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Exact Free Energy Functionals for Non-Simply-Connected Lattices

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We consider the nearest-neighbor Ising model in thermal equilibrium on a network with no required regularity or symmetry properties. Both coupling strengths and external fields are site-dependent. The objective is to describe this system in terms of a free energy magnetization functional whose conjugate variables are the external fields. For simply connected networks, this inverse problem has a local structure. On generalizing to loops, the local structure remains if the description is expanded in an overcomplete fashion to include a collective amplitude with respect to which the free energy is stationary. For more complex connectivity, a superbond representation is developed in terms of which the system can be described by a combined auxiliary set of branch and node collective variables.

KEY WORDS: Inhomogeneous Ising model; free-energy functional; collective modes.

1. INTRODUCTION

The classical Ising model on a lattice both models a variety of physical situations and, in various guises, represents a very broad class of equilibrium systems, discrete and continuous, classical and quantum. For obvious reasons, increasing attention has been paid to the spatial structure of such models. A prototypical format is that of the "profile equation," the relation between an applied potential field $\{-h_x\}$ in units of kT and the resulting magnetization field $\{m_x\}$. This relationship not only corresponds

Dedicated to Oliver Penrose, a master of long-range effects in many-body systems.

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to typical questions that one would ask, but can also be used to obtain the full multisite correlation structure of the system. The simplest spatial behavior is that of strict locality, in which $m_x = f_x(h_x)$ depends only upon the potential at the site in question; this can only hold if the sites are non-interacting. We will in fact restrict our attention to pair interactions which are as local as they can be: only nearest neighbors interact—but of course this is no restriction in the absence of imposed connection topology, since any interaction can be associated with a connection and thereby become nearest neighbor.

When interactions are only nearest neighbor, the concept of locality should certainly be extended to nearest neighbor as well, i.e., a relation of the form $m_x = f_x(h_x, \{h_y\})$ where $\langle y, x \rangle$ (read: y is a nearest neighbor of x) would be regarded as local. Although this particular form of locality does not in fact occur, the corresponding inverse profile has been shown[1-3] to take on a local form

$$h_x = f_x(m_x, \{m_y \mid \langle y, x \rangle\}) \tag{1.1}$$

for *any* simply connected lattice. The inverse profile form is particularly appropriate in the vicinity of thermodynamic singularities, where the $\{m_x\}$ depend sensitively upon the values of the $\{h_x\}$, but not vice versa, and has become the norm in continuous fluid approximations. But it has the additional advantage, as pointed out in refs. 1–3, of great simplicity for tree structures, e.g., Bethe lattices, which are prototypical reference systems for many approximation methods. The real interest, and difficulty, arises when there are interaction loops. In part, the change is deceptively simple[2,4,6]: each channel, i.e., sequence of vertices of coordination number two, has associated with it a collective amplitude, say C_α for channel α, so that for x in this channel, with neighbors x^+, x^-,

$$h_x = f_x(m_x/C_\alpha, m_{x^+}/C_\alpha, m_{x^-}/C_\alpha) \tag{1.2}$$

One can say that locality is maintained, but there is also a "hidden" parameter C_α. For a site A at a junction of channels, i.e., one whose coordination is greater than two, the situation is not so simple. A number of cases have been solved,[5,6] exhibiting the common structure

$$h_A = f_A(m_A, \{m_y \mid \langle y, A \rangle\}, \{C_i\}) \tag{1.3}$$

where $\{C_i\}$ is an expanded set of amplitudes, associated both with channels and interchannel junctions.

The aim of this paper is to develop a systematic approach for analyzing multiconnected Ising networks. For this purpose, we will make very explicit the nature of the collective amplitudes that have to be appended to maintain the nominally local form of (1.3). There will be an important by-product of this development, in the following context: the fields $\{h_x\}$ and magnetizations $\{m_x\}$ are conjugate sets of variables in the sense that

$$\partial h_x/\partial m_y = \partial h_y/\partial m_x \tag{1.4}$$

a consequence of the relation $\partial m_x/\partial h_y = -\partial^2\Omega/\partial h_x \partial h_y = \partial m_y/\partial h_x$, where Ω is the canonical thermodynamic potential of the lattice, i.e., $\Omega = -1/\beta \ln \sum_{\{\sigma_x\}} \exp -\beta\Phi\{\sigma_x\}$, where Φ is the total energy of the lattice. It follows that there is a free energy, recognized as the Legendre transform $\bar{F} = \Omega + \sum m_x h_x$, such that

$$h_x = \frac{\partial}{\partial m_x} \bar{F}\{m_y\} \tag{1.5}$$

for all x. Now by inspection, the profile equations (1.2), (1.3) also take the form

$$h_x = \frac{\partial}{\partial m_x} \bar{F}'\{m_y, C_i\}\bigg|_{\mathbf{C}} \tag{1.6}$$

for suitable $\bar{F}'$, as if one had an expanded space of magnetizations and collective amplitudes. It is not hard to establish the general result[4] that there must then exist a function $\Delta\{C_i\}$ of the collective amplitudes alone with the property that if

$$\bar{F}\{m_y, C_i\} = \bar{F}'\{m_y, C_i\} + \Delta\{C_i\}$$

then

$$\begin{aligned} h_x &= \frac{\partial}{\partial m_x} \bar{F}\{m_y, C_i\}\bigg|_{\mathbf{C}} \\ 0 &= \frac{\partial}{\partial C_i} \bar{F}\{m_y, C_i\}\bigg|_{\mathbf{m}} \end{aligned} \tag{1.7}$$

as well as $\bar{F}\{m_y, C_i\{m_y\}\} = \bar{F}\{m_y\}$ when the explicit form of the $\{C_i\}$ is inserted. In other words, we are indeed in an extended space, with the dependence of the $\{C_i\}$ on the $\{m_y\}$ resulting from the vanishing of the conjugates to the C_i. The problem of finding $\Delta\{C_i\}$, which has been non-trivial, is greatly simplified in the formulation to be described.

