New real-space renormalization-group calculation for the critical properties of lattice spin systems

Charles E. Hecht
Department of Chemistry, City University of New York, Hunter College, New York, New York 10021

Ryoichi Kikuchi
Hughes Research Laboratories, Malibu, California 90265

(Received 16 November 1981)

In evaluating the critical properties of lattice spin systems in the real-space renormalization-group theory we use the cluster variation method. A configuration in the transformed system is constrained and the probability of occurrence of this configuration is calculated both in the transformed system and in the original system. By equating the two probabilities and forming ratios of two such equalities (for two or more constrained configurations) the fixed point of the renormalization transformation is evaluated. The method can avoid the trouble due to different singularities in the original and transformed systems, and hence can obviate the possible development of spurious singularities in the transformation at low temperatures. The two-dimensional triangular Ising model is treated with numerical results comparable with those obtained by the cluster treatment of Niemeijer and van Leeuwen who used more and larger cluster types than those we introduce.

I. INTRODUCTION

We present a new implementation of Niemeijer and van Leeuwen's[1] real- (i.e., coordinate) space renormalization-group transformation for discrete spins on lattices. In this methodology one bundles groups of spins s^d together (d is the dimensionality) into cells and uses a rule that gives a composite cell spin, $\sigma' = \pm 1$ (as determined by the directions of the original s^d, often by a majority rule) at the center of the group. The new spins are distributed on a lattice isomorphic to the starting lattice but with a separation s times the old lattice distance. All quantities pertaining to the cell spin system will be denoted by primes. The number of cell spins, N' is related to the original number of spins, N by

$$N' s^d = N \ . \tag{1.1}$$

This is a transformation termed nonlinear in the literature[2] since the cell spin is not linearly related to the site spins of the cell. Transformations that linearly relate the cell spin to the site spins are dependent upon a parameter p appearing in the linear relation and this has been exploited to obtain excellent numerical results for critical-state property exponents in certain cases.[3] However, this linear method can lead to the development of spurious singularities in the transformation[4] perhaps related to a failure to preserve all the symmetries of the initial Hamiltonian,[5] H (for which the usual Boltzmann factor $-\beta = -1/k_B T$ has been included as multiplicative factor). It is of course essential in renormalization-group transformations from H to H' that not only the partition function be preserved but also that the free energy of the cell system exhibit the same singularities (if any) of the site system. The latter criterion is difficult to ensure for nonlinear transformations. In this work, we have been able to explicitly avoid this difficulty (to our knowledge for the first time) by using the technique suggested by van Leeuwen[6] of computing the free energy of the site spins under the constraint that the cell spins are either all of one sign or predominantly of one sign such that via the majority rule the site spins as well will always be predominantly of the same sign. Thus, we prevent the possibility of a magnetization in zero external magnetic field arising spontaneously (since it is always present) for both cells and sites. This obviates the possibility that the critical state for the sites will differ from that of the cells in the sense of having different critical point values for their respective nearest-neighbor interaction parameters. We treat the renormalization transformation as one from interaction parameters K_α to renormalized parameters K'_α where α labels interaction types for even numbers of spins. From the behavior of this transformation, linearized about its nontrivial fixed point, we determine the Ising-model critical point and thermal exponent (and follow this with a determination of its magnetic exponent) in the usual way.[1]

It is generally agreed[1,7] that cluster calculations are superior to finite-lattice and cumulant expansion methods for the calculation of K'_α in terms of K_α. In this paper we apply the cluster variation method (CVM)[8–10] to approximately evaluate the free energy

for the site spins on a triangular two-dimensional lattice. The cells between which renormalized interactions occur are triangles of three-nearest-neighbor spins such that $s=\sqrt{3}$ (see Fig. 1). From our results it is of particular interest to note that in order to obtain a fixed point it is necessary to work with clusters in the CVM at least as large as the cell chosen, i.e., a triangle in the present case, and it is necessary to correct the usual CVM entropy expression for the site spins to reflect the constraint that the cell distribution is fixed.

Denoting schematically a certain constrained spin distribution in the cell system as C_1 we calculate the probability $P(C_1)$ that the configuration C_1 appears. This is proportional to $\exp[H'(C_1,K_\alpha)]$. The same $P(C_1)$ is calculated in the site system as a partial sum of the partition function

$$P(C_1) \propto \sum_{\sigma \in C_1} \exp H(\sigma,K_\alpha) \ , \tag{1.2}$$

where the summation goes over the site spin configurations consistent with the cell spin distribution C_1. Thus we can write

$$\exp[G(K_\alpha)+H'(C_1,K'_\alpha)] = \sum_{\sigma \in C_1} \exp[H(\sigma,K_\alpha)] \ . \tag{1.3}$$

For any other constrained cell spin distribution C_2 we have another equation similar to (1.3) with C_1 replaced by C_2 such that in forming a ratio of the two equations $G(K_\alpha)$ drops out. Taking the logarithm of Eq. (1.3)

$$G(K_\alpha)+H'(C_1,K'_\alpha)=F(K_\alpha)=\frac{S}{k_B}-\frac{E}{k_BT} \tag{1.4}$$

we focus on the free energy (times $-\beta$), F of the site spin system. We numerically evaluate F as function of K_α using the CVM for as many constrained *cell* spin distributions (such as all +, fraction t + with further constraint of no + + first nearest-neighbor cell pairs) as is necessary to obtain numerical values for all the K'_α by taking differences of the respective Eq. (1.4) for pairs of F values. For each cell spin distribution the H' is explicitly written in terms of the K'_α and the numbers of the various interacting cell groups (first nearest-neighbor pairs, second nearest-neighbor pairs, etc) which numbers are either immediately given in terms of t or are obtainable from some of the numerical results for the equilibrium concentrations of various clusters of sites generated in evaluating F. We also eventually consider parameters h'_β and h_β where β labels interaction types for odd numbers of spins and which are nonzero only in external magnetic fields.

