] = \int m(\mathbf{r}) \, \mathscr{J}[\mathbf{r}, \{m\}] \, d\mathbf{r} + \mathscr{F}[\{\mathscr{J}(\mathbf{r}, \{m\})\}] \tag{1.4}$$

can be constructed and one then has

$$\Omega = \Gamma - \int hm \, d\mathbf{r} \tag{1.5}$$

This is the procedure described in many field-theory and statistical mechanics textbooks,[1-4] where it is also proven that $\Gamma[\{m\}]$ is the generating functional for the one-particle-irreducible (vertex) correlation functions. However, almost nothing is known about the general properties of the functional Γ at a critical point (or massless theory, in field-theoretic language) below the upper critical dimension. The ϵ expansion for a profile $m(\mathbf{r})$ involves, to first order in $\epsilon = 4 - d$, calculation of the determinant of the Schrödinger-type operator

$$-c\nabla^2 + 3um_0^2(\mathbf{r})$$

where $m_0(\mathbf{r})$ is the solution minimizing the zeroth-order mean-field functional (1.1). All the advances along this line of which we are aware, both in the theory of instantons[2,3] and of surface critical behavior,[5] were achieved for particular problems in which the zeroth-order profile m_0 allowed for explicit solution of the corresponding Schrödinger equation. These calculations prove to be strongly nonlocal in nature but give no direct information concerning the functional $\Gamma[\{m\}]$ itself.

On the other hand, several *local* but approximate functionals of the form

$$\tilde{\Omega}[t, \{m\}] = \int d\mathbf{r} \, \{\mathscr{A}_0[t, m(\mathbf{r})] + \mathscr{A}_1(\xi[t, m(\mathbf{r})] \, \nabla m)\} \tag{1.6}$$

have been proposed as generalizations of (1.1).[6,7],2 Here $\mathscr{A}_0(t, m)$ and $\xi(t, m)$ are, respectively, the bulk thermodynamic potential density and the

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2 See also the earlier work by Fisk and Widom,[8] which employed a simpler approximation.

bulk correlation length for the given reduced temperature $t = (T - T_c)/T_c$ and *homogeneous* magnetization m; both these functions may be regarded as known from the theory of the bulk critical phenomena. Beyond that, the function $\mathscr{A}_1$, which vanishes with ∇m, is constructed so as to satisfy as many known constraints as feasible.[6,7] This approach appears to be surprisingly effective for a number of problems concerning finite systems at criticality, near-critical adsorption, etc.,[7] despite the fact that the form (1.6) is presumably not the correct generating functional for the vertex functions. There are also certain fairly subtle physical aspects for which a functional of the form (1.6) has been shown to embody flaws[7,9] (see also comments in ref. 10).

However, a more profound shortcoming of *any local* free energy functional $\Omega(t, \{m\})$ utilising only the order-parameter profile $m(\mathbf{r})$ becomes apparent when one attempts to use it to calculate the wall free energy of a near-critical system *above* T_c, or to investigate the associated local perturbations to the bulk caused by a wall or interface, in the special but significant *symmetric case* in which the boundary conditions at the wall or interface do *not* break the (precise) order-parameter symmetry of the bulk (see, e.g., ref. 11). Important practical examples are provided by interfaces and walls in liquid helium-four near the transition to superfluidity[11,12] and by grain boundaries and surfaces in ferromagnetic materials in zero field or simple antiferromagnets in uniform fields.

More concretely, consider a semi-infinite system at an ordinary Ising-like bulk critical point[5] with a surface or wall that does not break the magnetic symmetry either explicitly, by imposition of a surface magnetic field, or by sufficiently strong surface enhancement of the surface ordering interactions. In this case the magnetization profile of the system above and at T_c is everywhere identically zero; thus the only contribution to a local Ω can come directly from the surface or wall itself. On the other hand, since the wall must in general change the exchange interactions locally (for example, by changing the number of neighbors for the surface spins), one expects a local *energy density perturbation*

$$\varepsilon(\mathbf{r}) \propto \langle s^2(\mathbf{r}) \rangle - \langle s^2(\infty) \rangle_c \tag{1.7}$$

which will decay with the normal distance z from the wall or interface as[4,6,13]

$$\varepsilon(\mathbf{r}) \sim 1/z^{\omega_\varepsilon} \quad \text{with} \quad \omega_\varepsilon = (1 - \alpha)/\nu \tag{1.8}$$

Clearly such a long-range tail in the local energy density cannot be understood on the basis of a local $\Omega[\{m\}]$. Furthermore, it is associated with a corresponding slow decay which leads to a *singular*, critical contribution

to the surface free energy[11] above T_c which cannot be obtained correctly from any local order-parameter functional like $\tilde{\Omega}[\{m\}]$.

To overcome this difficulty and provide a basis for practical computations for the symmetric case, we propose to investigate the conjugate, "microcanonical" thermodynamic potential $\mathscr{S}[\{m\}, \{\varepsilon\}]$, defined as a functional of *both* the local magnetization *and* the local energy density. Such an approach is rather natural from the viewpoint of general scaling theory.[4,13],3 Thus, one of the major defects of mean-field theory or Landau theory is the failure to predict truly singular critical behavior for the specific heat: the behavior of the energy is totally driven by the variation of the magnetization. This is, of course, built into (1.1). On the other hand, the nontrivial specific heat exponent seen in real systems and found in exactly solved models is represented in scaling theory and renormalization group analysis via the existence of *two independent* relevant critical operators (or densities) at a standard critical point, namely, the order parameter m and the energy ε. These are characterized by distinct scaling dimensions $\omega_m < \omega_\varepsilon < d$ or positive renormalization group eigenvalue exponents $\lambda_m = d - \omega_m > \lambda_\varepsilon = d - \omega_\varepsilon$. Accordingly, to obtain a complete, leading-order local description of critical behavior in nonhomogeneous situations, it seems appropriate to consider both relevant densities $m(\mathbf{r})$ and $\varepsilon(\mathbf{r})$, on an essentially similar footing.