2. ARTICULATION POINT REDUCTION

We will of course deal with connected networks. But they may have articulation points, vertices whose excision disconnects the lattice. The disconnected pieces created in this fashion, with articulation point vertices reinserted, may be regarded as basic components of the lattice, and we might anticipate that the profile relations and free energy of the full lattice would be expressible in terms of those of the components. Indeed, this will serve as a leading level of reduction and amalgamation for the purpose of organizing the analytic structure of the lattice.

Our first objective then is to see how free energies combine [see (2.8)] when a set of sublattices is combined via contact at single vertices. To start, suppose the lattice L has an articulation point x which decomposes L into sublattices A and B (Fig. 1):

$$A \cup B = L, \qquad A \cdot B = x \tag{2.1}$$

We will use the shorthand h^A for $\{h_y, y \in A\}$. Then the partition function Z^L for L can be decomposed, in obvious notation, into partition function fragments (hereafter, we choose units so that $\beta = 1$):

$$Z^L(h^L) = \sum_\sigma Z^A(h^{A-x}, \sigma)\, e^{h_x \sigma} Z^B(h^{B-x}, \sigma) \tag{2.2}$$

It follows that

$$1 \pm m_x = \langle 1 \pm \sigma_x \rangle = 2Z^A(h^{A-x}, \pm)\, e^{\pm h_x} Z^B(h^{B-x}, \pm)/Z^L(h^L)$$

and hence that

$$e^{h_x} = \left(\frac{1+m_x}{1-m_x}\right)^{1/2} \left(\frac{Z^A(h^{A-x}, -)\, Z^B(h^{B-x}, -)}{Z^A(h^{A-x}, +)\, Z^B(h^{B-x}, +)}\right)^{1/2} \tag{2.3}$$

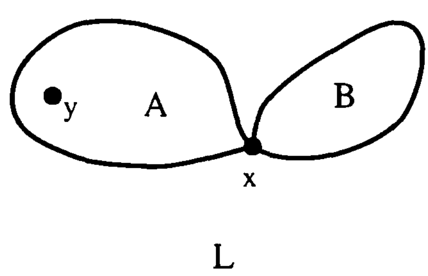

Fig. 1. Network with articulation point.

We can now use (2.3) to perform a partial Legendre transform to replace h_x by m_x: $\Lambda^{L-x,x}(h^{L-x}, m_x) = -\ln Z^L(h^L) + h_x m_x$, or

$$\begin{aligned}\Lambda^{L-x,x}(h^{L-x}, m_x) = {} & \frac{1+m_x}{2}\ln\frac{1+m_x}{2} + \frac{1-m_x}{2}\ln\frac{1-m_x}{2} \\ & -\left(\frac{1+m_x}{2}\ln Z^A(h^{A-x}, +) + \frac{1-m_x}{2}\ln Z^A(h^{A-x}, -)\right) \\ & -\left(\frac{1+m_x}{2}\ln Z^B(h^{B-x}, +) + \frac{1-m_x}{2}\ln Z^B(h^{B-x}, -)\right)\end{aligned} \tag{2.4}$$

The general partial transform $\Lambda^{L,M}(h^L, m^M)$ interpolates between grand potential and free energy in the sense that $\Lambda^{L,\varnothing}(h^L, \varnothing) = \Omega^L(h^L)$, while $\Lambda^{\varnothing,M}(\varnothing, m^M) = \bar{F}^M(m^M)$.

By successively setting $A - x = \varnothing$ and $B - x = \varnothing$ in (2.4) and subtracting from (2.4), we have the basic reduction formula

$$\begin{aligned}\Lambda^{L-x,x}(h^{L-x}, m_x) = {} & \Lambda^{A-x,x}(h^{A-x}, m_x) + \Lambda^{B-x,x}(h^{B-x}, m_x) \\ & -\left(\frac{1+m_x}{2}\ln\frac{1+m_x}{2} + \frac{1-m_x}{2}\ln\frac{1-m_x}{2}\right)\end{aligned} \tag{2.5}$$

In precisely the same way, if q_x sublattices meet at x, we find

$$\begin{aligned}\Lambda^{L-x,x}(h^{L-x}, m_x) = {} & \sum_{j=1}^{q_x} \Lambda^{A_j-x,x}(h^{A_j-x}, m_x) \\ & -(q_x - 1)\left(\frac{1+m_x}{2}\ln\frac{1+m_x}{2} + \frac{1-m_x}{2}\ln\frac{1-m_x}{2}\right)\end{aligned} \tag{2.6}$$

If $y \in A_j - x$, then applying $\partial/\partial h_y$ to (2.6) leads at once to

$$m_y^L(h^{L-x}, m_x) = m_y^{A_j}(h^{A_j-x}, m_x) \tag{2.7}$$

where the superscript in m^L means with respect to the lattice L. From (2.6) and (2.7), we can then Legendre-transform to replace all of the $\{h_y\}$ by $\{m_y\}$, obtaining

$$\bar{F}^L(m^L) = \sum_{j=1}^{q_x} \bar{F}^{A_j}(m^{A_j}) - (q_x - 1)\left(\frac{1+m_x}{2}\ln\frac{1+m_x}{2} + \frac{1-m_x}{2}\ln\frac{1-m_x}{2}\right) \tag{2.8}$$

or since the last expression in (2.8) is recognized as the one-site free energy, simply as

$$\bar{F}^L(m^L) = \sum_{j=1}^{q_x} \bar{F}^{A_j}(m^{A_j}) - (q_x - 1)\,\bar{F}^x(m_x) \tag{2.9}$$

Finally, if the complete set of articulation points is designated by $\{x_\alpha\}$ and the complete set of resulting components by $\{L_\gamma\}$, we have

$$\bar{F}^L(m^L) = \sum_\gamma \bar{F}^{L_\gamma}(m^{L_\gamma}) - \sum_\alpha (q_{x_\alpha} - 1)\,\bar{F}^{x_\alpha}(m_{x_\alpha}) \tag{2.10}$$