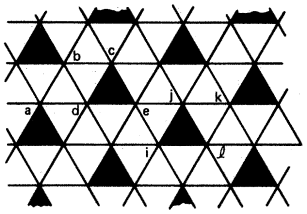


FIG. 1. Triangular lattice with cells shown shaded. Triangles type 1 are cells such as *i,j,l.* Triangles type 2 are like *b,c,d.* Triangles type 3 are like *a,b,d.* Rhombi type 1 are *i,j,k,l.* Rhombi type 2 are like *a,b,c,d.*

II. FIRST NEAREST-NEIGHBOR INTERACTIONS ONLY

We treat a triangular lattice in two dimensions with $3N$ sites (such that there will be $N'=N$ cells) for which the coordination number, c, of first, second, and third nearest neighbors (NN) is uniformly 6. Table I lists the total numbers of the various generic types of clusters for the CVM used in this paper. The first NN interaction energy is $-J_1$ if the spins are parallel and $+J_1$ if they are oppositely aligned and similarly for second NN pair energies of $\mp J_2$. The $K_i=(1/k_BT)J_1$. Since we are grouping the $3N$ sites into N cells which can assume four configurations with equal probabilities at infinite temperature, every

TABLE I. Generic cluster types.

Generic cluster		Generic variable	Total number
Site		x	$3N$
Intracell pair		y_1	$3N$
Intercell pair		y_2	$6N$
Triangle type 1		w_1	N
Triangle type 2		w_2	$3N$
Triangle type 3		w_3	$2N$
Rhombus type 1		u_1	$3N$
Rhombus type 2		u_2	$6N$

(F/N) for all $K_i=0$ should be ln4. This insures that our equations will have the trivial but physically important fixed point for all i:

$$K_i' = K_i = K_i^* = 0 \quad . \tag{2.1}$$

To effect this we must consider clusters at least as large as NN triangles and, if we limit the calculations only to first NN interactions, all larger clusters than these may be omitted. The entropy S/k_B of the N cells (of $3N$ sites) is written as the logarithm of the number of configurations Ω which is given[11] in the CVM by

$$\Omega = \frac{\{\quad\}^6 \{\quad\}^3}{\{\quad\}\{\quad\}^2\{\quad\}^3\{\quad\}^3} \quad . \tag{2.2}$$

For the case of N sites for which cells are not considered and all triangular NN clusters are alike, Eq. (2.2) reduces to Eq. (G.1) of Ref. 8:

$$\Omega = \frac{\{\quad\}^3}{\{\quad\}^2\{\cdot\}} \quad . \tag{2.3}$$

With reference to Tables II–IV, in which all the probability variables and their weights (q_j) are set out, the Stirling approximation applied to Eq. (2.2)

TABLE II. Site clusters. Circled signs refer to cell spins, uncircled signs refer to site spins.

Cluster	Variable
$\oplus$ $+$	x_1
$\oplus$ $-$	x_2
$\ominus$ $+$	x_3
$\ominus$ $-$	x_4

gives the entropy for the site spins as

$$S^{(1)} = Nk_B\Big[3\sum_j q_j \mathfrak{L}(y_{1j}) + 6\sum_j q_j \mathfrak{L}(y_{2j}) - 3\sum_j \mathfrak{L}(x_j) - \sum_j q_j \mathfrak{L}(w_{1j}) - 3\sum_j q_j \mathfrak{L}(w_{2j}) - 2\sum_j q_j \mathfrak{L}(w_{3j})\Big] \tag{2.4}$$

TABLE III. Intracell and intercell pair clusters.

Cluster	Variable	Weight	Cluster	Variable	Weight
$+\ \oplus\ +$	y_{11}	1	$+\ +\ \ominus$ / $\oplus$	y_{24}	2
$+\ \oplus\ -$	y_{12}	2	$+\ -\ \ominus$ / $\oplus$	y_{25}	2
$+\ \ominus\ -$	y_{13}	2	$-\ +\ \ominus$ / $\oplus$	y_{26}	2
$-\ \ominus\ -$	y_{14}	1	$-\ -\ \ominus$ / $\oplus$	y_{27}	2
$+\ +\ \oplus$ / $\oplus$	y_{21}	1	$+\ +\ \ominus$ / $\ominus$	y_{28}	1
$+\ -\ \oplus$ / $\oplus$	y_{22}	2	$+\ -\ \ominus$ / $\ominus$	y_{29}	2
$-\ -\ \oplus$ / $\oplus$	y_{23}	1	$-\ -\ \ominus$ / $\ominus$	y_{210}	1

TABLE IV. Triangle clusters.

Cluster	Variable	Weight	Pair energy	Magnetic energy
		Type 1		
	w_{11}	1	$\frac{3}{2}K_1$	$-\frac{1}{2}h_1$
	w_{12}	3	$\frac{1}{2}K_1$	$-\frac{1}{6}h_1$
	w_{13}	3	$\frac{1}{2}K_1$	$+\frac{1}{6}h_1$
	w_{14}	1	$-\frac{3}{2}K_1$	$+\frac{1}{2}h_1$
		Type 2		
	w_{21}	1	$-\frac{3}{2}K_1$	$-\frac{1}{2}h_1$
	w_{22}	1	$\frac{1}{2}K_1$	$-\frac{1}{6}h_1$
	w_{23}	2	$\frac{1}{2}K_1$	$-\frac{1}{6}h_1$
	w_{24}	2	$\frac{1}{2}K_1$	$\frac{1}{6}h_1$
	w_{25}	1	$-\frac{3}{2}K_1$	$-\frac{1}{2}h_1$
	w_{26}	1	$\frac{1}{2}K_1$	$-\frac{1}{6}h_1$
	w_{27}	2	$\frac{1}{2}K_1$	$-\frac{1}{6}h_1$
	w_{28}	2	$\frac{1}{2}K_1$	$\frac{1}{6}h_1$
	w_{29}	2	$\frac{1}{2}K_1$	$-\frac{1}{6}h_1$
	w_{210}	2	$\frac{1}{2}K_1$	$\frac{1}{6}h_1$
		Type 2		
	w_{211}	1	$\frac{1}{2}K_1$	$\frac{1}{6}h_1$
	w_{212}	1	$-\frac{3}{2}K_1$	$\frac{1}{2}h_1$
	w_{213}	2	$\frac{1}{2}K_1$	$-\frac{1}{6}h_1$
	w_{214}	2	$\frac{1}{2}K_1$	$\frac{1}{6}h_1$
	w_{215}	1	$\frac{1}{2}K_1$	$\frac{1}{6}h_1$
	w_{216}	1	$-\frac{3}{2}K_1$	$\frac{1}{2}h_1$
		Type 3		
	w_{31}	1	$-\frac{3}{2}K_1$	$-\frac{1}{2}h_1$
	w_{32}	3	$\frac{1}{2}K_1$	$-\frac{1}{6}h_1$
	w_{33}	3	$\frac{1}{2}K_1$	$\frac{1}{6}h_1$
	w_{34}	1	$-\frac{3}{2}K_1$	$\frac{1}{2}h_1$
	w_{35}	3	$-\frac{3}{2}K_1$	$-\frac{1}{2}h_1$
	w_{36}	6	$\frac{1}{2}K_1$	$-\frac{1}{6}h_1$
	w_{37}	3	$\frac{1}{2}K_1$	$-\frac{1}{6}h_1$