Of course, once this idea is accepted, a crucial issue is whether these two densities are sufficient to render the corresponding microcanonical functional $\mathscr{S}[\{m\}, \{\varepsilon\}]$ local. More modestly, one may hope that a significantly improved level of description, even if still only approximate, can be attained via suitable local functionals of m and ε together.

A few comments regarding terminology may be useful. If one deals with a particle system in a finite domain Δ, the terms grand canonical (gr), canonical (can.), and microcanonical (mic) for the corresponding *statistical mechanical ensembles* have well-established definite meanings, namely, the control variables are, respectively: $\text{gr} \equiv (T, \mu)$, $\text{can.} \equiv (T, N)$, and

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3 The need to go beyond a single order-parameter theory in discussing symmetric *critical endpoints*, as observed notably in superfluid helium (see, e.g., ref. 7), has been recognized independently by, in particular, Tavan and Widom.[12] Such a possibility is also especially clear in the phenomenological analysis of any *multi*component fluid system: Note the discussions in refs. 14 and 15. However, the essential point here, which we believe is novel, is the aim to treat the local *energy* and its fluctuations as *distinct* from the standard "symmetry-breaking" magnetic or compositional order parameters, which, even in symmetric cases, display a discontinuity below the critical point. (Recall that in a simple Ising-like or similar symmetric critical situation, the thermodynamic energy is *continuous* across the first-order transition boundary, as are the specific heat and all energy–energy correlation functions, etc.) Furthermore, independent, *non*driven critical behavior for $\varepsilon(\mathbf{r})$ should be represented in the formalism or arise transparently in the analysis.

mic $\equiv (U, N)$. Of course, the corresponding overall *thermodynamic poten-tials* are $Vp(T, \mu)$, $F_{tot}(T, N)$, and $S_{tot}(U, N)$. Nevertheless, if one contem-plates a magnetic system (such as an Ising model), the terminology is *not* so well established: however, the lattice gas–Ising ferromagnet analogy indicates that the natural correspondence is gr $\equiv (T, H)$, can. $\equiv (T, M)$, and mic $\equiv (U, M)$. As regards potentials, the notation $F(T, H)$ is standard; $A(T, M)$ has been proposed (originally by R. B. Griffiths); $S(U, M)$ is reasonable by analogy. In the more general situation where one envisages some general local order parameter $\Psi(\mathbf{r})$, it is natural to identify Ψ with M in the magnetic situation. Finally, recall that in the thermodynamic limit $V(\Delta) \to \infty$, suitably taken, all ensembles describe precisely the same physics.

Now the standard classical or Landau-type phenomenological theory for critical behavior, in which one expands in powers of Ψ and $(T - T_c)$, then addresses the thermodynamic potential $A(T, \Psi)$ which, if h is the con-jugate ordering field, satisfies $F(T, h) = \min_\Psi [A(T, \Psi) - h\Psi]$. While one leaves aside the question of calculating $A(T, \Psi)$ or $F(T, h)$ from statistical mechanics, for which the natural two ensembles would, by extension, be called canonical and grand canonical, the issue is only one of *ther-modynamic assemblies*: both would be called isothermal, since T is a con-trolled parameter, but, beyond that, there is no generally accepted ter-minology; *iso-ordering* and isochamp, respectively, are possible but we do not especially advocate these terms. More natural, we feel, is to extend the statistical mechanical usage so that: (i) a thermodynamic description or a calculation in which T and h are controlled is described as *grand canonical* and, likewise, if slowly varying $T(\mathbf{r})$ and $h(\mathbf{r})$ are specified; (ii) if T and Ψ, or $T(\mathbf{r})$ and $\Psi(\mathbf{r})$, are held fixed, as *canonical*; and (iii) if U and Ψ, or $\varepsilon(\mathbf{r})$ and $\Psi(\mathbf{r})$, are controlled, as *microcanonical*. In a thermodynamic functional formulation, then, we refer to $\mathscr{A}[T; \Psi(\mathbf{r})]$ ($\equiv \Gamma[\{\Psi\}]$) as a *canonical functional*; one functional minimization is required to compute the thermodynamic potential $F(T, h)$. By the same token, we call the entropy functional $\mathscr{S}[\varepsilon(\mathbf{r}), \Psi(\mathbf{r})]$ a *microcanonical functional*; a double functional minimization is required to compute $F(T, h)$, which, in all cases, we regard as the most basic thermodynamic potential.

In the slowly varying thermodynamic limit the various potentials and functionals will be well defined and related to one another via Legendre transformations. Of course, if these Legendre transformations are implemented in a finite system, the various results will *not* agree precisely. Thus, for example, one may compute the "microcanonical functional" $\mathscr{S}[\varepsilon, \Psi]$ grand canonically (as we will do) *or* canonically. For $V(\Delta) < \infty$ the exact results will differ; but these differences, which do not interest us here, will vanish in the thermodynamic limit.