Example 1. A simply connected lattice (Cayley tree, Bethe lattice,...) also has the property that *every* nonboundary vertex is an articulation point. The corresponding components are all nearest-neighbor pairs, so only $\bar{F}^{(x,y)}(m_x, m_y)$ for nearest neighbors $\langle x, y\rangle$ need be computed, and (2.10) then reduces to

$$\bar{F}^L(m^L) = \frac{1}{2} \sum_{\langle x,y\rangle} [\bar{F}^{(x,y)}(m_x, m_y) - \bar{F}^x(m_x) - \bar{F}^y(m_y)] + \sum_x \bar{F}^x(m_x) \tag{2.11}$$

For the basic two-site lattice, with Boltzmann weight $\exp(h_x\sigma_x + h_y\sigma_y + J_{xy}\sigma_x\sigma_y)$, it is trivial to find $m_x = \langle\sigma_x\rangle$ and $m_y = \langle\sigma_y\rangle$, from which

$$\frac{1+m_x}{1-m_x} = e^{2h_x} \frac{\cosh(h_y + J_{xy})}{\cosh(h_y - J_{xy})} \tag{2.12}$$

and similarly for $(1+m_y)/(1-m_y)$. These are readily solved to yield

$$e^{\pm 2h_x} = \frac{\pm t_{xy} + s_{xy}}{1 \mp m_x} \tag{2.13}$$

where

$$\begin{aligned} t_{xy} &= m_x \cosh 2J_{xy} - m_y \sinh 2J_{xy} \\ s_{xy}^2 &= s_{yx}^2 = 1 - m_x^2 + t_{xy}^2 \end{aligned} \tag{2.13}$$

with a corresponding expression for h_y. After a certain amount of algebra, one then finds that

$$Z^2 = 8\,\frac{\cosh 2J_{xy} - m_x m_y \sinh 2J_{xy} + s_{xy}}{(1-m_x^2)(1-m_y^2)} \tag{2.14}$$

and so concludes that (to within an additive constant)

$$\bar{F}^{(x,y)}(m_x, m_y) - \bar{F}^x(m_x) - \bar{F}^y(m_y)$$

$$= -\ln Z + h_x m_x + h_y m_y - \left(\frac{1+m_x}{2}\ln\frac{1+m_x}{2}\right.$$

$$\left. + \frac{1-m_x}{2}\ln\frac{1-m_x}{2} + \frac{1+m_y}{2}\ln\frac{1+m_y}{2} + \frac{1-m_y}{2}\ln\frac{1-m_y}{2}\right)$$

or

$$\bar{F}^{(x,y)}(m_x, m_y) - \bar{F}^x(m_x) - \bar{F}^y(m_y)$$

$$= \frac{1}{2}\left[m_x \ln\frac{t_{xy}+s_{xy}}{1+m_x} + m_y \ln\frac{t_{yx}+s_{xy}}{1+m_y} - \ln\frac{u_{xy}+s_{xy}}{2}\right] \tag{2.15}$$

where

$$u_{xy} = u_{yx} = \cosh 2J_{xy} - m_x m_y \sinh 2J_{xy}$$

which completes the evaluation of (2.11).

The construction of (2.15) can equally well proceed from the algebraic identities

$$\begin{aligned}
\frac{\partial}{\partial m_x}\ln(t_{xy}+s_{xy}) &= \frac{u_{xy}}{(1-m_x^2)s_{xy}} - \frac{m_x}{1-m_x^2} \\
\frac{\partial}{\partial m_x}\ln(t_{yx}+s_{xy}) &= -\frac{\sinh 2J_{xy}}{s_{xy}} \\
\frac{\partial}{\partial m_x}\ln(u_{xy}+s_{xy}) &= \frac{t_{xy}}{(1-m_x^2)s_{xy}} - \frac{m_x}{1-m_x^2}
\end{aligned} \tag{2.16}$$

and the immediate consequence that

$$\frac{\partial}{\partial m_x}\left[m_x \ln\frac{t_{xy}+s_{xy}}{1+m_x} + m_y \ln\frac{t_{yx}+x_{xy}}{1+m_y} - \ln\frac{u_{xy}+s_{xy}}{2}\right]$$

$$= \ln\frac{t_{xy}+s_{xy}}{1+m_x} \tag{2.17}$$

3. CHANNEL AMPLITUDES

If the network is not simply connected, then even if every vertex is an articulation point, the disconnected pieces created by their excision need no longer contain just one interaction bond, but may, for example, consist of loops. And if not every vertex is an articulation point—none are on a regular lattice—interconnected interaction loops are the norm. Nonetheless, some vestige of the locality of (2.11)—and the corresponding profile locality—will remain.

Consider a constituent chain of vertices of coordination number 2, and focus on a neighboring pair $\langle x, y\rangle$. Each vertex contributes a multiplicative weight

$$w_x(\sigma_x) = e^{h_x \sigma_x} \tag{3.1}$$

to the partition function, and hence to all expectations, whereas the pair contributes

$$E_{xy}(\sigma_x, \sigma_y) = e^{J_{xy}\sigma_x\sigma_y} \tag{3.2}$$

Now let us extend the pair x, y to the three-site sequence (see Fig. 2) and introduce normalized partition functions with gaps:

$$\xi_{xy}(\sigma_x, \sigma_y) = \sum_{\{\sigma_w \mid w \neq x, y\}} \rho\{\sigma\} \Big/ E_{xy}(\sigma_x, \sigma_y) \tag{3.3a}$$

$$\Lambda_{xz}(\sigma_x, \sigma_z) = \sum_{\{\sigma_w \mid w \neq x, y, z\}} \rho\{\sigma\} \Big/ [E_{xy}(\sigma_x, \sigma_y)\, w_y(\sigma_y)\, E_{yz}(\sigma_y, \sigma_z)] \tag{3.3b}$$

where $\rho\{\sigma\}$ is the full normalized Boltzmann weight. Denoting the 2×2 matrix $E_{xy}(\sigma_x, \sigma_y)$ by $\mathbf{E}_{xy}$, and representing $w_x(\sigma_x)$ as a diagonal matrix $\mathbf{w}_x$, we have at once, using the symmetry of $\mathbf{E}_{xy}$ in its arguments and indices,

$$\begin{aligned} &\mathrm{Tr}\, \xi_{xy}\mathbf{E}_{yx} = 1 \\ &\mathrm{Tr}\, \sigma\xi_{xy}\mathbf{E}_{yx} = m_x \\ &\mathrm{Tr}\, \xi_{xy}\sigma\mathbf{E}_{yx} = m_y \end{aligned} \tag{3.4}$$

where σ is the diagonal matrix of multiplication by σ.

