Journal of Statistical Physics, Vol. 73, Nos. 1/2, 1993

New Collective Modes of Interaction Nature in Inhomogeneous Ising Networks

L. Šamaj[1,3] and J. K. Percus[1,2]

Received May 4, 1993

We propose a vertex formulation of the Ising model with inhomogeneous external field on multiconnected networks possessing a superbond structure. The related technique based on gauge degrees of freedom enables us to recognize new collective modes of interaction nature, which provide an exact solution of the inverse profile problem and an explicit form of a local free-energy functional on an extended magnetization-mode space. Application is made to a square strip.

KEY WORDS: Inhomogeneous Ising network; profile equation; collective modes; free energy functional.

1. INTRODUCTION

Analysis of simplified model systems with a certain degree of spatial variation of model parameters[1,2] provides useful information about the role of inhomogeneity in thermal equilibrium. In particular, the free-energy functional format turns out to be a powerful instrument in detecting the role of locality and nonlocality in topologically significant exactly solvable examples. The complete solution of the inverse formulation of classical 1D lattice gases[3,4] was later recognized as a particular case of available inverse profiles for simply connected lattices, including the Bethe lattice.[5-7] Although the locality is broken for 1D Ising models with periodic boundary conditions, the existence of a topological collective mode permits the construction of a local free-energy functional on an extended space of site

[1] Courant Institute of Mathematical Sciences, New York University, New York, New York 10012.
[2] Physics Department, New York University, New York, New York 10012.
[3] Permanent address: Institute of Physics, Slovak Academy of Sciences, 842 28 Bratislava, Slovakia.

0022-4715/93/1000-0235$07.00/0

magnetizations and collective amplitudes.[8] The formalism of topological collective modes becomes substantially more laborious when generalizing the 1D periodic lattice to the simplest networks.[9] The entropy functional format[10,11] avoids, in certain restricted aspects, the problems associated with the nonsimple connectivity of the lattice structure.

The aim of this work is to overcome serious technical and conceptual problems in the theory of topological collective modes. The paper is based on a vertex representation of inhomogeneous Ising models and especially on a related gauge technique which is used to reduce substantially the effective number of microscopic states. We first treat the one-loop Ising network and find an intimate relationship between the structure of its free-energy functional and the implicit representation of the topological collective mode in the inhomogeneous regime. This relationship turns out to be of primary importance when we pass to more complicated many-loop networks with superbond structure. Together with the introduction of a new class of collective modes of interaction nature, it provides a simple "nearest-neighbor" form of the free-energy functional on the extended magnetization-mode space. The nonlocality is mirrored by a few collective modes of topological and interaction nature, determined by the stationarity of the free-energy functional. Application is made to a quasi-2D square ladder.

2. VERTEX FORMULATION OF THE ONE-LOOP ISING MODEL

2.1. Local Structure

We consider a one-dimensional closed chain, i.e., a ring, of Ising spins $\{\sigma_x\}$, $x=1,..., N$, with constant nearest-neighbor coupling J and in a varying field h_x (we set $1/kT$ to unity). In order to map the system onto a vertex model, we decorate each edge of the chain by a new vertex and attach to the resulting edge fragments the ordinary state variables $\sigma \in \{+,-\}$ (see Fig. 1). With each vertex of the original chain we associate a vertex weight $v_x(\sigma, \sigma') = \exp(h_x \sigma)\, \delta_{\sigma\sigma'}$. Then, the admissible vertex configurations with both incident edges in the same $+/-$ state are identified with the up/down state of the spin located at the corresponding site. To reflect the nearest-neighbor two-spin interactions, we attach to decorating sites the weight matrix with elements $E(\sigma, \sigma') = \exp(J\sigma\sigma')$. The statistical sum of the resulting system, defined by $Z = \sum_{\{\sigma,\sigma'\}} \prod$ (weights), is evidently identical to that of the Ising model. Let us express each $\mathbf{E}$-matrix as a product of two pair-dependent matrices, explicitly; for sites x, $x+1$ we set

$$\mathbf{E} = \mathbf{M}^T(g_{x,x+1}, g_{x+1,x})\, \mathbf{M}(g_{x+1,x}, g_{x,x+1}) \tag{2.1}$$

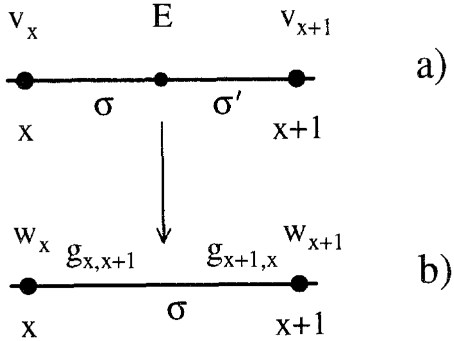

Fig. 1. A fragment of the Ising chain: (a) in the vertex representation with decorated bonds; (b) in the purely vertex representation.

Here, **M** is the invertible matrix parametrized by

$$\mathbf{M}(g_{x,y}, g_{y,x}) = \frac{1}{(1+g_{x,y}g_{y,x})^{1/2}} \begin{pmatrix} bg_{x,y}+a & ag_{x,y}+b \\ ag_{y,x}-b & bg_{y,x}-a \end{pmatrix} \tag{2.2}$$

($g_{x,y}g_{y,x} \neq -1$) with $a^2+b^2=\exp(J)$ and $2ab=\exp(-J)$. The columns (rows) of the matrix are indexed from left to right (from up to down) as $+$, $-$ and the indices in parameters $g_{x,y}$ indicate the corresponding bond as well as nearest-neighbor orientation. Grouping the couples of matrices **M** attached to an arbitrary original lattice node into new weights, we omit the decorating nodes and obtain the vertex model formulated on the original lattice with the following site-dependent vertex weights:

$$w_x(\sigma, \sigma') = \sum_{\sigma''=\pm} M_{\sigma\sigma''}(g_{x,x-1}, g_{x-1,x})\, M_{\sigma'\sigma''}(g_{x,x+1}, g_{x+1,x}) \exp(h_x\sigma'') \tag{2.3}$$