Now it is, of course, appropriate to check the proposed microcanonical approach first at the phenomenological or mean-field level. This is readily done.[16],4 Thus in the simplest symmetric situation the postulate (1.1) is replaced by

$$\mathscr{S}[\{m\}, \{\varepsilon\}] = \int d^d r \left\{ \tfrac{1}{2} c_m |\nabla m|^2 + \tfrac{1}{2} c_\varepsilon |\nabla \varepsilon|^2 + \tfrac{1}{2} c_{m\varepsilon} \nabla(m^2) \cdot \nabla \varepsilon \right.$$

$$- hm(\mathbf{r}) - t\varepsilon(\mathbf{r})$$

$$\left. + e_{20} \varepsilon^2(\mathbf{r}) + e_{12} \varepsilon(\mathbf{r}) m^2(\mathbf{r}) + e_{04} m^4(\mathbf{r}) + \cdots \right\} \qquad (1.9)$$

with the obvious generalizations for nonsymmetric cases. Of course, c_m, c_ε, and $c_{m\varepsilon}$ all remain finite through the critical region. One thence obtains a fully classical description of the critical point (or of a critical endpoint[7,11,12]) with the standard critical exponents $\beta = 1/2$, $\gamma = 1$, $\nu = 1/2$, etc. The only new feature is that energy profiles and energy–energy correlation functions can now be computed. However, even at the critical point, the energy profile and correlations decay *exponentially*; all long-distance, singular behavior is still controlled by the order parameter and its fluctuations in the usual classical way.

Thus, rather little of real interest arises at the classical or mean-field level. Various other lines of investigation, such as field-theoretic renormalization group analysis, are, however, quite open and are being pursued.[16] In this paper we test the approach by analyzing a continuum one-dimensional model equivalent to the linear ferromagnetic nearest-neighbor Ising model in the vicinity of its critical point at $T = 0$, $h = 0$.[17] We are able to calculate explicitly the microcanonical functional $\mathscr{S}[\{m\}, \{\varepsilon\}]$ and find that, indeed, it is completely local! It must be noted, however, that an elegant, explicitly local exact expression for the entropy functional of the discrete, one-dimensional nearest-neighbor Ising model has recently been obtained by Percus.[18],5 Nevertheless the discrete form of $\mathscr{S}$ does not exhibit the important universal features, specifically *scale invariance* and (asymptotic) *conformal covariance*, that we uncover. In our calculation we implement the required Legendre transformations directly on the original

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4 See also footnote 3 above.

5 See also the references therein. The calculations undertaken by Percus were motivated by his program to construct the entropy for particle systems as a functional of the *one*-point and *two*-point *correlation functions*, the latter being thermodynamically conjugate to the two-point or particle–particle interaction potential. In general, this choice of second density and conjugate thermodynamic field is quite distinct from what we are proposing, in terms of a local energy density. However, in the case of the nearest-neighbor Ising model the pair-interaction potential reduces to a local scalar and the two definitions of entropy functional coincide.

continuum model, reducing it, in the process, to a two-level quantum mechanical system in continuous imaginary time. In the end, of course, we check that our results may be obtained from Percus' expression by taking an appropriate continuum limit.

Beyond its scaling character our functional assumes the postulated form[6,7] (1.6), but with t replaced by $\varepsilon(\mathbf{r})$. In other words, gradient terms involving $\nabla\varepsilon$ do *not* contribute to $\mathscr{S}$. This result, which is somewhat surprising, is certainly special to the one-dimensional case $d = 1$. However, it could be a hint that the way in which local gradients of $\varepsilon(\mathbf{r})$ enter $\mathscr{S}$ for $4 > d > 1$ (supposing that they do) may be significantly more complex than the customary gradient expansions tend to suggest. In any event, we hope that this explicit calculation for a simple linear system will clarify the little-explored nature of the critical thermodynamic potential of an inhomogeneous system. Such exact studies have, for one-dimensional systems, previously been enlightening in uncovering the operations of renormalization groups,[17] in the density functional theory of fluids,[18,19] and in the theory of critical interfaces.[20]

2. THE ONE-DIMENSIONAL MODEL

The procedure of calculating $\mathscr{S}[\{m\}, \{\varepsilon\}]$ which we use here is a straightforward generalization of the definition of $\Gamma[\{m\}]$ given in the Introduction; see (1.4). However, we will now need to supplement the Hamiltonian with two external or source terms, namely,

$$+ \tfrac{1}{2}\int d\mathbf{r}\, t(\mathbf{r})\, s^2(\mathbf{r})$$

which embodies an arbitrary position-dependent "temperature deviation" $t(\mathbf{r})$ and

$$- \int d\mathbf{r}\, h(\mathbf{r})\, s(\mathbf{r})$$

as discussed previously. The resulting "grand canonical" free energy or thermodynamic potential $\mathscr{F}[\{h\}, \{t\}]$ will be subject to a double Legendre transform with respect to both h and t, to yield the desired "microcanonical" functional $\mathscr{S}[\{m\}, \{\varepsilon\}]$.

Specifically, we consider a long linear chain of sites $j = 1,..., N$ with a discrete Ising variable $s_j = \pm 1$ located at each site j. Each spin interacts with a local external field h_j and also with its nearest neighbors, so that a pair of *anti*parallel neighbors with $s_j s_{j+1} < 0$ increases the energy by t_k,

where $k \equiv (j, j+1)$ labels the *bonds* of the spin chain. The Hamiltonian of the model is thus

$$\mathscr{H} = -\sum_j h_j s_j + \tfrac{1}{2} \sum_{k \equiv (j, j+1)} t_k(1 - s_j s_{j+1}) \qquad (2.1)$$

where, in more standard notation, the $t_k = 2J_k$ are all positive. For convenience, the thermal energy $k_B T$ will be used to scale all the energies in the calculation, so the free energy is just

$$\mathscr{F}[\{h\}, \{t\}] = -\ln \left(\sum_{\{s_i = \pm 1\}} \exp[-\mathscr{H}] \right) \qquad (2.2)$$

The mean energy density defined in this way, namely,

$$\varepsilon_k = \partial \mathscr{F}/\partial t_k = \tfrac{1}{2}(1 - \langle s_j s_{j+1} \rangle) \qquad (2.3)$$

has the clear meaning of the density of "broken bonds" or "domain walls."