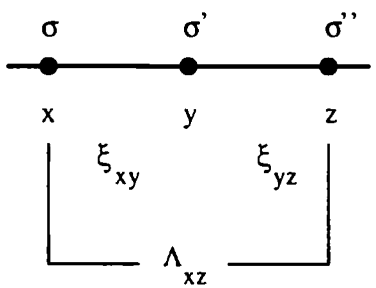

Fig. 2. Normalized partition functions with gaps.

Equations (3.4) are not enough to determine the four elements of ξ_{xy}. However, we also observe that

$$\xi_{xy} = \Lambda_{xz} \mathbf{E}_{zy} \mathbf{w}_y \tag{3.5a}$$

$$\xi_{yz} = \mathbf{w}_y \mathbf{E}_{yx} \Lambda_{xz} \tag{3.5b}$$

It follows that Det ξ_{xy} Det $\mathbf{E}_{yx}$ = Det ξ_{yz} Det $\mathbf{E}_{zy}$ has a constant value along the chain; we denote this by

$$K = \text{Det } \xi_{yz} \text{ Det } \mathbf{E}_{zy} \tag{3.6}$$

Since $\text{Tr}(\xi_{xy}\mathbf{E}_{yx}) = 1$ and all elements are nonnegative, the determinant $\text{Det}(\xi_{xy}\mathbf{E}_{yx}) = K$ is bounded from above by 1/4, allowing us to define $C \geqslant 0$ by

$$C^2 = 1 - 4K \tag{3.7}$$

Given C, the solution of (3.4) and (3.6) is immediate, and we find

$$\begin{aligned} \eta_{xy} \equiv \xi_{xy}\mathbf{E}_{yx} &= \frac{1}{2}\begin{pmatrix} 1 + m_x & C[t_{xy}(C) + s_{xy}(C)] \\ C[-t_{xy}(C) + s_{xy}(C)] & 1 - m_x \end{pmatrix} \\ \bar{\eta}_{xy} \equiv \mathbf{E}_{yx}\xi_{xy} &= \frac{1}{2}\begin{pmatrix} 1 + m_y & C[-t_{yx}(C) + s_{yx}(C)] \\ C[t_{yx}(C) + s_{yx}(C)] & 1 - m_y \end{pmatrix} \end{aligned} \tag{3.8}$$

where

$$\begin{aligned} t_{xy}(C) &= \left(\frac{m_x}{C}\right)\cosh 2J_{xy} - \left(\frac{m_y}{C}\right)\sinh 2J_{xy} \\ s_{xy}(C)^2 &= t_{xy}(C)^2 + 1 - \frac{m_x^2}{C^2} = t_{yx}(C)^2 + 1 - \frac{m_y^2}{C^2} \\ u_{xy}(C) &= \cosh 2J_{xy} - \left(\frac{m_x}{C}\right)\left(\frac{m_y}{C}\right)\sinh 2J_{xy} \end{aligned} \tag{3.9}$$

Clearly, $t_{xy}(C \mid \{m\}) = t_{xy}(\{m/C\})$, $s_{xy}(C \mid \{m\}) = s_{xy}(\{m/C\})$ in terms of the functions of (2.12), (2.15); we will need $u_{xy}(C \mid \{m\}) = u_{xy}(\{m/C\})$ in a moment.

Now, according to (3.5), we have $\mathbf{w}_y \bar{\eta}_{xy} = \eta_{yz}\mathbf{w}_y$, and so conclude that

$$e^{-h_y}[t_{yx}(C) + s_{yx}(C)] = e^{h_y}[-t_{yz}(C) + s_{yz}(C)]$$

or

$$h_y = \tfrac{1}{2}\ln[t_{yx}(C) + s_{yx}(C)] + \tfrac{1}{2}\ln[t_{yz}(C) + s_{yz}(C)] - \tfrac{1}{2}\ln(1 - m_y^2/C^2) \tag{3.10}$$

in which C enters only as a uniform multiplier: m_x/C. The identities (2.16) then allow us to deduce at once that the explicitly m_y-dependent part of the free energy is given by

$$\begin{aligned}\bar{F}_y = &\frac{1}{2} m_y \ln[t_{yx}(C) + s_{yx}(C)] + \frac{1}{2} m_x \ln[t_{xy}(C) + s_{xy}(C)] \\ &+ \frac{1}{2} m_y \ln[t_{yz}(C) + s_{yz}(C)] + \frac{1}{2} m_z \ln[t_{zy}(C) + s_{zy}(C)] \\ &- \frac{C}{2}\ln[u_{yx}(C) + s_{yx}(C)] - \frac{C}{2}\ln[u_{yz}(C) + s_{yz}(C)] \\ &+ \frac{C}{2}\left(1 - \frac{m_y}{C}\right)\ln\left(1 - \frac{m_y^2}{C^2}\right)\end{aligned} \tag{3.11}$$

in the sense that

$$h_y = \left.\frac{\partial \bar{F}_y}{\partial m_y}\right|_C \tag{3.12}$$

Example 2. Suppose that the lattice is a polygon—a discrete ring—of N sites (Fig. 3). Then (3.12) will hold for each site if (with periodic boundary conditions: $N + 1 = 1$)

$$\begin{aligned}\bar{F}(\{m\}, C) = &\sum_x \frac{C}{2}\left(1 - \frac{m_x}{C}\right)\ln\left(1 - \frac{m_x^2}{C^2}\right) \\ &+ \frac{1}{2}\sum_x \{m_x \ln[t_{x,x+1}(C) + s_{x,x+1}(C)] \\ &+ m_{x+1}\ln[t_{x+1,x}(C) + s_{x+1,x}(C)] \\ &- C\ln[u_{x,x+1}(C) + s_{x,x+1}(C)]\}\end{aligned} \tag{3.13}$$