The parameters g play the role of the free gauge parameters leaving the partition function of the system invariant.[12-14]

Let us take advantage of the gauge degrees of freedom to eliminate substantially the number of microscopic states. With this aim, we nullify off-diagonal vertex weights at each site x,

$$w_x(+,-)=0 \tag{2.4a}$$

$$w_x(-,+)=0 \tag{2.4b}$$

Using the notation

$$G^+_{x,y} = \frac{a+bg_{x,y}}{ag_{x,y}+b} \tag{2.5a}$$

$$G^-_{x,y} = \frac{ag_{x,y}-b}{a-bg_{x,y}} \tag{2.5b}$$

we can write conditions (2.4a), (2.4b) in the form

$$\exp(-2h_x) = G^+_{x,x-1} G^+_{x,x+1} \left(\frac{G^-_{x+\delta,x}}{G^+_{x,x+\delta}} \right), \qquad \delta = \pm 1 \tag{2.6}$$

indicating the one-site character of the direction-independent ratios $G^-_{x+\delta,x}/G^+_{x,x+\delta}$. Since every edge provides a pair of gauge parameters, (2.6) determines unambiguously $\{g_{x,y}\}$ as functions of $\{h_x\}$. It is easy to show that the nonzero diagonal vertex weights $w_x(+,+)$ and $w_x(-,-)$, determined by (2.3), (2.6) satisfy the relations

$$w_x(+,+)\, w_x(-,-) = (e^{2J} - e^{-2J}) \tag{2.7a}$$

$$\frac{w_x(-,-)}{w_x(+,+)} = \frac{(a - bg_{x-1,x})(a - bg_{x+1,x})}{(ag_{x,x-1} + b)(ag_{x,x+1} + b)} \left(\frac{G^-_{x+\delta,x}}{G^+_{x,x+\delta}} \right) \tag{2.7b}$$

Having imposed a strictly diagonal form of local vertex weights, only two "macroscopic" states—with all edges in either $(+)$ or $(-)$ state—are allowed. The calculation of statistical quantities is then rather trivial. The statistical sum is evidently given by

$$Z = \prod_x w_x(+,+) + \prod_x w_x(-,-) \tag{2.8}$$

The magnetization at a given site x, m_x, can be calculated in terms of the statistical sum with modified Ising-like vertex weight at site x, $v_x \to \tilde{v}_x(\sigma, \sigma') = \sigma \exp(h_x \sigma)\, \delta_{\sigma\sigma'}$, implying

$$\tilde{w}_x(\sigma, \sigma') = \sum_{\sigma'' = \pm} M_{\sigma\sigma''}(g_{x,x-1}, g_{x-1,x})\, M_{\sigma'\sigma''}(g_{x,x+1}, g_{x+1,x})\, \sigma'' \exp(h_x \sigma'') \tag{2.9}$$

and the ordinary statistical sum (2.8). The admissible $(+)$ and $(-)$ lattice edge configurations contribute elements $\tilde{w}_x(+,+)$ and $\tilde{w}_x(-,-)$, respectively. Using the independence of $G^-_{x+\delta,x}/G^+_{x,x+\delta}$ on the nearest-neighbor direction $\delta = \pm 1$, we find

$$\frac{\tilde{w}_x(+,+)}{w_x(+,+)} = \frac{1 - G^-_{x+\delta,x}/G^+_{x,x+\delta}}{1 + G^-_{x+\delta,x}/G^+_{x,x+\delta}} \tag{2.10a}$$

$$\frac{\tilde{w}_x(-,-)}{w_x(-,-)} = -\frac{\tilde{w}_x(+,+)}{w_x(+,+)} \tag{2.10b}$$

and immediately arrive at

$$m_x = \sqrt{C} \left(\frac{1 - G^-_{x+\delta,x}/G^+_{x,x+\delta}}{1 + G^-_{x+\delta,x}/G^+_{x,x+\delta}} \right) \tag{2.11a}$$

with

$$\sqrt{C}=\left[\prod_y w_y(+,+)-\prod_y w_y(-,-)\right]\Big/\left[\prod_y w_y(+,+)+\prod_y w_y(-,-)\right] \tag{2.11b}$$

These relations confirm the expected one-site dependence of the ratios $G^-_{x+\delta,x}/G^+_{x,x+\delta}$,

$$\frac{G^-_{x+\delta,x}}{G^+_{x,x+\delta}}=\frac{\sqrt{C}-m_x}{\sqrt{C}+m_x} \tag{2.12}$$

Equation (2.11a) provides a direct solution of the inverse problem, i.e., finding h_x as a function of the magnetization profile. For one bond, say between sites x and $x+1$, the boundary magnetizations m_x and m_{x+1} can be expressed in terms of the same pair of gauge parameters $g_{x,x+1}$ and $g_{x+1,x}$ contained in the auxiliary variables $G^\pm_{x,x+1}$ and $G^\pm_{x+1,x}$ consequently yielding the explicit form of $g_{x,x+1}$ and $g_{x+1,x}$ as local functions of the magnetizations $\{m_x, m_{x+1}\}$. In particular, e.g., for $G^+_{x,y}$ one gets

$$G^+_{x,y}=\frac{\sqrt{C}+m_x}{t_{x,y}(J)+[t^2_{x,y}(J)-m_x^2+C]^{1/2}} \tag{2.13a}$$

$$t_{x,y}(J)=\cosh(2J)\,m_x-\sinh(2J)\,m_y \tag{2.13b}$$

Having determined the magnetization dependence of the gauge parameters, we return to formula (2.6) and obtain, with the aid of Eqs. (2.12), (2.13a), and (2.13b), the local profile equation for the applied field,

$$\begin{aligned}h_x=&-\tfrac{1}{2}\ln(C-m_x^2)+\tfrac{1}{2}\ln\{t_{x,x+1}(J)+[t^2_{x,x+1}(J)-m_x^2+C]^{1/2}\}\\&+\tfrac{1}{2}\ln\{t_{x,x-1}(J)+[t^2_{x,x-1}(J)-m_x^2+C]^{1/2}\}\end{aligned} \tag{2.14}$$