The problem of calculating the free energy in (2.2) is readily reexpressed using the transfer matrices

$$\mathbf{T}_j = \begin{bmatrix} e^{h_j} & 0 \\ 0 & e^{-h_j} \end{bmatrix}, \qquad \mathbf{T}'_k = \begin{bmatrix} 1 & \zeta_k \\ \zeta_k & 1 \end{bmatrix} \qquad (2.4)$$

$$F = -\ln Z = -\ln \mathrm{Tr} \left(\prod_{j=1}^{N} \mathbf{T}_j \mathbf{T}'_{(j, j+1)} \right) \qquad (2.5)$$

where we have introduced the local fugacity of a domain wall via

$$\zeta_k = \exp(-t_k) = \exp(-2J_k/k_B T) \qquad (2.6)$$

The critical point of the model is at $T_c = 0$ and zero field,[17,20] so that the approach to overall criticality is described by $h_j \to 0$ and $t_k \to \infty$ or $\zeta_k \to 0$. To obtain the desired continuum limit, we must restrict the fields h_j and ζ_k so that the important lengths arising thermodynamically are much greater than the lattice spacing a. That means that each factor in the matrix product in (2.5) should differ little from the unit matrix, so that significant changes in the state vector accumulate only over large distances. Physically, one may think of an Ising chain at any $h > 0$ and t as a gas of clusters (or domains) of magnetization of opposite sign to h. When h increases, the size of such a cluster decreases like $1/h$, while generally the distance between two neighboring clusters is of order $1/\zeta$. Since both these distances must greatly exceed a, we suppose the fields h_j and ζ_k (which are otherwise arbitrary) satisfy

$$|h_{j+1} - h_j| \ll |h_j| \ll 1, \qquad 0 < \zeta_k \ll 1 \qquad (2.7)$$

that is, they are small in absolute value and vary slowly on the scale of the lattice spacing, which we set to unity below. (Of course, the positivity of ζ follows from its definition above.)

Under these conditions we go over to a continuum description. We define the matrix

$$\tilde{\mathbf{T}}_{k=(j,\,j+1)} = \mathbf{T}_j^{1/2}\mathbf{T}_k'\mathbf{T}_{j+1}^{1/2} \approx \mathbf{I} + \begin{bmatrix} h_k & \zeta_k \\ \zeta_k & -h_k \end{bmatrix} \tag{2.8}$$

where $h_k = \frac{1}{2}(h_j + h_{j+1})$ and we have neglected terms of order $|h_{j+1} - h_j|$ and h_k^2 in the expansion about the unit matrix $\mathbf{I}$. On introducing the matrix product

$$\mathbf{Z}(x) = \prod_{k<x} \tilde{\mathbf{T}}_k \tag{2.9}$$

we may use (2.7), which implies $Z(x+1) - Z(x) \ll Z(x)$, and then consider $x = n$ as a continuous variable. Thence we obtain

$$\frac{d}{dx}\mathbf{Z}(x) = \begin{bmatrix} h(x) & \zeta(x) \\ \zeta(x) & -h(x) \end{bmatrix} \mathbf{Z}(x) = [\zeta(x)\,\sigma_1 + h(x)\,\sigma_3]\,\mathbf{Z}(x) \tag{2.10}$$

where the σ_i are the standard Pauli matrices. For an initial condition it is adequate to take $\mathbf{Z}(0) = \mathbf{I}$.

The relations (2.5) and (2.10), with $Z = \mathrm{Tr}\{\mathbf{Z}(N)\}$ define the model. The idea of writing a differential equation for the incomplete partition sum matrix $\mathbf{Z}(x)$ was inspired by the work of Percus,[19] who considered classical hard-core particles on a line in an arbitrary external potential. Evidently (2.10) can be regarded as a Schrödinger equation in imaginary time x for a two-state quantum mechanical system in a time-dependent external field and with a time-varying tunneling probability.

3. CALCULATION OF THE FREE ENERGY

The representation of the "equation of motion" (2.10) via the Pauli matrices reveals a notable symmetry between the field h and the fugacity ζ (which, indeed, is also a known feature of the discrete model). Another representation of (2.10), making this symmetry even more transparent, is obtained by mapping the columns of the matrix $\mathbf{Z}(x) \equiv [Z_{ij}(x)]$ $(i, j = 1, 2)$ onto two complex numbers via the definitions

$$z_l(x) = Z_{1l}(x) + iZ_{2l}(x) \qquad \text{with} \quad l = 1, 2 \tag{3.1}$$

so that

$$z_1(0) = 1, \qquad z_2(0) = i \qquad (3.2)$$

Then we have

$$dz_l/dx = \mu(x)\, z_l^* \qquad (l = 1, 2) \qquad (3.3)$$

where the varying magnetic and thermal fields are embodied in the local external potential

$$\mu(x) = h(x) + i\zeta(x) \qquad (3.4)$$

while the asterisk denotes complex conjugation. By introducing polar coordinates in the complex plane through

$$\mu(x) = \rho(x)\, e^{i\varphi(x)}, \qquad z_l(x) = r_l(x)\, e^{i\theta_l(x)} \qquad (3.5)$$

we may rewrite (3.3) as the pair of equations

$$\frac{1}{r_l}\frac{dr_l}{dx} = \rho\,\cos(\varphi - 2\theta_l), \qquad r_l(0) = 1 \qquad (3.6)$$

$$\frac{d\theta_l}{dx} = \rho\,\sin(\varphi - 2\theta_l) \qquad (l = 1, 2) \qquad (3.7)$$

Note that by the definitions (3.4) and (3.5) and the positivity of ζ, the angle of φ is strictly bounded by

$$0 < \varphi < \pi \qquad (3.8)$$

while $\theta_1(0) = 0$ and $\theta_2(0) = \frac{1}{2}\pi$.