But how is C to be determined? We know (see Appendix A) that $\Delta(C)$ can be found such that

$$\begin{aligned}&\text{if} \quad \bar{F}_{\mathrm{TOT}}(\{m\}, C) = \bar{F}(\{m\}, C) + \Delta(C) \\ &\text{then} \quad \bar{F}(\{m\}) = \bar{F}_{\mathrm{TOT}}(\{m\}, C\{m\}) \\ &\text{and} \quad 0 = \partial\bar{F}_{\mathrm{TOT}}(\{m\}, C)/\partial C\end{aligned} \tag{3.14}$$

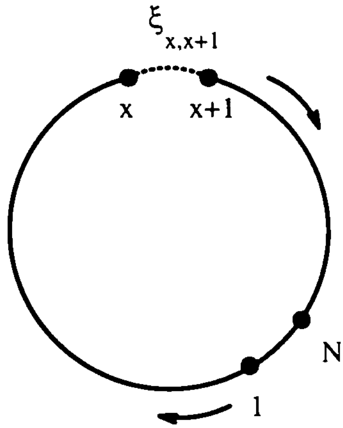

Fig. 3. Ring lattice.

and so it is $\Delta(C)$ that supplies the implicit relationship for C. To find $\Delta(C)$, we first observe that because of the special form of (3.13), we can write

$$\bar{F}_{\mathrm{TOT}}(\{m\}, C) = C\bar{f}(\{m/C\}) + \Delta(C) \tag{3.15}$$

The "profile equation" for C then becomes

$$\begin{aligned} 0 &= \partial\bar{F}_{\mathrm{TOT}}(\{m\}, C)/\partial C \\ &= \bar{f}(\{m/C\}) + \Delta'(C) - \sum h_x m_x \Big/ C \\ &= \Big(\bar{F} - \sum h_x m_x\Big)\Big/ C + \Delta'(C) - \Delta(C)/C \\ &= \Omega/C + \Delta'(C) - \Delta(C)/C \end{aligned}$$

Hence

$$\Omega = \Delta(C) - C\Delta'(C) \tag{3.16}$$

a function of C alone.

On the other hand, it is clear that

$$\xi_{x,x+1}(\sigma, \sigma') = (\mathbf{w}_{x+1}\mathbf{E}_{x+1,x+2}\mathbf{w}_{x+2}\cdots\mathbf{w}_{x-1}\mathbf{E}_{x-1,x}\mathbf{w}_x)(\sigma', \sigma)/Z \tag{3.17}$$

Since $\mathrm{Det}\,\mathbf{w}_x = 1$; then

$$\mathrm{Det}\,\xi_{x,x+1}(\sigma, \sigma') = \Big(\prod_{y \neq x} \mathrm{Det}\,\mathbf{E}_{y,y+1}\Big)\Big/ Z^2 \tag{3.18}$$

from which

$$K=\left(\prod_{y} \text{Det}\, \mathbf{E}_{y,y+1}\right)\Big/ Z^2 \tag{3.19}$$

or

$$\Omega=\frac{1}{2}\ln\frac{1-C^2}{4}-\frac{1}{2}\sum_{y}\ln\text{Det}\,\mathbf{E}_{y,y+1} \tag{3.20}$$

with obvious modification when $C>1$. On comparing with (3.16), imposing the condition $\Delta(1)=-\sum_{y}(\ln 2)/2$ obtained by the $J_{x,x+1}\to 0$ limit of independent spins with $\bar{F}=\sum \bar{F}^{x}(m_{x})$, we find at once

$$\Delta(C)=\frac{1+C}{2}\ln\frac{1+C}{2}+\frac{1-C}{2}\ln\frac{1-C}{2}$$
$$-\frac{1-C}{2}\sum_{y}\ln(\sinh 2J_{y,y+1})-\frac{1}{2}\sum_{y}\ln 2 \tag{3.21}$$

The determination of Δ, and hence implicitly of C, is complete.

Example 3. By a *cactus*, we mean a network in which *all* nonboundary vertices are articulation points (Fig. 4). The components obtained by splitting at the vertices need not be links with two vertices, but may be any polygons, serving as supervertices of a generalized tree. The definition can be extended with no loss of malleability by replacing nonboundary vertices in the definition by vertices of nonboundary polygons. Now we can apply (2.10) together with (3.13), (3.14), (3.21). If the supervertex α has N_α

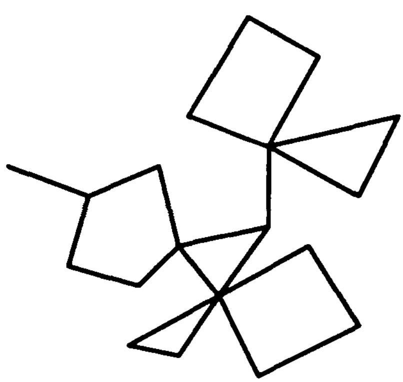

Fig. 4. Typical cactus.

vertices and q_x is the number of polygons intersecting at x, the incorporation of channel amplitudes changes nothing in (2.10), and we have at once

$$\bar{F}=\sum_{\alpha} C_\alpha[\bar{f}_\alpha(\{m/C_\alpha\})+\Delta_\alpha(C_\alpha)]-\sum_{x}(q_x-1)\,\bar{F}^x(m_x) \tag{3.22}$$

where $\bar{f}_\alpha$ is given by (3.13), $\bar{F}^x$ by (2.8), and $\Delta(C)$ by (3.21).