TABLE IV (*Continued*).

Cluster	Variable	Weight	Pair energy	Magnetic energy
		Type 3		
	w_{38}	3	$\frac{1}{2}K_1$	$\frac{1}{6}h_1$
	w_{39}	6	$\frac{1}{2}K_1$	$\frac{1}{6}h_1$
	w_{310}	3	$-\frac{3}{2}K_1$	$\frac{1}{2}h_1$
	w_{311}	3	$-\frac{3}{2}K_1$	$-\frac{1}{2}h_1$
	w_{312}	6	$\frac{1}{2}K_1$	$-\frac{1}{6}h_1$
	w_{313}	3	$\frac{1}{2}K_1$	$-\frac{1}{6}h_1$
	w_{314}	3	$\frac{1}{2}K_1$	$\frac{1}{6}h_1$
	w_{315}	6	$\frac{1}{2}K_1$	$\frac{1}{6}h_1$
	w_{316}	3	$-\frac{3}{2}K_1$	$\frac{1}{2}h_1$
	w_{317}	1	$-\frac{3}{2}K_1$	$-\frac{1}{2}h_1$
	w_{318}	3	$\frac{1}{2}K_1$	$-\frac{1}{6}h_1$
	w_{319}	3	$\frac{1}{2}K_1$	$\frac{1}{6}h_1$
	w_{320}	1	$-\frac{3}{2}K_1$	$\frac{1}{2}h_1$

in which

$$\mathfrak{L}(x) \equiv x \ln x - x \tag{2.5}$$

and where the sum on j is over those configurations of a cluster set allowed by the various constraints on the cells. Since each set of cluster probability variables $(x,y_1,y_2, \ldots ,u_2)$ times their respective weights are separately normalized to unity the number for example of triangular clusters with probability variable w_{39} is (with reference to Table I) explicitly $(2N)(6)(w_{39})$.

A. All cells of positive spin

Constraints on the cell spins are important for reasons given in the introduction and they are also helpful in limiting the number of variables in the CVM. With all cells positive there are only ten triangular cluster variables and the energy may be written by inspection as

$$E = -3NJ_1[(y_{11}-2y_{12})+2(y_{21}+y_{23}-2y_{22})] \ . \tag{2.6}$$

In the natural iteration (NI) technique[12,13] for maximizing the F of Eq. (1.4) one chooses all the largest cluster variables as independent and introduces as many Lagrangian parameters as are needed to satisfy all the constraints. As shown in Appendix A it is straightforward to obtain $F_{++}(K_1)/N$ and to show that it is ln4 for $K_1=0$.

B. Fraction t of cells of positive spin with no first NN +cell, +cell pairs

The triangular cluster variables, now 26 in number, are w_{11}, w_{12}, w_{13}, w_{14}; w_{25}, . . . w_{216}; and w_{311}, . . . w_{320}. Since t is the fraction of cells with cell spin (by majority rule of the site spins) positive and with the further constraint of no first NN (+ cell, + cell) pairs, the geometry of the triangular lattice dictates that t can range between 0 and $\frac{1}{3}$. Furthermore, the fraction of first NN (cell, cell) pairs that are (+,−), i.e., f_{1+-}, must be

$$f_{1+-}=2t \ . \tag{2.7}$$

The entropy $S^{(1)}$ of Eq. (2.4) is the entropy when the positions of the cells are not fixed, i.e., it contains a contribution $S^{(2)}$ for the distribution of the N cells over the lattice which must be subtracted from $S^{(1)}$ when the cell distribution is frozen as it must be for our renormalization-group calculation. Thus, the entropy S for the site spins is

$$\frac{S}{Nk_B} = \frac{S^{(1)}}{Nk_B} - \frac{S^{(2)}}{Nk_B} \ . \tag{2.8}$$

The cell-distribution entropy is given by the analog of Eq. (2.3) for *cell* clusters in terms of the probability variables given in Table V

$$\frac{S^{(2)}}{Nk_B}=\ln\Omega(\text{cells})$$
$$=3[2\mathfrak{L}(y_{c2})+\mathfrak{L}(y_{c3})]-2[3\mathfrak{L}(w_{c3})+\mathfrak{L}(w_{c4})]$$
$$-[\mathfrak{L}(x_{c1})+\mathfrak{L}(x_{c2})]\ . \tag{2.9}$$

Since from Table V $2y_{c2}$ has the same meaning as f_{1+-} we have

$$y_{c2}=t\ , \tag{2.10a}$$

and by normalization

$$y_{c3}=1-2t\ . \tag{2.10b}$$

In addition

$$x_{c1}=x_1+x_2=w_{11}+3w_{12}=t\ , \tag{2.10c}$$
$$x_{c2}=x_3+x_4=w_{14}+3w_{13}=1-t\ , \tag{2.10d}$$

and from the obvious consistency relations

$$3Ny_{c3}=2N[3w_{c3}(1)+w_{c4}(3)](\tfrac{1}{2})\ ,$$
$$3N(2y_{c2})=2N[3w_{c3}(2)](\tfrac{1}{2})\ ,$$

we have

$$w_{c3}=t\ , \tag{2.10e}$$
$$w_{c4}=1-3t\ , \tag{2.10f}$$

such that

$$S^{(2)}/Nk_B=-t\ln t+3(1-2t)\ln(1-2t)$$
$$-2(1-3t)\ln(1-3t)\ -(1-t)\ln(1-t)\ . \tag{2.11}$$