The nonlocal collective mode C reflects the global character of the magnetization profile due to chain closing, which manifests itself as a magnetization rescaling by the factor $1/\sqrt{C}$. Taking into account (2.7a), (2.8), and (2.11b), it can be expressed as

$$C=1-\frac{4}{Z^2}(e^{2J}-e^{-2J})^N \tag{2.15}$$

2.2. Free Energy

For fixed C, the inverse relation (2.14) possesses the integrability property $\partial h_x/\partial m_y|_C=\partial h_y/\partial m_x|_C$, which[8,9] guarantees the existence of a free-energy functional F on the extended $\{\mathbf{m}, C\}$ space such that

$$h_x = \frac{\partial}{\partial m_x} F[\mathbf{m}, C] \tag{2.16a}$$

$$0 = \frac{\partial}{\partial C} F[\mathbf{m}, C]\bigg|_{C=C(m)} \tag{2.16b}$$

Within the proposed formalism it is possible to introduce naturally the quantity conjugate to the collective mode C (more precisely, to $\sqrt{C}$). First, let us study how the above mechanism manifests itself in the direct calculation of $m_x = \partial \ln Z/\partial h_x$. A straightforward calculation using formula (2.3) shows that besides the gauge invariance of Z as a whole, there holds for its separate parts

$$\frac{\partial}{\partial g_{x,y}} \prod_z w_z(+,+) = 0 \tag{2.17a}$$

$$\frac{\partial}{\partial g_{x,y}} \prod_z w_z(-,-) = 0 \tag{2.17b}$$

This fact permits us to obtain explicitly the derivatives

$$\frac{\partial}{\partial h_x} \prod_y w_y(+,+) = \prod_{y \neq x} w_y(+,+)\, \tilde{w}_x(+,+) \tag{2.18a}$$

$$\frac{\partial}{\partial h_x} \prod_y w_y(-,-) = \prod_{y \neq x} w_y(-,-)\, \tilde{w}_x(-,-) \tag{2.18b}$$

and so arrive at the final formula for m_x (2.11). In the spirit of the vertex approach, we now define the variable ϕ which controls the polarity of the circuit: $\prod_x w_x(+,+) \to e^{\phi} \prod_x w_x(+,+)$, $\prod_x w_x(-,-) \to e^{-\phi} \prod_x w_x(-,-)$. The logarithm of the corresponding statistical sum

$$Z(\mathbf{h}, \phi) = e^{\phi} \prod_x w_x(+,+) + e^{-\phi} \prod_x w_x(-,-) \tag{2.19}$$

is the generating function for magnetization $m_x = \partial \ln Z(\mathbf{h}, \phi)/\partial h_x$, which, owing to (2.18a) and (2.18b), takes the form of (2.11a) with

$$\sqrt{C} = \frac{[e^{\phi} \prod_y w_y(+,+) - e^{-\phi} \prod_y w_y(-,-)]}{[e^{\phi} \prod_y w_y(+,+) + e^{-\phi} \prod_y w_y(-,-)]} \tag{2.20}$$

Since $\sqrt{C} = \partial \ln Z(\mathbf{h}, \phi)/\partial \phi$, ϕ is the conjugate quantity of $\sqrt{C}$. According to (2.20), it satisfies the relation

$$2\phi = -\ln\left(\frac{1-\sqrt{C}}{1+\sqrt{C}}\right) + \sum_x \ln\left[\frac{w_x(-,-)}{w_x(+,+)}\right] \tag{2.21}$$

Inverse relation (2.21) is of interest not only in a potential nonequilibrium description ($\phi \neq 0$) of a finite Ising ring, but also in the equilibrium conditions ($\phi = 0$) where it provides, using (2.7b) and the results for $g_{x,y}$, an implicit form of C as a function of magnetizations:

$$\ln\left(\frac{1-\sqrt{C}}{1+\sqrt{C}}\right) = \sum_x \ln(C - m_x^2) - \sum_{\langle x, x+1\rangle} \ln \lambda_{x,x+1}(J, C) \qquad (2.22a)$$

where the bond quantity $\lambda_{x,x+1}$, given by

$$\lambda_{x,x+1}(J, C) = \frac{1}{\sinh(2J)} \{C \cosh(2J) - m_x m_{x+1} \sinh(2J) + \sqrt{C}\,[t_{x,x+1}^2(J) - m_x^2 + C]^{1/2}\} \qquad (2.22b)$$

is a symmetric function of neighboring magnetizations m_x, m_{x+1} [see the definition of $t_{x,y}$, (2.13b)]. After lengthy algebra it can then be shown that the free-energy functional on the extended $\{\mathbf{m}, C\}$ space, defined via (2.16a) and the inverse relation (2.14), takes the form

$$F[\mathbf{m}, C] = \sum_x m_x h_x + \frac{\sqrt{C}}{2}\left[\sum_x \ln(C - m_x^2) - \sum_{\langle x, x+1\rangle} \ln \lambda_{x,x+1}(J, C)\right] + f(C) \qquad (2.23)$$

where $f(C)$ is an as-yet-undetermined function of the collective mode, ensuring the stationarity condition (2.16b). The striking correspondence between the rhs of Eq. (2.22a) and the term in the square brackets in Eq. (2.23) permits to us specify $f(C)$ immediately by taking into account the fact that $F[\mathbf{m}, C]$ satisfying (2.16) is related to the ordinary free-energy functional $F[\mathbf{m}]$ by[8,9] $F[\mathbf{m}, C(\mathbf{m})] = F[\mathbf{m}]$. Since

$$\begin{aligned} F[\mathbf{m}] &= \sum_x m_x h_x - \ln Z \\ &= \sum_x m_x h_x + \tfrac{1}{2}\ln(1 - C) + \text{const} \end{aligned} \qquad (2.24)$$

we readily get

$$f(C) = \tfrac{1}{2}[(1+\sqrt{C})\ln(1+\sqrt{C}) + (1-\sqrt{C})\ln(1-\sqrt{C})] \qquad (2.25)$$

The intimate relationship between the implicit representation of collective modes and the structure of the free-energy functional on the extended space in the *inhomogeneous* regime is of primary interest when formulating the functional theory in its variational form for more complicated structures.