It is now easily seen that (3.7) describes the relaxation of θ_1 and θ_2 toward the value $\frac{1}{2}\varphi$, the variation of both being strictly bounded by

$$0 < \theta_l < \tfrac{1}{2}\pi \qquad \text{for all} \quad x > 0 \qquad (3.9)$$

For a homogeneous system, with $\varphi(x)$ and $\rho(x)$ constant, both θ_l relax toward $\frac{1}{2}\varphi$ at a rate corresponding to a spatial correlation length given (in units of the lattice spacing a) by

$$\xi = \rho^{-1} = (h^2 + \zeta^2)^{-1/2} \qquad (3.10)$$

while $d(\ln r_l)/dx$ attains the maximal value

$$\rho = \rho_0 \equiv (h^2 + \zeta^2)^{1/2} \qquad (3.11)$$

Consequently we find $r_l(x) \sim \exp(\rho_0 x)$ and thus we have

$$-F = \rho_0 L + O(1) \qquad \text{as} \quad L \equiv Na \to \infty \tag{3.12}$$

Of course, this expression for the free energy is equivalent to the well-known result.[17] It can be checked easily by noting that $(h^2 + \zeta^2)^{1/2}$ is the largest eigenvalue of $\tilde{T}$, as defined in (2.8), in this uniform limit. Note also that the conditions (2.7) imply that the correlation length satisfies $\xi \gg 1$, as anticipated.

When $\varphi(x)$ varies, however, the $\theta_l(x)$ are not able to follow $\frac{1}{2}\varphi(x)$ exactly. Thus, the right-hand side of (3.6) falls below $\rho(x)$ and one has

$$r_l(x) = \exp\left\{ \int^x \rho(y) \cos[\varphi(y) - 2\theta_l(y)] \, dy \right\} < \exp\left[\int^x \rho(y) \, dy \right] \tag{3.13}$$

It follows that the free energy, which is given by

$$\begin{aligned} F = -\ln\Bigg[&\exp\left\{ \int_0^L \rho(x) \cos[\varphi(x) - 2\theta_1(x)] \, dx \right\} \cos\theta_1(L) \\ &+ \exp\left\{ \int_0^L \rho(x) \cos[\varphi(x) - 2\theta_2(x)] \, dx \right\} \sin\theta_2(L) \Bigg] \end{aligned} \tag{3.14}$$

[see (2.5), (3.1), (3.5), (3.6)] is larger than the natural local approximation, namely

$$F_{\text{loc}} = -\int_0^L \rho(x) \, dx \tag{3.15}$$

We can obtain further insight by linearizing (3.7), which, we will show, is justified when $d\varphi/dx \ll \rho(x)$. The linearized equation is readily solved to yield

$$\begin{aligned} \theta_l(x) = \theta_l(0) \exp\left[-2\int_0^x \rho(y) \, dy \right] \\ + \int_0^x dy\, \rho(y)\, \varphi(y) \exp\left[-2\int_y^x \rho(y') \, dy' \right] \end{aligned} \tag{3.16}$$

The main conclusion to be drawn is that if

$$\int_0^x \rho(y) \, dy \to \infty \qquad \text{when} \quad x \to \infty \tag{3.17}$$

i.e., the integral of $\rho(x)$ grows without bound as x increases, then the dependence on the initial conditions is eventually lost. [Note that $\rho(x)$ is

strictly positive.] For sufficiently large x, one thus has $\theta_1(x) = \theta_2(x) \equiv \theta(x)$ and (3.14) immediately yields

$$-F = \int_0^L dx \, \rho(x) \cos[\varphi(x) - 2\theta(x)] + O(1) \tag{3.18}$$

Now the expansion in $d\varphi/dx$, embodied in the linearized form (3.16) to leading order, can be formally carried to any order. This is most conveniently done by putting $2\theta_l(x) = \varphi(x) - \psi_l(x)$, so that from (3.7) one has, as the equation of motion for $\psi_l(x)$,

$$\frac{d\psi_l}{dx} + 2\rho \sin \psi_l = \frac{d\psi_l}{dx} + 2\rho\psi_l - \frac{1}{3}\rho\psi_l^3 + \cdots = \frac{d\varphi}{dx} \tag{3.19}$$

When $d\varphi/dx$ is small, the angles ψ_l will also be small, so that the nonlinear terms on the left-hand side of (3.19) may be treated perturbatively. By induction we find that to any fixed order the result has a form similar to (3.16), namely,

$$\theta_l(x) = \Theta_l[\theta_l(0), \{\varphi\}, x] \exp\left[-2\int_0^x \rho(y)\,dy\right] + \Theta_0(\{\varphi\}, x) \tag{3.20}$$

where Θ_0 does not depend on the initial conditions, while the part carrying that information carries an explicit exponential extinction factor. Since the variation of Θ_l is bounded via (3.9), the results (3.17) and (3.20) formally imply the convergence $\theta_1(x), \theta_2(x) \to \Theta_0(x)$ as x increases. That, in turn, justifies (3.18).