At any fixed t, this contribution (see Fig. 2) will not affect the equation for maximizing F of Eq. (1.4) (nor the iterative method of calculation discussed in Appendix B). However, the correction is necessary for obtaining the correct numerical value of $F(t,K_1)$ and, in particular, for obtaining at any allowed t

$$\frac{F(t,0)}{N}=\ln 4\ .$$

$S^{(2)}/Nk_B$ is zero for $t=0$ and so does not enter the calculation for the all negative cell case (which is equivalent to all the positive cell case of Appendix A in zero external magnetic field). We note that for $t>0.296\,08\ldots$, $S^{(2)}/Nk_B$ is negative and this is so independent of temperature. This must be connected with a transition to triangle ordering with + cells predominantly on only one of the three sublattices of the triangular lattice for $t>0.296\,08\ldots$. Baxter[14] has recently published an exact solution of this case at zero temperature for which this critical

TABLE V. Cell clusters.

Cell cluster	Variable	Weight	Total number of cell clusters
⊕	x_{c1}	1	N
⊖	x_{c2}	1	
⊕ ⊖	y_{c2}	2	$3N$
⊖ ⊖	y_{c3}	1	
⊕ / ⊖ ⊖	w_{c3}	3	$2N$
⊖ / ⊖ ⊖	w_{c4}	1	

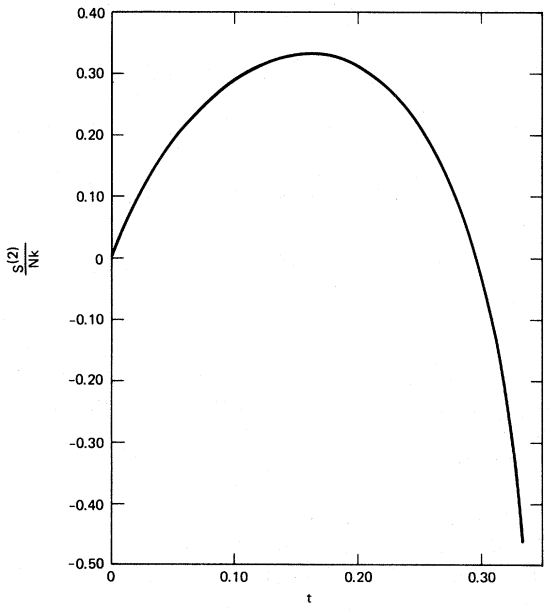


FIG. 2. Cell distribution entropy as function of t, the fraction of the N cells with cell spin positive by virtue of the majority rule.

$t=\frac{1}{10}(5-\sqrt{5})=0.27639$. [This is so because no physical model can have a negative entropy and means that the CVM parameters of Table V could no longer serve to describe the constrained cell-distribution situation if treated as an independent problem. However subtracting $S^{(2)}$ in Eq. (2.8) continues to correctly cancel contributions included in $S^{(1)}$ when Eq. (2.4) is used even when $t>0.29608$.]

C. Fixed point and thermal exponent

The following additional glossary is useful for the general situation including magnetic interaction terms: H'_{ex}, effective external magnetic field in cells; m' effective magnetic moment per cell; p', effective cell spin three-body interaction term for triangles of first NN cell spins taken with minus (plus) sign in the energy expression if triple product of the cell spins is positive (minus); f_{i+-}, fraction of ith NN (cell, cell) pairs that are $(+,-)$; N'_s, number of cells of sign s where s is $+$ or $-$; $N'_{iss'}$, number of ith NN (cell, cell) pairs of signs s,s'; $h'_1=m'H'_{ex}/k_BT$; $h'_2=p'H'_{ex}/k_BT$; H'_+ effective Hamiltonian for the all $+$ cell case; H'_t effective Hamiltonian for fraction t of cells of $+$ spin and no first NN ($+$ cell, $+$ cell) pairs. Reference to Eqs. (2.10e) and (2.10f) shows

$$H'_t=\frac{-1}{k_BT}\{-J'_1N'_{1--}+J'_1N'_{1+-}-m'H'_{ex}(N'_+-N'_-)$$
$$-J'_2(N'_{2++}+N'_{2--})+J'_2N'_{2+-}$$
$$-p'H'_{ex}(2N)[3t-(1-3t)]\} \tag{2.12}$$

which from Eq. (2.7) and the glossary becomes

$$H'_t=\frac{Nc}{2}(K'_1+K'_2)-N(h'_1+2h'_2)-2NcK'_1t$$
$$-NcK'_2f_{2+-}+2Nh'_1t+12Nh'_2t\ . \tag{2.13}$$

Similarly for all the $+$ cell case

$$H'_+=\frac{Nc}{2}(K'_1+K'_2)+N(h'_1+2h'_2) \tag{2.14}$$

which differs, in an external magnetic field, from $H'_{t=0}$ since the latter corresponds to the case with all spins down (minus).

Taking differences of Eq. (1.4) for any two situations solved for, allows the cancellation of the $G(K_\alpha)$ function and, for only first NN interactions in the absence of external magnetic fields, it gives the one necessary equation for K'_1 in terms of K_1. Using the all plus cell case and a fraction t case this equation is, from Eqs. (2.13) and (2.14),

$$12K'_1t=\frac{F_{++}(K_1)}{N}-\frac{F(t,K_1)}{N} \tag{2.15}$$

or using two different t cases (t_1,t_2) this equation is

$$12K'_1(t_2-t_1)=\frac{F(t_1,K_1)}{N}-\frac{F(t_2,K_1)}{N}\ . \tag{2.16}$$

Using the numerical methods described in Appendices A and B it is a straightforward calculation to obtain the fixed point of our transformation

$$K'_1=K_1=K_1^* \tag{2.17}$$

which in a one even interaction parameter case is identical to K_c, the Ising model critical point of the lattice. The thermal exponent y_T is obtained from