3. MULTICONNECTED NETWORKS WITH SUPERBOND STRUCTURE

3.1. Profile Equations

The prototype for introducing the problems arising when one passes to more general structures is the many-loop case drawn in Fig. 2. Here, each channel $\alpha = 1,..., q$, possessing N_α internal points $x\alpha$ ($x = 1,..., N_\alpha$) ends at points $A = 0\alpha$ and $B = (N_\alpha + 1)\alpha$, which thus become q-coordinated. In order to simplify the notation associated with channels, in what follows the summation $\sum_{x\alpha}$ means the sum over all internal points of the αth channel (i.e., $x = 1,..., N_\alpha$), while the summation over nearest neighbors $\sum_{\langle x\alpha, (x+1)\alpha \rangle}$ will include also pair contributions with adjacent sites A and B (i.e., $x = 0,..., N_\alpha$).

It is easy to find $h_{x\alpha}$ inside the αth channel ($x = 1,..., N_\alpha$). Namely, we can introduce a superbond matrix $\bar{\mathbf{S}}_\alpha$ between sites A, B which reflects their effective interaction as well as effective field contributions at A and B induced by all channels $\beta \neq \alpha$ (Fig. 3a). We then proceed as in the one-loop case and arrive at the local inversion relation

$$h_{x\alpha} = -\tfrac{1}{2} \ln(C_\alpha - m_{x\alpha}^2) + \tfrac{1}{2} \ln\{t_{x\alpha,(x+1)\alpha}(J) + [t_{x\alpha,(x+1)\alpha}^2(J) - m_x^2 + C_\alpha]^{1/2}\}$$
$$+ \tfrac{1}{2} \ln\{t_{x\alpha,(x-1)\alpha}(J) + [t_{x\alpha,(x-1)\alpha}^2(J) - m_x^2 + C_\alpha]^{1/2}\} \qquad (3.1)$$

The formula for collective mode (2.15) modifies slightly owing to the variation of interaction between A, B sites to

$$C_\alpha = 1 - \frac{4}{Z^2} (e^{2J} - e^{-2J})^{N_\alpha + 1} \operatorname{Det}(\bar{\mathbf{S}}_\alpha) \qquad (3.2)$$

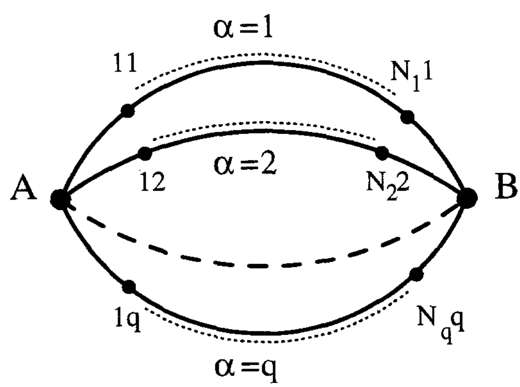

Fig. 2. The q-channel network.

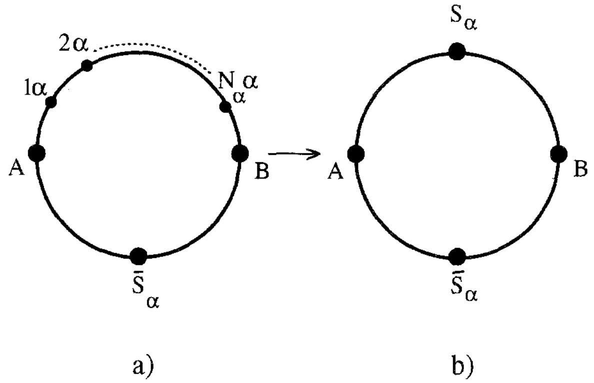

Fig. 3. Two equivalent representations of the q-channel network when the αth channel is the reference: (a) with the αth channel composed of N_α nodes and the superbond $\bar{\mathbf{S}}_\alpha$; (b) with superbonds $\mathbf{S}_\alpha$ and $\bar{\mathbf{S}}_\alpha$.

The complication comes when studying the profile problem for sites A, B. We return to the αth channel and concentrate on its superbond representation $\mathbf{S}_\alpha$ with respect to A, B sites (Fig. 3b). Within the gauge technique it is easy to perform the diagonalization of the channel together with nodes A, B and then put back the edge matrices $\mathbf{M}$, which results in

$$\mathbf{S}_\alpha = \mathbf{M}^T(g_{A,1\alpha}, g_{1\alpha,A}) \begin{pmatrix} \prod_{x\alpha} w_{x\alpha}(+,+) & 0 \\ 0 & \prod_{x\alpha} w_{x\alpha}(-,-) \end{pmatrix} \times \mathbf{M}(g_{B,N_\alpha\alpha}, g_{N_\alpha\alpha,B}) \tag{3.3}$$

This superbond matrix induces an effective A–B pair interaction J_α and additional fields h_A^α and h_B^α to sites A and B, respectively, defined by

$$\mathbf{S}_\alpha = n_\alpha^{1/2} \begin{pmatrix} \exp(h_A^\alpha + h_B^\alpha + J_\alpha) & \exp(h_A^\alpha - h_B^\alpha - J_\alpha) \\ \exp(-h_A^\alpha + h_B^\alpha - J_\alpha) & \exp(-h_A^\alpha - h_B^\alpha + J_\alpha) \end{pmatrix} \tag{3.4}$$