4. SUPERBOND REDUCTION

An internal chain of bonds $A, A+1,..., B$ is characterized by a common collective amplitude C such that h_x is expressible in terms of m_x/C, $m_{x\pm 1}/C$ at each interior site of the chain. Hence the partition function component

$$Z_{AB}(\sigma_A, \sigma_B)=\sum_{\{\sigma_x \mid x=A+1,..., B-1\}} \prod_{A+1}^{B-1} e^{h_x\sigma_x} \prod_{A}^{B-1} e^{\sigma_x J_{x,x+1}\sigma_{x+1}} \tag{4.1}$$

can in principle be written explicitly in terms of $\sigma_A, m_A/C$, $m_{A+1}/C,..., m_B/C, \sigma_B$. If we represent this component as

$$Z_{AB}(\sigma_A, \sigma_B)=n_{AB}\exp(\Delta h_A\sigma_A+\Delta h_B\sigma_B+J_{AB}\sigma_A\sigma_B) \tag{4.2}$$

which we can always do, the chain has therefore been replaced, insofar as expectations are concerned, by a "superbond" J_{AB}, together with "edge fields" Δh_A and Δh_B (Fig. 5). To determine the four parameters in (4.2), let us embed the chain in an otherwise arbitrary (periodic boundary) ring with collective amplitude C. We have seen that for this ring,

$$\bar{F}_{\mathrm{TOT}}(\{m\}, C)=C\bar{f}\left(\left\{\frac{m}{C}\right\}\right)+\frac{1+C}{2}\ln\frac{1+C}{2}+\frac{1-C}{2}\ln\frac{1-C}{2}$$
$$-\frac{1-C}{2}\sum_{x}\ln\sinh(2J_{x,x+1}) \tag{4.3}$$

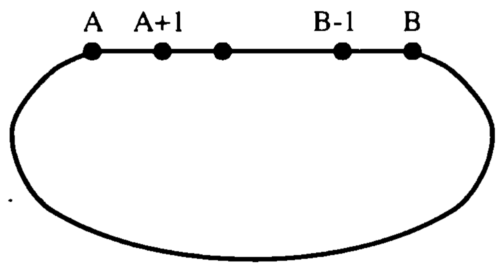

Fig. 5. Isolated superbond.

so that, using

$$(\partial/\partial C)[C\bar{f}(\{m/C\})]=\bar{f}(\{m/C\})-\sum h_x(\{m/C\})\,m_x/C$$

the "profile equation" $(\partial/\partial C)\,\bar{F}_{\mathrm{TOT}}(\{m\},C)=0$ reads

$$\ln\frac{1-C}{1+C}=\sum_x\left[\ln\left(1-\frac{m_x^2}{C^2}\right)-\ln[u_{x,x+1}(C)+s_{x,x+1}(C)]+\ln\sinh(2J_{x,x+1})\right] \tag{4.4}$$

On the other hand, with $A+1,\ldots,B-1$ replaced by the superbond, we have

$$\ln\frac{1-C}{1+C}=\sum_{A\geqslant x\geqslant B}\ln\left(1-\frac{m_x^2}{C^2}\right)-\sum_{A-1\geqslant x\geqslant B}\ln\frac{u_{x,x+1}(C)+s_{x,x+1}(C)}{\sinh(2J_{x,x+1})}-\ln\frac{u_{A,B}(C)+s_{A,B}(C)}{\sinh(2J_{AB})} \tag{4.5}$$

and so conclude that

$$\ln\frac{u_{A,B}(C)+s_{A,B}(C)}{\sinh(2J_{A,B})}=-\sum_{A+1\leqslant x\leqslant B-1}\ln\left(1-\frac{m_x^2}{C^2}\right)+\sum_{A\leqslant x\leqslant B-1}\ln\frac{u_{x,x+1}(C)+s_{x,x+1}(C)}{\sinh(2J_{x,x+1})} \tag{4.6}$$

This is of course an equation for $J_{A,B}$. Since

$$\frac{u_{x,y}(C)+s_{x,y}(C)}{\sinh(2J_{x,y})}=p_{x,y}(C) \tag{4.7}$$

has the solution

$$e^{4J_{x,y}}=\left[p_{x,y}(C)+\left(1+\frac{m_x}{C}\right)\left(1+\frac{m_y}{C}\right)\right]\times\left[p_{x,y}(C)+\left(1-\frac{m_x}{C}\right)\left(1-\frac{m_y}{C}\right)\right]\Big/\left\{\left[p_{x,y}(C)-\left(1+\frac{m_x}{C}\right)\left(1-\frac{m_y}{C}\right)\right]\times\left[p_{x,y}(C)-\left(1-\frac{m_x}{C}\right)\left(1+\frac{m_y}{C}\right)\right]\right\} \tag{4.8}$$

$J_{A,B}$ is determined by

$$e^{4J_{A,B}(C)} = \left[p_{A,B}(C) + \left(1 + \frac{m_A}{C}\right)\left(1 + \frac{m_B}{C}\right) \right] \times \left[p_{A,B}(C) + \left(1 - \frac{m_A}{C}\right)\left(1 - \frac{m_B}{C}\right) \right] \Big/ \left\{ \left[p_{A,B}(C) - \left(1 + \frac{m_A}{C}\right)\left(1 - \frac{m_B}{C}\right) \right] \times \left[p_{A,B}(C) - \left(1 - \frac{m_A}{C}\right)\left(1 + \frac{m_B}{C}\right) \right] \right\} \tag{4.9}$$

where

$$p_{A,B}(C) = \prod_A^{B-1} \frac{u_{x,x+1}(C) + s_{x,x+1}(C)}{\sinh(2J_{x,x+1})} \Big/ \prod_{A+1}^{B-1} \left[1 - \left(\frac{m_x}{C}\right)^2 \right]$$

Continuing, we know that for the multisite chain, one has

$$h_A = \tfrac{1}{2} \ln[t_{A,A-1}(C) + s_{A,A-1}(C)] + \tfrac{1}{2} \ln[t_{A,A+1}(C) + s_{A,A+1}(C)] - \tfrac{1}{2} \ln(1 - m_A^2/C^2) \tag{4.10}$$

whereas for the single link superbond, we require

$$h_A + \Delta h_A(C) = \tfrac{1}{2} \ln[t_{A,A-1}(C) + s_{A,A-1}(C)] + \tfrac{1}{2} \ln[t_{A,B}(C) + s_{A,B}(C)] - \tfrac{1}{2} \ln(1 - m_A^2/C^2) \tag{4.11}$$