$$\left(\frac{dK'_1}{dK_1}\right)_{K_1^*}=(\sqrt{3})^{y_T}\ . \tag{2.18}$$

Calculations were carried out for three cases: all plus cells, $t=\frac{1}{3}$, and $t=0.16$ which permitted the calculation of three sets of K_c and y_T values. Results are listed in Table VI in which the all plus cell case is denoted by $t=1$. They are comparable in accuracy to a four cell cluster calculation of van Leeuwen and Niemeijer[15] which involved first and second NN pair interaction parameters and one four site (rhombus) interaction. We believed the approximate nature of our calculation was the reason for these fixed-point results to vary as the pairs of t values varied. These last were chosen simply for convenience to span the range $0\leq t\leq\frac{1}{3}$. However a comment has redirected our attention to the question of whether a unique approximate fixed point is obtainable. We conjecture that this is so for by expanding the second term on the right of Eq. (2.16) about $t_2=t_1$ we obtain

$$K'_1=-\frac{1}{12}\frac{\partial}{\partial t}\left(\frac{F(t,K_1)}{N}\right)$$

and for $K_1=K_1^*$ the derivative may be independent of t as is the case for the trivial fixed point at infinite temperature. *(Noted Added in Proof.* The derivative is not independent of t at $K_1=K_1^*$.)

TABLE VI. Results for the Ising model on the triangular lattice using first NN interactions only and single-site spin effects in an external magnetic field.

Case	K_c	y_T	y_h
$t=1$; $t=0.16$	0.2372	0.8908	1.732
$t=1$; $t=\frac{1}{3}$	0.2472	0.8478	1.758
$t=0.16$; $t=\frac{1}{3}$	0.2582	0.8094	1.800
Exact	0.27465	1.0000	1.875

D. Magnetic exponent

Considering only the single-site spin-energy terms in an external magnetic field H_{ex} the added term in the energy is

$$-mH_{ex}(3N)(x_1+x_3-x_2-x_4)$$

which gives as added term in $F(t,K_1)/N$,

$$3h_1(x_1+x_3-x_2-x_4) \ .$$

On expressing the x's as explained in Appendix A in the most symmetrical way in terms of all the independent w's and taking derivatives with respect to each w the only change in the calculation for magnetic field is to introduce obvious factors into every $\hat{w}$ expression [of, for example, Eq. (A7)]. These factors are, respectively, the exponential of minus the magnetic energy term for each w variable listed in Table IV. For example, looking at the diagram for w_{22} one reads off a net magnetic energy contribution of $-mH_{ex}$ multiplies by $1/6k_BT$ (since every site is in six triangles) and takes the exponential with sign change to arrive at a factor $e^{1/6h_1}$ multiplying the previous $\hat{w}_{22}$ expression for the iterative calculation in zero magnetic field.

One computes at the fixed point $F_{++}(K_1^*,h_1)/N$ and $F(t,K_1^*,h_1)/N$ to obtain h_1' as function of h_1. Explicitly for example using the all + cell case and the $t=0.16$ fraction we have

$$1.68h_1' = \frac{F_{++}}{N}(K_1^*,h_1) - \frac{F(0.16;K_1^*,h_1)}{N} - 1.92K_1^* \ . \tag{2.19}$$

Choosing a set of h_1 values in the vicinity of $h_1=0$ (where $h_1'=0$ as well) one computes the magnetic exponent y_h of our renormalization-group transformation from

$$\left(\frac{dh_1'}{dh_1}\right)_{h_1=h_1'=0} = (\sqrt{3})^{y_h} \ . \tag{2.20}$$

The results are given in Table VI. As observed previously[15] y_h is quite sensitive to the value of K_c becoming more accurate as K_c approaches its exact value. This behavior is not shown by y_T.

III. FIRST AND SECOND NEAREST-NEIGHBOR INTERACTIONS

To include second NN interactons one must go to rhombi of site spins (as illustrated in Fig. 1) for which the CVM gives the corresponding $S^{(1)}/Nk_B$ of Eq. (2.8) as

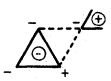
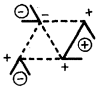
$$S^{(1)}/Nk_B = \ln\Omega \tag{3.1}$$

in which

$$\Omega = \frac{\left\{\triangle\right\}^2 \left\{\triangledown\right\}^6 \left\{\triangle\!\!\triangledown\right\}^4}{\left\{\triangle\!\!\triangledown\right\}^3 \left\{\triangle\!\!\triangledown\right\}^6 \left\{\triangle\right\}^3} \tag{3.2}$$

and then when the cells (which remain triangles) are frozen the entropy of the site spins is obtained as before from Eqs. (2.8) and (2.11) using now Eqs. (3.1) and (3.2). There are many rhombus cluster variables to be treated independently. In the all + cell case we have 6 of type u_1, and 12 of type u_2. In the case of fraction t of + cells with the added constraint of Sec. II B there are 18 more of type u_1 and 48 more of type u_2. The detailed listing of these variables and their interconnections are given in a supplementary publication.[16] However in Table VII we list two examples of rhombi that enter the calculation labeled u_{118} and u_{221}, respectively. In arriving at the pair energy for a cluster symmetry constraints discussed in SP require first NN pairs on the edge of the rhombus to be weighted by a factor $\frac{1}{6}$ and the first NN pair on the diagonal of the rhombus to be weighted by a factor $\frac{1}{3}$. Each rhombus has one second NN pair (weight unity). The magnetic energy in an external field has a weight factor $(\frac{1}{12})$ for single sites and a weight factor $(\frac{1}{3})$ for triples of which there are two in each rhombus cluster. Since the Ω of Eq. (3.2) involves beside rhombi only the points (x variables) and triangles (w variables) the two $\hat{u}$ of Table VII comparable to the $\hat{w}$ of Eq. (B7) are with reference to the explicit

TABLE VII. Two examples of rhombi used when second nearest-neighbor pair interactions are included.