It is plausible that the expansion underlying (3.20) normally has a nonzero radius of convergence: in other words, if for all x the ratio $|d\varphi/dx|/\rho$ is bounded by a suitable constant of order unity, then (3.20) is fully valid. Since the variation of 2θ excludes the endpoints 0 and π [see (3.9)], it is even plausible that the relaxational dynamics of (3.7) always ensures the convergence of θ_1 and θ_2 to $\theta(x)$ on some bounded length scale determined by the growth of the integral in (3.17).

Being unable to make more definitive statements at present, we will limit our considerations to the "smooth" or "steady" regime, in which θ_1 and θ_2 do indeed converge on a finite scale to a definite $\theta(x)$, so that (3.18) is valid. Physically this means that the influence of the boundary conditions is limited to the appearance of surface terms of order unity in the total free energy. One might also, for example, suppose that a sufficiently thick slab of a homogeneous phase, with some $\varphi = \text{const}$, is placed at the origin, so providing effectively for relaxation to $\theta_1 = \theta_2 = \frac{1}{2}\varphi$ before the inhomogeneous region is reached. We also expect that unsteady or fluctuating

regimes, if present, will be revealed as solutions of the final Euler–Lagrange equations (see Section 4 below) of a similar character.

Consequently, (3.7) and (3.18) constitute the main result of this section: to obtain the total free energy $F \equiv \mathscr{F}[\{h\}, \{t\}]$ up to corrections of order unity, one has to solve (3.7) for $\theta(x)$ with *any* initial condition and then substitute in (3.18). We will show in the next section that this procedure is at least self-consistent, yielding an unambiguous local expression for $\mathscr{S}[\{m\}, \{\varepsilon\}]$.

We close this section with two comments:

(a) The argument $\psi(x)$ of the cosine in (3.18), as determined by (3.7) or (3.19), depends on all values of $\varphi(x') = \cot^{-1}(h/\zeta)$ in the interval $x - \rho^{-1} \lesssim x' < x$ [as seen by comparison with (3.16) and (3.10)]. When ρ becomes small, the free energy $\mathscr{F}[\{h\}, \{t\}]$ thus becomes highly nonlocal, as was to be anticipated in view of (3.10).

(b) However, the effects of nonlocality are induced by variation of $\varphi(x)$ only. If h and t conspire so as to keep the ratio h/ζ constant, the free energy is precisely given by the local approximation (3.15). Noting that $-\delta F_{\text{loc}}/\delta h(x) = m(x) = \cos \varphi(x)$, we see that $\varphi = \text{const}$ is equivalent to $m = \text{const}$. Consequently, we learn that $\mathscr{S}[\{m\}, \{\varepsilon\}]$ cannot contain additive terms depending solely on $d\varepsilon/dx$, the gradient of the energy density. We will confirm this explicitly in the next section.

4. THE MICROCANONICAL THERMODYNAMIC POTENTIAL

In order to perform the double Legendre transform from the magnetic and thermal fields

$$h(x) = \rho(x) \cos \varphi(x) \tag{4.1}$$

$$t(x) = -\ln[\rho(x)] - \ln[\sin \varphi(x)] \tag{4.2}$$

to the corresponding conjugate magnetization $m(x)$ and (domain wall) energy $\varepsilon(x)$ densities, we use (3.18) and the covariant representation

$$\mathscr{S}[\{m\}, \{\varepsilon\}] = \max_{\rho, \varphi} \int dx \, [m\rho \cos \varphi + \varepsilon \ln \rho + \varepsilon \ln \sin \varphi - \rho \cos(2\theta - \varphi)] \tag{4.3}$$

where $\theta(x)$ satisfies (3.7); this latter equation of motion allows one to make the replacement

$$\varphi(x) = 2\theta(x) + \sin^{-1}[\rho^{-1}(d\theta/dx)] \tag{4.4}$$

The remaining calculation just entails solving the variational equations for (4.3) as a functional of $\rho(x)$, $\theta(x)$, and $(d\theta/dx)$. The main stages of an elementary but somewhat involved calculation are outlined in the Appendix. As regards principles, the derivation relies strongly on discarding the surface terms resulting after integration by parts: according to the discussion at the end of the previous section, we believe that these terms will contribute to the free energy of the boundaries, which is beyond the scope of the present analysis.

The result is found to be

$$
\mathscr{S}[\{m\}, \{\varepsilon\}] = \int dx \left\{ \varepsilon \ln\left(\frac{\varepsilon}{e}\right) - \tfrac{1}{2}\varepsilon \ln(1 - m^2) \right.
$$

$$
+ \tfrac{1}{2}\varepsilon \left[\left(1 + \frac{1}{2\varepsilon}\frac{dm}{dx}\right) \ln\left(1 + \frac{1}{2\varepsilon}\frac{dm}{dx}\right) \right.
$$

$$
\left. \left. + \left(1 - \frac{1}{2\varepsilon}\frac{dm}{dx}\right) \ln\left(1 - \frac{1}{2\varepsilon}\frac{dm}{dx}\right) \right] \right\} \tag{4.5}
$$

The "equations of motion," obtained by variation of

$$
\mathscr{Q} = \mathscr{S} + \int (t\varepsilon - hm)\, dx \tag{4.6}
$$

take the form

$$
\frac{\delta\mathscr{S}}{\delta\varepsilon(x)} = \tfrac{1}{2}\ln\left[\varepsilon^2 - \tfrac{1}{4}\left(\frac{dm}{dx}\right)^2\right] - \tfrac{1}{2}\ln(1 - m^2) = -t(x) \tag{4.7}
$$

$$
\frac{\delta\mathscr{S}}{\delta m(x)} - \frac{d}{dx}\left[\frac{\delta\mathscr{S}}{\delta(dm/dx)}\right] = \frac{\varepsilon m}{1 - m^2} - \tfrac{1}{2}\frac{d}{dx}\left[\tanh^{-1}\left(\frac{1}{2\varepsilon}\frac{dm}{dx}\right)\right] = h(x) \tag{4.8}
$$