Hence, in more explicit notation,

$$\Delta h_{A,B}(\mathbf{m}, C) = \frac{1}{2} \ln \frac{t_{A,B}(C) + s_{A,B}(C)}{t_{A,A+1}(C) + s_{A,A+1}(C)} \tag{4.12}$$

and similarly

$$\Delta h_{B,A}(\mathbf{m}, C) = \frac{1}{2} \ln \frac{t_{B,A}(C) + s_{B,A}(C)}{t_{B,B-1}(C) + s_{B,B-1}(C)} \tag{4.13}$$

Finally, it is clear that

$$\text{Det } Z_{A,B} = \prod_A^{B-1} \text{Det}(e^{\sigma J_{x,x+1} \sigma'}) = \prod_A^{B-1} 2 \sinh(2J_{x,x+1})$$

but Det $Z_{A,B} = 2n^2_{A,B} \sinh 2J_{A,B}$, and so we have

$$n_{A,B}(C) = \left(\prod_A^{B-1} 2\sinh(2J_{x,x+1}) \Big/ 2\sinh J_{A,B}(C) \right)^{1/2} \tag{4.14}$$

Now that we have found $Z_{A,B}(\sigma_A, \sigma_B)$, there is in principle no difficulty in producing the full partition function. Numerically, it is simply

$$Z(\mathbf{h}, \mathbf{m}, \mathbf{C}) = \sum_{\{\sigma_A \mid q_A > 2\}} \left(\prod_A e^{h_A \sigma_A} \right) \prod_{(A,B)}{}' Z_{A,B}(\sigma_A, \sigma_B) \tag{4.15}$$

where $\prod'$ indicates that only one order of a pair is included, and that $B \neq A$. But $h_A(\mathbf{m})$ is not known. One option is to use a mixed thermodynamic potential, as in (2.4), which is direct in the h_A but inverse in $\{\mathbf{m}, \mathbf{C}\}$. However, if one wants a fully inverse free energy formulation, a simple device is that of regarding h_A as a collective variable as well; consider

$$\bar{F}(\mathbf{H}, \mathbf{m}, \mathbf{C}) = \sum_{\{z \mid q_z \leq 2\}} h_z(\mathbf{m}, \mathbf{C}) m_z + \sum_{\{A \mid q_A > 2\}} H_A m_A - \ln Z(\mathbf{H}, \mathbf{m}, \mathbf{C}) \tag{4.16}$$

a function of all m_z, the H_A, and the C_{AB}. From the definition of $Z_{A,B}$, we know that

$$Z(\mathbf{H}, \mathbf{m}, \mathbf{C}) = \sum_{\left\{ \substack{\sigma_z \mid q_z \leq 2 \\ \sigma_A \mid q_A > 2} \right\}} \prod_{\langle x,y \rangle} e^{J_{xy}\sigma_x\sigma_y} e^{\sum H_A \sigma_A} e^{\sum h_z(\mathbf{m},\mathbf{C})\sigma_z} \tag{4.17}$$

and we readily find the variational properties of $\bar{F}(\mathbf{H}, \mathbf{m}, \mathbf{C})$. By direct computation, we have

$$\partial \bar{F}/\partial m_z = h_z(\mathbf{m}, \mathbf{C}) + \sum_{z'} \partial h_{z'}(\mathbf{m}, \mathbf{C})/\partial m_z (m_{z'} - \langle \sigma_{z'} \rangle_{\mathbf{H},\mathbf{m},\mathbf{C}})$$

$$\partial \bar{F}/\partial m_A = H_A + \sum_z \partial h_z(\mathbf{m}, \mathbf{C})/\partial m_A (m_z - \langle \sigma_z \rangle_{\mathbf{H},\mathbf{m},\mathbf{C}})$$

$$\partial \bar{F}/\partial H_A = m_A - \langle \sigma_A \rangle_{\mathbf{H},\mathbf{m},\mathbf{C}}$$

$$\partial \bar{F}/\partial C_{AB} = \sum_z \partial h_z(\mathbf{m}, \mathbf{C})/\partial C_{AB} (m_z - \langle \sigma_z \rangle_{\mathbf{H},\mathbf{m},\mathbf{C}}) \tag{4.18}$$

where the subscript **H**, **m**, **C** denotes an average over the kernel of (4.15). It is clear that imposing $\partial\bar{F}/\partial H_A = 0$ is sufficient to enforce $H_A = h_A$. Thus the set (4.18) becomes

$$h_z = \left.\frac{\partial \bar{F}(\mathbf{H}, \mathbf{m}, \mathbf{C})}{\partial m_z}\right|_{\mathbf{H}=\mathbf{h}}, \qquad h_A = \left.\frac{\partial \bar{F}(\mathbf{H}, \mathbf{m}, \mathbf{C})}{\partial m_A}\right|_{\mathbf{H}=\mathbf{h}}$$
$$0 = \left.\frac{\partial \bar{F}(\mathbf{H}, \mathbf{m}, \mathbf{C})}{\partial H_A}\right|_{\mathbf{H}=\mathbf{h}}, \qquad 0 = \left.\frac{\partial \bar{F}(\mathbf{H}, \mathbf{m}, \mathbf{C})}{\partial C_{AB}}\right|_{\mathbf{H}=\mathbf{h}} \tag{4.19}$$

and $\bar{F}(\mathbf{H}, \mathbf{m}, \mathbf{C})|_{\mathbf{H}=\mathbf{h}} = \bar{F}(\mathbf{m})$ as well. We thus have an explicit extended free energy functional for the lattice, but one that is structurally simple only if (unlike a regular grid) there are relatively few vertices of coordination number greater than 2.