We now intuitively suggest that the A–B effective interaction J_α is a relevant collective variable. Once this assumption has been accepted, comparing Eqs. (3.3) and (3.4) and using the gauge formalism developed in the previous section [mainly Eq. (2.12) applied to $G_{1\alpha,A}^-/G_{A,1\alpha}^+$, $G_{N_\alpha\alpha,B}^-/G_{B,N_\alpha\alpha}^+$ and the explicit results (2.13a), (2.13b) for $G_{A,1\alpha}^+$, $G_{B,N_\alpha\alpha}^+$], we first express, from the relation determining J_α, the quantity

$$\frac{(a - bg_{1\alpha,A})(a - bg_{N_\alpha\alpha,B})}{(ag_{A,1\alpha} + b)(ag_{B,N_\alpha\alpha} + b)} \prod_{x\alpha} \left[\frac{w_{x\alpha}(-,-)}{w_{x\alpha}(+,+)}\right]$$

as a function of $\{J_\alpha, C_\alpha, m_A, m_B\}$ and then consider this dependence in the relations for h_A^α, h_B^α. The algebra yields

$$n_\alpha = (e^{2J} - e^{-2J})^{N_\alpha+1}/(e^{2J_\alpha} - e^{-2J_\alpha}) \tag{3.5a}$$

$$h_A^\alpha = \tfrac{1}{2}(\ln\{t_{AB}(J_\alpha) + [t_{AB}^2(J_\alpha) - m_A^2 + C_\alpha]^{1/2}\} \\ - \ln\{t_{A,1\alpha}(J) + [t_{A,1\alpha}^2(J) - m_A^2 + C_\alpha]^{1/2}\}) \tag{3.5b}$$

with a similar formula for h_B^α under the interchange $A \leftrightarrow B$ and $1\alpha \to N_\alpha\alpha$. Here $t_{AB}(J_\alpha)$ is the obvious generalization of definition (2.13b). The simplicity of the resulting relations is remarkable in that the effect of inhomogeneity inside the whole channel is now represented by only one parameter. Having specified all superbonds $\mathbf{S}_1, \dots, \mathbf{S}_q$, the total effect of all spins between sites A and B is represented by superbond $\mathbf{S}$ (Fig. 4) given by

$$\mathbf{S} = \left(\prod_\alpha n_\alpha\right)^{1/2} \begin{pmatrix} \exp \sum_\alpha (h_A^\alpha + h_B^\alpha + J_\alpha) & \exp \sum_\alpha (h_A^\alpha - h_B^\alpha - J_\alpha) \\ \exp \sum_\alpha (-h_A^\alpha + h_B^\alpha - J_\alpha) & \exp \sum_\alpha (-h_A^\alpha - h_B^\alpha + J_\alpha) \end{pmatrix} \tag{3.6}$$

Thus, our task reduces to the two-site inverse problem for nodes A, B with respective magnetizations m_A, m_B and in respective fields $h_A + \sum_\alpha h_A^\alpha$, $h_B + \sum_\alpha h_B^\alpha$, coupled by $\sum_\alpha J_\alpha$. A straightforward solution takes the form

$$h_A = -\tfrac{1}{2}\ln(1 - m_A) + \tfrac{1}{2}\ln\left\{t_{AB}\left(\sum_\alpha J_\alpha\right) + \left[t_{AB}^2\left(\sum_\alpha J_\alpha\right) - m_A^2 + 1\right]^{1/2}\right\} \\ + \tfrac{1}{2}\sum_\alpha (\ln\{t_{A,1\alpha}(J) + [t_{A,1\alpha}^2(J) - m_A^2 + C_\alpha]^{1/2}\} \\ - \ln\{t_{AB}(J_\alpha) + [t_{AB}^2(J_\alpha) - m_A^2 + C_\alpha]^{1/2}\}) \tag{3.7}$$

A similar formula with interchange $A \leftrightarrow B$ and $1\alpha \to N_\alpha\alpha$ holds for h_B. It is clear that the integrability conditions $\partial h_A/\partial m_{x\alpha} = \partial h_{x\alpha}/\partial m_A$, $\partial h_A/\partial m_B =$

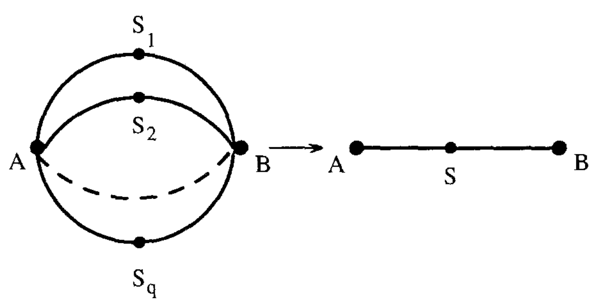

Fig. 4. The superbond representations of spins between sites A and B.

$\partial h_B/\partial m_A$ are fulfilled: the terms on the rhs of (3.7) which express the dependence on magnetizations at sites 1α are simply the correct counterparts of the corresponding terms in the inverse relations for $h_{1\alpha}$, while the remaining terms have either one-site character or describe the magnetization dependence of the "nearest-neighbor type" between sites A and B. We therefore conclude that $\{J_\alpha\}$ are true collective modes.

3.2. Structure of Free Energy

Inversion relations (3.1), (3.7) imply the following form of the free-energy functional on the combined $\{\mathbf{m}, \mathbf{J}, \mathbf{C}\}$ space:

$$\begin{aligned} F[\mathbf{m}, \mathbf{J}, \mathbf{C}] = {} & \sum_\alpha \sum_{x\alpha} m_{x\alpha} h_{x\alpha} + m_A h_A + m_B h_B \\ & + \frac{1}{2}\left\{\ln(1-m_A^2) + \ln(1-m_B^2) - \ln \lambda_{AB}\left(\sum_\alpha J_\alpha, 1\right)\right\} \\ & + \sum_\alpha \frac{\sqrt{C_\alpha}}{2}\left[\sum_{x\alpha} \ln(C_\alpha - m_{x\alpha}^2) - \sum_{\langle x\alpha, (x+1)\alpha\rangle} \ln \lambda_{x\alpha,(x+1)\alpha}(J, C_\alpha) \right. \\ & \left. + \ln \lambda_{AB}(J_\alpha, C_\alpha)\right] + f(\mathbf{J}, \mathbf{C}) \end{aligned} \tag{3.8}$$