Cluster	Variable	Weight	Pair energy	Magnetic energy
	u_{118}	2	$\frac{1}{3}K_1-K_2$	$\frac{1}{6}h_1-\frac{2}{3}h_2$
	u_{221}	1	$\frac{1}{3}K_1-K_2$	$-\frac{1}{6}h_1+\frac{2}{3}h_2$

enumeration of Table IV transparently,

$$\hat{u}_{118}=\frac{(w_{13}w_{210})^{2/3}e^{-K_1/3+K_2}}{(x_2x_3x_4^2)^{1/12}}\ ,$$
$$\hat{u}_{221}=\frac{(w_{312}w_{26})^{2/3}e^{-K_1/3+K_2}}{(x_1^2x_3x_4)^{1/12}}\ , \tag{3.3}$$

and with additional factors $\exp(-1/6h_1+2/3h_2)$ and $\exp(+1/6h_1-2/3h_2)$, respectively, for calculations in an external magnetic field. The more complex part of the calculation is obtaining all the necessary linear constraints among the independent u variables and the proper insertion of all the Lagrangian parameters. This has been done[16] and the numerical equality of the appropriate F/N of Eq. (1.4) to ln4 checked at various values of t when $K_1=K_2=0$.

A minimum of three cases must be calculated to obtain two independent differences of Eq. (1.4) to obtain K_1' and K_2' in terms of K_1 and K_2. These were chosen as $t=1$ (all + cell case), $t=0.16$ and 0.30. We did not carry through calculations for $t=\frac{1}{3}$ since in this limit the necessary Lagrangian parameter μ [comparable to that of Eq. (B8)] must be taken so large that convergence is hard to achieve and exponent overflow occurred in several runs. The working equations from Eq. (2.14) less Eq. (2.13) become

$$1.92K_1'+aK_2'=\frac{F_{++}(K_1,K_2)}{N}-\frac{F(0.16,K_1,K_2)}{N}\ ,$$
$$3.60K_1'+bK_2'=\frac{F_{++}(K_1,K_2)}{N}-\frac{F(0.30,K_1,K_2)}{N}\ , \tag{3.4}$$

in which

$$a=6f_{2+-}\ \text{for}\ t=0.16\ ,$$
$$b=6f_{2+-}\ \text{for}\ t=0.30\ . \tag{3.5}$$

The parameters a,b are determined in good approximation from the results for the u values obtained at the end of each calculation of $F(t,K_1,K_2)/N$ as shown in SP.

To solve Eq. (3.4) start with $K_1=K_{10}$ (an initial guess for K_c) and $K_2=0$ and iterate. If the K_1's and K_2's grow larger and larger $K_{10}>K_c$. If they fall away toward zero $K_{10}<K_c$. In this process good approximations will eventually be generated for the fixed-point values K_1^* and K_2^* as those K_1,K_2 values which change very slightly in successive iterations. In this way we find for the Ising-model critical point,

$$K_c=0.2303\ , \tag{3.6}$$

and the approximate K_1^*,K_2^* values are easily refined by standard methods for dealing with a pair of nonlinear equations to give for the fixed point

$$K_1^*=0.218\,365\,6;\quad K_2^*=0.008\,941\,9\ . \tag{3.7}$$

The thermal matrix (here 2×2) is obtained from appropriate derivatives evaluated at the above fixed point and has one eigenvalue greater than unity from which we find for the thermal exponent

$$y_T=0.9229\ . \tag{3.8}$$

The equations corresponding to Eq. (3.4) in a magnetic field are written down and the 2×2 magnetic matrix obtained from which we find for the magnetic exponent

$$y_h=1.704\ . \tag{3.9}$$

IV. DISCUSSION AND OUTLOOK

By presenting a method of real-space renormalization-group calculations with constrained fraction of cell spins of one sign we believe that we have eliminated the problems and uncertainties associated with competing ground states at low temperatures (discussed by van Leeuwen and Niemeijer[17] and by Griffiths[18]), which may cause the original spin system free energy to have a singularity different from that of the cell spin free energy. Some examples from the literature of these difficulties are: a five cell cluster treatment of the Ising model gives no (nontrivial) fixed point if very small four spin interactions are omitted[15]; a simplest cumulant expansion for spin-glasses gives a fixed point but if a simple cluster calculation is made no fixed point is obtained[19]; a second-order cumulant expansion for the two-dimensional spin-$\frac{1}{2}$ Heisenberg model gives a fixed point while the first-order expansion does not.[20] Our results using a first NN interaction parameter are comparable in accuracy to calculations using three types of even spin number parameters. However our results in Sec. III in which second NN interactions and a triple spin magnetic term are added are disappointing in giving a poor value for K_c (and thus a poorer value for y_h) than any of those listed in Table VI although the y_T value is improved. We believe including the second NN terms without simultaneously including the third NN terms which involve an equal number of sites only 1.15 times further distant than the second NN sites of a given spin has skewed our results. To include third NN interactions one must treat hexagons of seven site spins each. The numerical method of calculating the free energy used in this paper would probably not be feasible for this due to the great increase in the number of Lagrangian parameters if all the largest cluster variables are kept independent. A higher degree of automation of the calculation will be necessary to eliminate most of these variables in terms of a truly independent set and then to solve the resulting nonlinear equations by Newton's method. Recently several papers treating this approach for CVM calculations have appeared[21–23] and we plan to extend our renormalization-group calculations to include third NN interactions and to three-dimensional lattices using the techniques therein presented.

ACKNOWLEDGMENT

One of us (C.E.H.) wishes to thank Professor J. M. J. van Leeuwen for suggesting this research.

APPENDIX A

We treat the case of only positive cells permitted and only first NN interactions between site spins. The possible triangular cluster variables are $w_{11}, w_{12}, w_{21}, w_{22}, w_{23}, w_{24}, w_{31}, w_{32}, w_{33}, w_{34}$. We take all of these as independent variables (subject to constraints). The other cluster variables appearing in the entropy and energy expressions must be expressed in terms of them but in such a way as shown in what follows to preserve all the symmetries of all the cluster figures.