Example 4. The basic multiconnected network consists of r parallel branches b_α between two vertices (Fig. 6). According to (4.2), (4.16) (but using α to distinguish the various branches between A and B),

$$\begin{aligned}\bar{F}(\mathbf{h}, \mathbf{m}, \mathbf{C}) = {} & \sum_{\alpha} \sum_{z \in b_\alpha} h_z(\mathbf{m}, C_\alpha) m_z + h_A m_A + h_B m_B \\ & - \ln \left\{ \prod_{\alpha} n_\alpha(\mathbf{m}, \mathbf{C}_\alpha) \sum_{\sigma_A, \sigma_B} \exp\left[\left(h_A + \sum_{\alpha} \Delta h_{A,\alpha}(\mathbf{m}, \mathbf{C}_\alpha)\right)\sigma_A\right] \right. \\ & \left. \times \exp\left[\left(h_B + \sum_{\alpha} \Delta h_{B,\alpha}(\mathbf{m}, \mathbf{C}_\alpha)\right)\sigma_B\right] \exp\left[\sum_{\alpha} J_\alpha(\mathbf{m}, \mathbf{C})\, \sigma_A \sigma_B\right]\right\}\end{aligned} \tag{4.20}$$

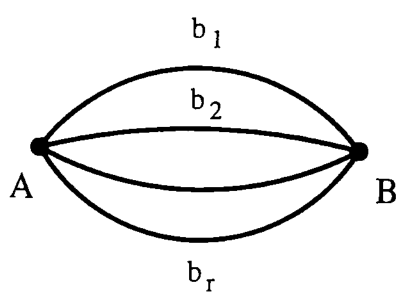

Fig. 6. Multiconnected network, prototype.

or, in obvious notation,

$$\bar{F}(\mathbf{h}, \mathbf{m}, \mathbf{C}) = h_A m_A + h_B m_B + \sum_\alpha \left[\sum_{z \in b_\alpha} h_z(\mathbf{m}, C_\alpha) m_z - \ln n_\alpha(\mathbf{m}, C_\alpha) \right]$$
$$- \ln \left[\sum_{\sigma, \sigma'} e^{(h_A + \Delta h_A(\mathbf{m}, \mathbf{C}))\sigma} e^{(h_B + \Delta h_B(\mathbf{m}, \mathbf{C}))\sigma'} e^{J(\mathbf{m}, \mathbf{C})\sigma\sigma'} \right] \quad (4.21)$$

The profile equations follow at once.

5. CONCLUDING REMARKS

As we have shown, the remarkable locality of the nearest-neighbor Ising-model free energy for simply connected networks not only extends to simple loops when a collective amplitude is allowed for, but also extends to multiconnected networks. The price to be paid is that the fields at the "mesoscopic" nodes of the network are themselves treated as subsidiary collective variables. For such more complicated networks, the major task is that of computing

$$Z(\mathbf{h}, \mathbf{m}, \mathbf{C}) = \left[\prod_{\{A, B\}}' n_{AB}(C_{AB}) \right]$$
$$\times \sum_{\{\sigma_A \mid q_A > 2\}} \left\{ \prod_A \exp\left[\left(h_A + \sum_B \Delta h_{A,B}(\mathbf{m}, \mathbf{C}) \right) \sigma_A \right] \right.$$
$$\left. \times \prod_{\{A, B\}}' \exp[J_{A,B}(\mathbf{m}, \mathbf{C})\, \sigma_A \sigma_B] \right\} \quad (5.1)$$

This is equivalent to solving the skeleton model whose only vertices are those of coordination number greater than two.

But the skeleton model has facets that are significant. In particular, parallel superbonds may have been created in the process of constructing (5.1), and these may be combined in the fashion that was used for (4.21). There may then exist chains of superbonds that have their own collective amplitudes, and in this series—parallel reduction technique, a hierarchy of collective amplitudes can be produced before the process grinds to a halt at an irreducible skeleton. If this does not happen before the network collapses to triviality, one is working with a member of the CHNC hierarchy of graphs, built recursively from links by series and parallel operations alone. It would be both interesting and more than a bit valuable if the complications of the hierarchical reduction could be organized so that it does not have to be carried out explicitly, use being made only of the fact that the network belongs to this class. Equation (2.11) illustrates this strategy for a much narrower class of networks. Work along these lines is now proceeding.

APPENDIX[4]

Suppose that the profile equation can be written in the form

$$h_x = \partial \bar{F}(\{m\}, \{C\})/\partial m_x \tag{A1}$$

where the C_α are themselves independent functions of the $\{m_x\}$. If $\bar{F}\{m\}$ is the unknown but complex free energy that generates the profile, we will also have

$$h_x = \partial \bar{F}\{m\}/\partial m_x \tag{A2}$$

Hence

$$\frac{\partial}{\partial m_x}(\bar{F}(\{m\}, \{C\{m\}\}) - \bar{F}\{m\}) = \sum \frac{\partial \bar{F}(\{m\}, \{C\})}{\partial C_\alpha}\frac{\partial C_\alpha}{\partial m_x} \tag{A3}$$

The independent $\{C_\alpha\}$ can be enlarged to the full space of functions of $\{m_x\}$ by appending the set $\{D_\beta\}$; carrying out the operation $\sum_x (\partial m_x/\partial D_\beta)$ on (A3), we have $(\partial/\partial D_\beta)(\bar{F}(\{m\{C, D\}\}, \{C\}) - \bar{F}\{m\{C, D\}\}) = 0$. Hence

$$\bar{F}\{m\} = \bar{F}(\{m\}, \{C\{m\}\}) + \Delta\{C\{m\}\} \tag{A4}$$

for some function Δ of the $\{C_\alpha\}$ alone, with

$$\partial \bar{F}(\{m\}, \{C\})/\partial C_\alpha = -\partial \Delta/\partial C_\alpha \tag{A5}$$

Furthermore, writing

$$\bar{F}_{\mathrm{TOT}}(\{m\}, \{C\}) = \bar{F}(\{m\}, \{C\}) + \Delta\{C\} \tag{A6}$$

we have

$$\sum \partial \bar{F}_{\mathrm{TOT}}/\partial m_x \, dm_x + \sum \partial \bar{F}_{\mathrm{TOT}}/\partial C_\alpha \, dC_\alpha$$
$$= \sum \partial \bar{F}/\partial m_x \, dm_x + \sum \partial \bar{F}/\partial C_\alpha \, dC_\alpha + \sum \partial \Delta/\partial C_\alpha \, dC_\alpha$$

Using (A2) and (A5), we see then that

$$\frac{\partial \bar{F}_{\mathrm{TOT}}}{\partial m_x} = h_x, \qquad \frac{\partial \bar{F}_{\mathrm{TOT}}}{\partial C_\alpha} = 0 \tag{A7}$$

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