with the obvious extension of the definition of λ, (2.22b). In order to determine $f(\mathbf{J}, \mathbf{C})$, we have to find the relationship between $F[\mathbf{m}, \mathbf{J}, \mathbf{C}]$ and the implicit representation of collective modes. Let us note that the collective mode C_α can be represented implicitly by a counterpart of (2.22a) in two ways: (I) in the ordinary picture with the αth channel composed of N_α nodes and the superbond $\bar{\mathbf{S}}_\alpha$ (Fig. 3a); (II) in the purely superbond picture with superbonds $\mathbf{S}_\alpha$ and $\bar{\mathbf{S}}_\alpha$ (Fig. 3b). For the case (I) we have

$$\begin{aligned} \ln\left(\frac{1-\sqrt{C_\alpha}}{1+\sqrt{C_\alpha}}\right) = {} & \sum_{x\alpha} \ln(C_\alpha - m_{x\alpha}^2) + \ln(C_\alpha - m_A^2) + \ln(C_\alpha - m_B^2) \\ & - \sum_{\langle x\alpha, (x+1)\alpha\rangle} \ln \lambda_{x\alpha,(x+1)\alpha}(J, C_\alpha) - \ln \lambda_{AB}\left(\sum_{\beta\neq\alpha} J_\beta, C_\alpha\right) \end{aligned} \tag{3.9}$$

while for the case (II) the implicit representation of C_α reads

$$\begin{aligned} \ln\left(\frac{1-\sqrt{C_\alpha}}{1+\sqrt{C_\alpha}}\right) = {} & \ln(C_\alpha - m_A^2) + \ln(C_\alpha - m_B^2) \\ & - \ln \lambda_{AB}(J_\alpha, C_\alpha) - \ln \lambda_{AB}\left(\sum_{\beta\neq\alpha} J_\beta, C_\alpha\right) \end{aligned} \tag{3.10}$$

Subtraction of (3.9) and (3.10) cancels the "unwanted" terms and results in the equality

$$\sum_{x\alpha} \ln(C_\alpha - m_{x\alpha}^2) - \sum_{\langle x\alpha, (x+1)\alpha \rangle} \ln \lambda_{x\alpha,(x+1)\alpha}(J, C_\alpha) + \ln \lambda_{AB}(J_\alpha, C_\alpha) = 0 \quad (3.11)$$

From the two-site picture (Fig. 4) with superbond S, (3.6), one gets after some algebra

$$\frac{1}{2}\left\{\ln(1-m_A^2) + \ln(1-m_B^2) - \ln \lambda_{AB}\left(\sum_\alpha J_\alpha, 1\right)\right\}$$
$$= \frac{1}{2}\left[\ln \sinh\left(\sum_\alpha 2J_\alpha\right) - \sum_\alpha \ln \sinh(2J_\alpha)\right] - \ln Z + \text{const} \quad (3.12)$$

Finally, taking into account the equality

$$F[\mathbf{m}, \mathbf{J}(\mathbf{m}), \mathbf{C}(\mathbf{m})] = \sum_\alpha \sum_{x\alpha} m_{x\alpha} h_{x\alpha} + m_A h_A + m_B h_B - \ln Z \quad (3.13)$$

and combining Eqs. (3.8), (3.11), and (3.12), we arrive at

$$f(\mathbf{J}, \mathbf{C}) = \frac{1}{2}\left[\sum_\alpha \ln \sinh(2J_\alpha) - \ln \sinh\left(\sum_\alpha 2J_\alpha\right)\right] \quad (3.14)$$

The free-energy functional (3.8) with $f(\mathbf{J}, \mathbf{C})$ given by (3.14) determines the inhomogeneous external field and collective variables through

$$h_x = \frac{\partial F[\mathbf{m}, \mathbf{J}, \mathbf{C}]}{\partial m_x} \quad (3.15\text{a})$$

$$0 = \left.\frac{\partial F[\mathbf{m}, \mathbf{J}, \mathbf{C}]}{\partial \mathbf{J}}\right|_{J=J(m), C=C(m)} \quad (3.15\text{b})$$

$$0 = \left.\frac{\partial F[\mathbf{m}, \mathbf{J}, \mathbf{C}]}{\partial \mathbf{C}}\right|_{J=J(m), C=C(m)} \quad (3.15\text{c})$$

We notice that there exists a relationship among the collective modes. Within the superbond formalism we have

$$\text{Det}(\bar{\mathbf{S}}_\alpha) = \left(\prod_{\beta \neq \alpha} n_\beta\right)\left[\exp\left(\sum_{\beta \neq \alpha} 2J_\beta\right) - \exp\left(-\sum_{\beta \neq \alpha} 2J_\beta\right)\right]$$

and, consequently, Eq. (3.2) can be written as

$$C_\alpha = 1 - C_0 \frac{\exp(\sum_{\beta \neq \alpha} 2J_\beta) - \exp(-\sum_{\beta \neq \alpha} 2J_\beta)}{\prod_{\beta \neq \alpha}[\exp(2J_\beta) - \exp(-2J_\beta)]} \quad (3.16\text{a})$$

($\alpha = 1, \ldots, q$) with C_0 defined by

$$C_0 = \frac{4}{Z^2} \prod_\alpha (e^{2J} - e^{-2J})^{N_\alpha + 1} \tag{3.16b}$$

Using Eqs. (3.16a) and (3.16b), we can reduce the number of collective modes, e.g., by restricting ourselves to "interaction" collective modes $\{\mathbf{J}\}$ and to C_0 related directly to the partition function. Since J_α is easily expressible, using the superbond representation (3.3), as a function of the magnetization profile inside the αth channel and of the C_α-mode, this suggests an alternative construction of the ordinary free-energy functional $F[\mathbf{m}]$ with a complete set of equations determining collective modes. We consider the formalism of the free-energy functional on the extended space more simple and efficient, so we will not discuss this alternative.