Various points may now be made. First, consider the exact result of Percus for the discrete Ising model or lattice gas, namely, Eq. (2.12) of ref. 18. After expressing the lattice-gas one- and two-particle densities used in ref. 18 in terms of our magnetic variables via $n_x = \tfrac{1}{2}(1 - m_x)$ and

$$
n_{x,x+1} = \tfrac{1}{2}\left[1 + \tfrac{1}{2}(m_x + m_{x+1}) - \tfrac{1}{2}\varepsilon_{x,x+1}\right]
$$

and making the standard change to continuum notation via

$$
m(x) = \tfrac{1}{2}(m_x + m_{x+1}), \qquad \frac{dm}{dx} = m_{x+1} - m_x
$$

we can write Percus' expression as

$$\mathcal{S} = \int dx \left\{ \varepsilon \ln \varepsilon - \tfrac{1}{2}\varepsilon \ln[(1-\varepsilon)^2 - m^2] \right.$$

$$+ \frac{1-m}{2} \ln\left(1 - \frac{\varepsilon}{1-m}\right) + \frac{1+m}{2} \ln\left(1 - \frac{\varepsilon}{1+m}\right)$$

$$+ \tfrac{1}{2}\varepsilon \left[\left(1 + \frac{1}{2\varepsilon}\frac{dm}{dx}\right) \ln\left(1 + \frac{1}{2\varepsilon}\frac{dm}{dx}\right)\right.$$

$$\left.\left. + \left(1 - \frac{1}{2\varepsilon}\frac{dm}{dx}\right) \ln\left(1 - \frac{1}{2\varepsilon}\frac{dm}{dx}\right)\right]\right\} \qquad (4.9)$$

Note that the terms independent of dm/dx simply represent the exact entropy expression for a uniform Ising chain. Now the full expression reduces to (4.5) under the condition

$$\varepsilon \ll 1 - |m| \qquad (4.10)$$

which, following the discussion preceding (2.7), means physically that the typical size of a domain fluctuation is much larger than the lattice spacing. Indeed, (4.10) is equivalent to our original restriction $h \ll 1$ in (2.7), since $1 - |m|$ is of order ε/h when $\varepsilon \ll |h| \ll 1$.

Note, second, that the advantage of accepting the restriction (4.10) is that the entropy functional becomes *conformally covariant*. The conformal group in one dimension consists of all diffeomorphisms $x \to x'$. Conformal invariance of the critical state[21] means that any correlation function of the densities $\varphi_j(x)$ remains invariant under any conformal transformation if the densities are simultaneously rescaled according to

$$\varphi_j(x) \to \left(\frac{dx'}{dx}\right)^{\omega_j} \varphi_j(x') \qquad (4.11)$$

where ω_j is the scaling dimension of φ_j [see e.g., (1.8)]. Recalling the relation between $\mathcal{S}[\{m\}, \{\varepsilon\}]$ and $F[\{h\}, \{t\}]$, the latter being the generating functional for the correlation functions in question,[1,16] we may formulate the principle of conformal covariance of the entropy functional as follows: the functional $\mathcal{Q}$ in (4.6), taken at the critical point values of the fields t and h ($h = 0$ and $t = +\infty$ in our case), must be invariant under any conformal transformation

$$x = f(x') \qquad (4.12)$$

provided the densities m and ε are transformed according to (4.11) while the fields are rescaled locally via

$$h \to (dx'/dx)^{d-\omega_m} h(x'), \qquad t \to (dx'/dx)^{d-\omega_\varepsilon} t(x') \qquad (4.13)$$

It is easily seen that the form (4.5) is indeed conformally covariant if $\omega_m = 0$ and $\omega_\varepsilon = 1$: all elements of length dx enter (4.5) only in combination with $\varepsilon(x)$, so that the factors dx'/dx compensate each other. The term $\int dx' \, \varepsilon(x') \, \ln(dx'/dx)$, generated by rescaling of the energy density in the argument of the logarithm, contributes to the source term $\int dx' \, t(x') \, \varepsilon(x')$ and does not change its critical point value $t = +\infty$. The well-known[17] values of the scaling dimensions $\omega_m = 0$, $\omega_\varepsilon = 1$ can be easily verified by noting that the decay of the spin–spin correlation function in $d = 1$ is always purely exponential (implying $\eta = 1$), and that $\nu = 1/\lambda_\varepsilon = 1/(d - \omega_\varepsilon) = \infty$.

Third, most striking in the light of the discussion in the Introduction, is the fact that the microcanonical functional (4.5) is entirely *local*. Furthermore, it depends only on the *first* derivative of the local magnetization. Note, however, that Percus[18] has also managed to obtain a local, although rather complicated, expression for the *canonical* functional $\mathscr{A}[\{m\}, \{t\}]$ for the $d = 1$ Ising chain. Indeed, rearrangement of (4.7) expresses $\varepsilon(x)$ in terms of $t(x)$, $m(x)$, and (dm/dx); substitution in (4.5) then confirms canonical locality in the continuum limit.