4. GENERALIZATION

The proposed procedure for finding the free-energy functional on the extended space is applicable to an arbitrary structure which can be transformed by a successive reduction via superbonds into an exactly solvable case. Two examples of this kind—the ring with a superbond hierarchy and the ladder strip—are presented in Fig. 5. The elimination of a superbond (with collective variables $\{C_\alpha, J_\alpha\}$ introduced for each of its channels) induces an effective interaction $\sum_\alpha J_\alpha$ and field contributions of type (3.5b) for the pair of edge sites of the superbond and provides an explicit inverse relation for internal sites. We observe that internal sites at a given level

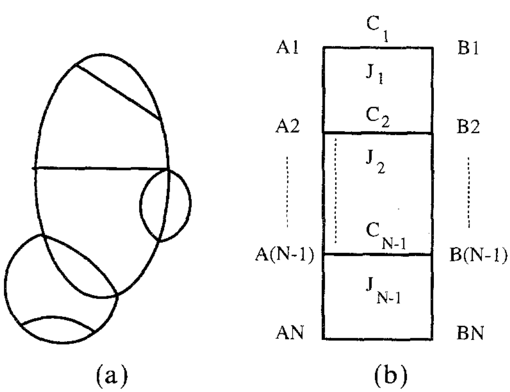

Fig. 5. Two examples of exactly solvable inhomogeneous Ising networks with superbond structure: (a) the ring with a hierarchy of superbonds (we note that between the crossing points with coordination >2 there can be an arbitrary number of two-coordinated nodes); (b) the ladder strip.

may have had coordination number >2 at a previous level, and therefore may have additional field contributions, as in (3.5b). We proceed in this way to a structure solvable by ordinary means, in our examples to a ring (Fig. 5a) and to a two-site lattice (Fig. 5b). The corresponding free-energy functional possesses a structure analogous to that presented in formula (3.8)—it is composed of one-site and symmetric "nearest-neighbor" contributions which are produced by the hierarchy of superbond elimination as well as by the exact solution of the final structure. To obtain the unknown function $f(\mathbf{J}, \mathbf{C})$ it is necessary to consider, at each level of the superbond elimination, two possible representations (I) and (II) of the collective variables C_α introduced. In this way, we are able to derive identities like (3.11) [the field contributions of type (3.5b) manifest themselves in the free-energy functional in such a way that the subtraction mechanism is automatically available] and express, using the results of the previous section, the terms given by the exact solution of the final structure through collective modes.

To be more specific, we present briefly the explicit results for the square ladder (Fig. 5b). Let us eliminate successively the superbonds from up to down, introducing before every elimination a new pair of collective modes $\{C_x, J_x\}$ as indicated in the figure. Observing that after the elimination of sites Ax, Bx the total effective interaction between sites $A(x+1)$, $B(x+1)$ is equal to $(J+J_x)$, we readily find

$$\begin{aligned} h_{A1} = & -\tfrac{1}{2}\ln(C_1 - m_{A1}^2) + \tfrac{1}{2}\ln\{t_{A1,A2}(J) + [t_{A1,A2}^2(J) - m_{A1}^2 + C_1]^{1/2}\} \\ & + \tfrac{1}{2}\ln\{t_{A1,B1}(J) + [t_{A1,B1}^2(J) - m_{A1}^2 + C_1]^{1/2}\} \end{aligned} \tag{4.1a}$$

$$\begin{aligned} h_{Ax} = & -\tfrac{1}{2}\ln(C_x - m_{Ax}^2) + \tfrac{1}{2}\ln\{t_{Ax,A(x+1)}(J) \\ & + [t_{Ax,A(x+1)}^2(J) - m_{Ax}^2 + C_x]^{1/2}\} \\ & + \tfrac{1}{2}\ln\{t_{Ax,Bx}(J+J_{x-1}) + [t_{Ax,Bx}^2(J+J_{x-1}) - m_{Ax}^2 + C_x]^{1/2}\} \\ & + \tfrac{1}{2}\ln\{t_{Ax,A(x-1)}(J) + [t_{Ax,A(x-1)}^2(J) - m_{Ax}^2 + C_{x-1}]^{1/2}\} \\ & - \tfrac{1}{2}\ln\{t_{Ax,Bx}(J_{x-1}) + [t_{Ax,Bx}^2(J_{x-1}) - m_{Ax}^2 + C_{x-1}]^{1/2}\} \\ & (x = 2,..., N-1) \end{aligned} \tag{4.1b}$$

$$\begin{aligned} h_{AN} = & -\tfrac{1}{2}\ln(1 - m_{AN}) + \tfrac{1}{2}\ln\{t_{AN,BN}(J+J_{N-1}) \\ & + [t_{AN,BN}^2(J+J_{N-1}) - m_{AN}^2 + 1]^{1/2}\} \\ & + \tfrac{1}{2}\ln\{t_{AN,A(N-1)}(J) + [t_{AN,A(N-1)}^2(J) - m_{AN}^2 + C_{N-1}]^{1/2}\} \\ & - \tfrac{1}{2}\ln\{t_{AN,BN}(J_{N-1}) + [t_{AN,BN}^2(J_{N-1}) - m_{AN}^2 + C_{N-1}]^{1/2}\} \end{aligned} \tag{4.1c}$$

The corresponding free-energy functional reads

$$F=\sum_x (m_{Ax}h_{Ax}+m_{Bx}h_{Bx})$$
$$+\sum_{x=1}^{N-1}\frac{\sqrt{C_x}}{2}\{\ln(C_x-m_{Ax}^2)+\ln(C_x-m_{Bx}^2)-\ln\lambda_{Ax,A(x+1)}(J,C_x)$$
$$-\ln\lambda_{Bx,B(x+1)}(J,C_x)-\ln\lambda_{Ax,Bx}(J+J_{x-1},C_x)$$
$$+\ln\lambda_{A(x+1),B(x+1)}(J_x,C_x)\}$$
$$+\frac{1}{2}\{\ln(1-m_{AN}^2)+\ln(1-m_{BN}^2)-\ln\lambda_{AN,BN}(J+J_{N-1},1)\}+f(\mathbf{J},\mathbf{C}) \tag{4.2}$$

Here, J_0 is identically equal to 0 and $f(\mathbf{J},\mathbf{C})$ has to be determined. By considering two possible implicit representations of the collective mode C_x at the xth level, we obtain

$$\ln(C_x-m_{Ax}^2)+\ln(C_x-m_{Bx}^2)-\ln\lambda_{Ax,A(x+1)}(J,C_x)-\ln\lambda_{Bx,B(x+1)}(J,C_x)$$
$$-\ln\lambda_{Ax,Bx}(J+J_{x-1},C_x)+\ln\lambda_{A(x+1),B(x+1)}(J_x,C_x)=0 \tag{4.3}$$

Evaluating the prefactors of superbond matrices at every elimination level, we see that

$$\tfrac{1}{2}\{\ln(1-m_{AN}^2)+\ln(1-m_{BN}^2)-\ln\lambda_{AN,BN}(J+J_{N-1},1)\}$$
$$=\tfrac{1}{2}\sum_{x=1}^{N-1}[\ln\sinh 2(J+J_x)-\ln\sinh 2J_x]-\ln Z+\text{const} \tag{4.4}$$

Finally, the equality

$$F[\mathbf{m},\mathbf{J}(\mathbf{m}),\mathbf{C}(\mathbf{m})]=\sum_x (m_{Ax}h_{Ax}+m_{Bx}h_{Bx})-\ln Z$$

implies the following form of $f(\mathbf{J},\mathbf{C})$:

$$f(\mathbf{J},\mathbf{C})=\tfrac{1}{2}\sum_{x=1}^{N-1}[\ln\sinh 2J_x-\ln\sinh 2(J+J_x)] \tag{4.5}$$

A similar procedure can be applied to the triangle strip, which is equivalent to the inhomogeneous Ising chain with NN and NNN two-spin interactions.

It is to be noted that the external fields themselves can be considered, in principle and sometimes also in practice, as collective variables. Indeed, putting $h_x = H_x$, we find that the integrability conditions $\partial h_x/\partial m_y|_H = \partial h_y/\partial m_x|_H$ $(=0)$ are fulfilled. The free-energy functional on the combined $(\mathbf{m}, \mathbf{H})$ space reads

$$F[\mathbf{m}, \mathbf{H}] = \sum_x m_x H_x - \ln Z(h_x = H_x) \tag{4.6}$$

so that we have

$$h_x = \frac{\partial}{\partial m_x} F[\mathbf{m}, \mathbf{H}], \qquad 0 = \frac{\partial}{\partial H_x} F[\mathbf{m}, \mathbf{H}]\bigg|_{H = H(m)} \tag{4.7}$$

This indicates a general criterion for choosing appropriate collective modes. For small lattices with complicated topological structure, the available explicit form of $\ln Z$ as a function of $\{H_x\}$ can make the formulation (4.6) the most appropriate one. For large lattices an explicit form of $\ln Z(h_x = H_x)$ is not at our disposal and so the application of collective modes of topological or interaction nature is inevitable. They substantionally decrease the number of variational parameters and/or make the free-energy functional expressible in a simple way. The latter feature is clearly seen in the case of the square ladder, where the formulation (4.6) is intractable, while the proposed combination of topological and interaction modes leads to a very simple form of the free-energy functional (4.2), (4.5) possessing formally the structure of the original model Hamiltonian. For more complicated lattices, $\{H_x\}$ may be used as complementary collective variables and could help to solve some topological nontrivialities.

5. CONCLUSION

The vertex formulation of the inhomogeneous Ising model enables us to pass from the local site-to-site recurrence approach to the formalism of interplaying chain fragments. The related technique of gauge parameters turns out to be a powerful method even in the relatively well-understood case of the closed Ising chain, for which it provides the natural introduction of the quantity conjugate to the collective mode and the establishment of the close relationship between the implicit representation of the collective mode and the structure of the free-energy functional on the extended magnetization-mode space in the inhomogeneous regime. For nontrivial generalization of the superbond type, we have found new interaction collective modes which imply "integrable" profile equations and maintain the simple "nearest-neighbor" form of the free-energy functional on the extended space. The observed relationship between the structure of the free-energy functional and the possible implicit representation of collective modes is of primary importance. It confirms that there is a harmony in the inverse treatment—the extremely complicated nonlocal effect of inhomogeneity and nonlinearity is encompassed by a few collective modes whose dependence on the magnetization profile can be generated, according to a variational principle, from a simple free-energy functional. The simple form of the functional evokes the possibility of its construction for general structures by topological rules, with a hierarchy of collective modes of various kinds governing the statistics of the system. Investigation as to whether such a simple picture is realistic is left for the future.

ACKNOWLEDGMENT

This work was supported by a grant from the National Science Foundation.

REFERENCES

1. M. Mendes-France, *J. Stat. Phys.* **45**:89 (1986).
2. B. Derrida, M. Mendes-France, and J. Peyriere, *J. Stat. Phys.* **45**:439 (1986).
3. J. K. Percus, *J. Stat. Phys.* **16**:299 (1977).
4. J. K. Percus, *J. Math. Phys.* **23**:1162 (1982).
5. J. K. Percus, *J. Stat. Phys.* **55**:1263 (1989).
6. L. Šamaj, *Physica A* **153**:517 (1988).
7. L. Šamaj, *J. Phys.* (Paris) **50**:273 (1989).
8. J. K. Percus and M. Q. Zhang, *Phys. Rev. B* **38**:11737 (1988).
9. M. Q. Zhang and J. K. Percus, *J. Stat. Phys.* **56**:695 (1989).
10. J. K. Percus, *J. Stat. Phys.* **60**:221 (1990).
11. M. Q. Zhang, *J. Phys. A Math. Gen.* **23**:2173 (1990).
12. F. J. Wegner, *Physica* **68**:570 (1973).
13. X. N. Wu and F. Y. Wu, *J. Phys. A Math. Gen.* **22**:L55 (1989).
14. L. Šamaj and M. Kolesík, *Physica A* **182**:455 (1992).