The absence of any $(d\varepsilon/dx)^2$ terms and of other gradients of the density $\varepsilon(x)$ agrees with the physical picture that in the absence of a mean overall magnetization the system is essentially just an *ideal* gas of *non*interacting domain walls: clearly this is special to linear Ising-like models.

It is also interesting that the microcanonical functional embodies a basic feature of the Fisher–de Gennes[6,7] canonical form (1.5), namely that the gradient of the magnetization density is always scaled by the *local* correlation length, which is seen to be simply $\varepsilon^{-1}(x)$. Nevertheless, such a form could well break down in higher dimensions. (Recall, for comparison, van der Waals' excluded-volume approximation, which is exact in $d = 1$, but no longer fully correct in higher dimensions, although qualitatively valid.)

There are singularities in (4.5) as a function of ε that are all quite physical. That at $\varepsilon = 0$ corresponds to the suppression of all thermal excitations at $|m| = 1$ (complete saturation); those at $2\varepsilon = |dm/dx|$ reflect the fact that a jump of magnetization from $+1$ to -1 (or vice versa) can be achieved only at a domain wall. In both of these limits the continuum model becomes a less faithful representation the original Ising chain.

In conclusion, the conformally covariant microcanonical functional for a one-dimensional Ising-like system can be evaluated exactly in the vicinity of the zero-temperature, zero-field critical point; the functional is local and has an appealing scaled form.[6,7] Approximations for more general situations might profitably embody these features; but, even if they do not, the formulations should, ideally, reproduce the present results in the limit $d = 1$.

APPENDIX. DERIVATION OF THE MICROCANONICAL FUNCTIONAL

In order to derive $\mathscr{S}(\{m\}, \{\varepsilon\})$ from $\mathscr{F}(\{h\}, \{t\})$ as given by (4.3) with (4.4), we may start by substituting for $\rho(x)$ and $\theta(x)$ via

$$u(x) = [\rho^2(x) - (d\theta/dx)^2]^{1/2}, \qquad w(x) = \sin 2\theta(x) \qquad \text{(A1)}$$

For brevity we will denote (d/dx) by an overdot. Then the integrand in (4.3) may be written

$$\mathscr{L}(u, w, \dot{w}) = (1 - w^2)^{1/2} (mu - \tfrac{1}{2}\dot{m}) + \varepsilon \ln(uw + \tfrac{1}{2}\dot{w}) - u \qquad \text{(A2)}$$

where one integration by parts has been performed in (4.3) to obtain the term $\dot{m}(1 - w^2)^{1/2}$. The first Euler–Lagrange equation is simply $(\partial \mathscr{L}/\partial u) = 0$, which yields

$$\varepsilon/(uw + \tfrac{1}{2}\dot{w}) = 1 - m(1 - w^2)^{1/2} \qquad \text{(A3)}$$

The second one, derived using an integration by parts in the standard way, is $(\partial \mathscr{L}/\partial w) = (\partial \mathscr{L}/\partial \dot{w})^{\cdot}$. Upon repeated substitution of (A3) this eventually reduces to

$$\frac{\dot{m}}{2w(1 - w^2)^{1/2}} - \frac{w}{(1 - w^2)^{1/2}} \frac{m\varepsilon}{1 - m(1 - w^2)^{1/2}} + \frac{\varepsilon}{w} = 0 \qquad \text{(A4)}$$

Note that all terms involving $\dot{w}$ have cancelled, so providing a *local* expression for w in terms of m, $\dot{m}$, and ε, namely

$$w = (1 - m^2)^{1/2} [1 - (\dot{m}/2\varepsilon)^2]^{1/2}/|1 - (m\dot{m}/2\varepsilon)| \qquad \text{(A5)}$$

while (A3) then yields

$$u = (\varepsilon - \tfrac{1}{2}m\dot{m})/(1 - m^2) - \tfrac{1}{2}\dot{w}/w \qquad \text{(A6)}$$

Now note that in substituting for u and w in (A2), the last term in (A6) cancels in the argument of the logarithm. The same $\dot{w}/w$ term in u

may be discarded in the last term in (A2) as a perfect derivative, while in the first term it may be grouped with $-\dot{m}(1-w^2)^{1/2}$ to yield

$$-\frac{m\dot{w}}{2w(1-w^2)^{1/2}} - \tfrac{1}{2}\frac{d}{dx}\left[m(1-w^2)^{1/2}\right]$$

$$= -\tfrac{1}{2}m\frac{d}{dx}\ln\left\{\frac{w}{1+(1-w^2)^{1/2}}\right\} + \dot{D}_1(x) \qquad (A7)$$

where $\dot{D}_1(x)$ denotes a perfect derivative. Now, considering a further integration by parts, this can be rewritten as

$$\tfrac{1}{2}\dot{m}\ln\left(\frac{w}{1+(1-w^2)^{1/2}}\right) + \dot{D}_2(x)$$

$$= \tfrac{1}{4}\dot{m}\ln\left(\frac{1-m}{1+m}\right) + \tfrac{1}{4}\dot{m}\ln\left(\frac{1+(\dot{m}/2\varepsilon)}{1-(\dot{m}/2\varepsilon)}\right) + \dot{D}_2(x) \qquad (A8)$$

where $D_2(x)$ is a further perfect derivative and (A5) has been used to eliminate w. The first term on the right-hand side here is also a perfect derivative, since

$$\dot{m}f(m) = \frac{d}{dx}\int f(m)\,dm \qquad (A9)$$

and so may likewise be discarded. The remaining parts of (A5) and (A6) may be substituted into (A2) straightforwardly. On recalling that $\dot{m} = dm/dx$, this finally reproduces the form of the microcanonical functional as recorded in (4.5).

ACKNOWLEDGMENTS

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