We begin by counting up subcluster figures in alternative ways, e.g.,

$$3Nx_1 = N[w_{11}(3) + 3w_{12}(2)] \ ,$$

$$6N(2y_{22}) = 2N[3w_{32}(2) + 3w_{33}(2)] \ .$$

By including also, relations of the x's to the y's we obtain finally

$$\begin{aligned} x_1 &= w_{11} + 2w_{12} \ , \\ x_2 &= w_{12} \ , \\ x_1 &= w_{21} + w_{22} + w_{23} + w_{24} = w_{21} + 2w_{23} \ , \\ x_2 &= w_{23} + w_{24} = w_{22} + 2w_{24} \\ x_1 &= w_{31} + 2w_{32} + w_{33} \ , \\ x_2 &= w_{32} + 2w_{33} + w_{34} \ , \end{aligned} \tag{A1}$$

and also

$$\begin{aligned} y_{11} &= w_{11} + w_{12} = w_{21} + w_{22} \ , \\ y_{12} &= w_{12} = w_{23} + w_{24} \ , \\ y_{21} &= w_{21} + w_{23} = w_{31} + w_{32} \ , \\ y_{22} &= w_{23} = w_{32} + w_{33} = w_{22} + w_{24} \ , \\ y_{23} &= w_{24} = w_{33} + w_{34} \ . \end{aligned} \tag{A2}$$

These relations are used to rewrite the energy Eq. (2.6) in a most symmetrical way as

$$E = -3NJ_1(\tfrac{1}{2}w_{11} - \tfrac{1}{2}w_{12} + \tfrac{3}{2}w_{21} - \tfrac{1}{2}w_{22} - w_{23} - w_{24} + w_{31} - w_{32} - w_{33} + w_{34}) \ . \tag{A3}$$

This form is obtained by writing y_{11} and y_{12} (with equal weights) once in terms of w_1's and once in terms of w_2's from Eq. (A2). Similarly y_{21} and y_{23} are written once in terms of w_2's and once in terms of w_3's. However y_{22} being expressible from (A2) in two ways in terms of w_2's is written in Eq. (2.6) to obtain (A3) as

$$-4y_{22} = -w_{23} - w_{22} - w_{24} - 2w_{32} - 2w_{33} \ .$$

Similarly in writing the entropy $S^{(1)}$ from Eq. (2.4) we use

$$3\sum_j q_j \mathcal{L}(y_{1j}) \equiv \tfrac{3}{2}[\mathcal{L}(y_{11} = w_{11} + w_{12}) + 2\mathcal{L}(y_{12} = w_{12}) + \mathcal{L}(y_{11} = w_{21} + w_{22}) + 2\mathcal{L}(y_{12} = w_{23} + w_{24})] \tag{A4}$$

and

$$\begin{aligned} 6\sum_j q_j \mathcal{L}(y_{2j}) \equiv 3[&\mathcal{L}(y_{21} = w_{21} + w_{23}) + \mathcal{L}(y_{22} = w_{22} + w_{24}) + \mathcal{L}(y_{22} = w_{23}) + \mathcal{L}(y_{23} = w_{24}) \\ &+ \mathcal{L}(y_{21} = w_{31} + w_{32}) + 2\mathcal{L}(y_{22} = w_{32} + w_{33}) + \mathcal{L}(y_{23} = w_{33} + w_{34})] \ . \end{aligned} \tag{A5}$$

Less obviously but with a little trial and error and for reasons given below we also use in Eq. (2.4)

$$\begin{aligned} -3\sum_j \mathcal{L}(x_j) = &-\tfrac{1}{2}[\mathcal{L}(x_1 = w_{11} + 2w_{12}) + \mathcal{L}(x_2 = w_{12})] - [\mathcal{L}(x_1 = w_{21} + w_{22} + w_{23} + w_{24}) + \mathcal{L}(x_2 = w_{23} + w_{24})] \\ &- \tfrac{1}{2}[\mathcal{L}(x_1 = w_{21} + 2w_{23}) + \mathcal{L}(x_2 = w_{22} + 2w_{24})] \\ &- [\mathcal{L}(x_1 = w_{31} + 2w_{32} + w_{33}) + \mathcal{L}(x_2 = w_{32} + 2w_{33} + w_{34})] \ . \end{aligned} \tag{A6}$$

To satisfy the constraints that exist among the w's from Eqs. (A1) and (A2) we add to $F_{++}(K_1)/N$ of Eq. (1.4) (the double sign subscript indicating that there are only ++NN cell-cell pairs) the terms

$$\begin{aligned} &6\alpha_1(w_{11} + w_{12} - w_{21} - w_{22}) + 6\alpha_2(w_{12} - w_{23} - w_{24}) + 6\beta_1(w_{21} + w_{23} - w_{31} - w_{32}) + 6\beta_2(w_{23} - w_{32} - w_{33}) \\ &\qquad + 6\beta_3(w_{24} - w_{33} - w_{34}) + 6\gamma(w_{22} + w_{24} - w_{23}) \ , \end{aligned}$$

and to account for normalization of the w's we add further

$$\lambda_1(1-w_{11}-3w_{12})+3\lambda_2(1-w_{21}-w_{22}-2w_{23}-2w_{24}) +2\lambda_3(1-w_{31}-3w_{32}-3w_{33}-w_{34})$$

in which the α's, β's, γ, and λ's are Lagrangian parameters. Setting the derivatives of this augmented $F_{++}(K_1)/N$ expression with respect to each of the w's equal to zero gives the following equations for iteration:

$$\begin{aligned}
w_{11}&=e^{-\lambda_1}\hat{w}_{11}e^{6\alpha_1}\ ,\\
\hat{w}_{11}&=(y_{11}^3)^{1/2}e^{3K_1/2}/(x_1^3)^{1/6}\ ,\\
w_{12}&=e^{-\lambda_1}\hat{w}_{12}e^{2\alpha_1+2\alpha_2}\ ,\\
\hat{w}_{12}&=(y_{11}y_{12}^2)^{1/2}e^{-K_1/2}/(x_1^2x_2)^{1/6}\ ,\\
w_{21}&=e^{-\lambda_2}\hat{w}_{21}e^{-2\alpha_1+2\beta_1}\ ,\\
\hat{w}_{21}&=(y_{11}y_{21}^2)^{1/2}e^{3K_1/2}/(x_1^3)^{1/6}\ ,\\
w_{22}&=e^{-\lambda_2}\hat{w}_{22}e^{-2\alpha_1+2\gamma}\ ,\\
\hat{w}_{22}&=(y_{11}y_{22}^2)^{1/2}e^{-K_1/2}/(x_1^2x_2)^{1/6}\ ,\\
w_{23}&=e^{-\lambda_2}\hat{w}_{23}\exp(-\alpha_2+\beta_1+\beta_2-\gamma)\ ,\\
\hat{w}_{23}&=(y_{12}y_{21}y_{22})^{1/2}e^{-K_1/2}/(x_1^2x_2)^{1/6}\ ,\\
w_{24}&=e^{-\lambda_2}\hat{w}_{24}\exp(-\alpha_2+\beta_3+\gamma)\ ,\\
\hat{w}_{24}&=(y_{12}y_{22}y_{23})^{1/2}e^{-K_1/2}/(x_1x_2^2)^{1/6}\ ,\\
w_{31}&=e^{-\lambda_3}\hat{w}_{31}e^{-3\beta_1}\ ,\\
\hat{w}_{31}&=(y_{21}^3)^{1/2}e^{3K_1/2}/(x_1^3)^{1/6}\ ,\\
w_{32}&=e^{-\lambda_3}\hat{w}_{32}e^{-\beta_1-\beta_2}\ ,\\
\hat{w}_{32}&=(y_{21}y_{22}^2)^{1/2}e^{-K_1/2}/(x_1^2x_2)^{1/6}\ ,\\
w_{33}&=e^{-\lambda_3}\hat{w}_{33}e^{-\beta_2-\beta_3}\ ,\\
\hat{w}_{33}&=(y_{22}^2y_{23})^{1/2}e^{-K_1/2}/(x_1x_2^2)^{1/6}\ ,\\
w_{34}&=e^{-\lambda_3}\hat{w}_{34}e^{-3\beta_3}\ ,\\
\hat{w}_{34}&=(y_{23}^3)^{1/2}e^{3K_1/2}/(x_2^3)^{1/6}\ .
\end{aligned}\tag{A7}$$

Now the symmetry relations in the $\hat{w}$'s are obvious [and were the reasons for writing Eq. (A6) with its particular weights]. For example, reference to Tables II–IV shows that in w_{23} bonds y_{12}, y_{21}, and y_{22} each shared by two triangles make up the triangle of two x_1 and one x_2 site, each site shared by six triangles. Further the three pair energies of w_{23} sum to J_1 and then times $(+1)/2k_BT$ gives the weighted pair energy in Table IV type-triangle clusters with division by 2 since this energy is bond by bond shared by two triangles and finally with a sign change in $\hat{w}_{23}$ since all probability variables are weighted by the exponent of minus the free-energy contribution.

Algebraically subtracting in succession from our augmented $F_{++}(K_1)/N$ expression the $w_i(\partial/\partial w_i)(F_{++}/N)$ terms (each of which will be numerically zero) shows that the only terms to survive are those independent of the w's

$$F_{++}(K_1)/N=\lambda_1+3\lambda_2+2\lambda_3\ .\tag{A8}$$

In order to start the major iteration for a given K_1 value it is sufficient to put $x_1=\frac{3}{4}$ and $x_2=\frac{1}{4}$ characteristic of the infinite-temperature limit and then assign the y's as random Bragg-Williams–type products

$$y_{11}=\tfrac{1}{2};\ y_{12}=\tfrac{1}{4}\ ;\ y_{21}=\tfrac{9}{16};\ y_{22}=\tfrac{3}{16};\ y_{23}=\tfrac{1}{16}\ .$$

We then proceed to the minor iteration for the Lagrangian parameters (all of which can be started from zero). We note first that since there is only one independent normalization when all the constraints on the w's are enforced if we keep all three λ's then two of the Lagrangian parameters (say α_2 and β_3) may be omitted. Then we determine α_1, for example, by defining

$$A_{L1}=(w_{11}+w_{12})e^{\lambda_1},\quad A_{R1}=(w_{21}+w_{22})e^{\lambda_2}\ ,$$

$$A_{L2}=(w_{12}e^{\lambda_1}),\quad A_{R2}=(w_{23}+w_{24})e^{\lambda_2}\ ,$$

from which the constraints require that the ratios (which are independent of the λ's) be equal

$$\frac{A_{L1}}{A_{L2}}=\frac{A_{R1}}{A_{R2}}$$

or

$$\frac{A_{L1}e^{-2\alpha_1}(e^{2\alpha_1})}{A_{L2}}=\frac{A_{R1}e^{2\alpha_1}(e^{-2\alpha_1})}{A_{R2}}\ ,$$

$$\alpha_1^{(1)}=\tfrac{1}{4}\ln\frac{(A_{R1})(A_{L2})}{(A_{L1})(A_{R2})}+\alpha_1^{(0)}$$

such that for purpose of convergence

$$\hat{\alpha}_1=\tfrac{1}{2}(\alpha_1^{(1)}+\alpha_1^{(0)})=\tfrac{1}{8}\ln\frac{(A_{R1})(A_{L2})}{(A_{L1})(A_{R2})}+\alpha_1^{(0)}\tag{A9}$$

in which $\hat{\alpha}_1$ serves as input for α_1 in the next minor iteration step. With the other parameters found in like manner the λ_i are obtained from the normalization conditions, e.g.,

$$\lambda_1=\ln(\hat{w}_{11}e^{6\alpha_1}+3\hat{w}_{12}e^{2\alpha_1})\ .\tag{A10}$$

The w_i's are obtained from (A7) and Eqs. (A1) and (A2) generate new x's and y's for the next step of the major iteration. When successive sets of w's differ by less than a predetermined amount the free energy is calculated from Eq. (A8). This equation

gives

$$F_{++}(0)/N = \ln 4$$

as it should.

APPENDIX B

We treat the case of fraction t of the cells of positive spin and no first NN + cell, + cell pairs for which there are 26 triangular variables. Without formulating the energy expression or $S^{(1)}$ explicitly one can immediately write down all the necessary $\hat{w}_i$ expressions analogous to those of Eq. (A7) in terms of the appropriate y's and x's by referring to Tables II–IV. Parameters γ are used for constraints between the w_2's which add terms to $F(t,K_1)/N$ as follows:

$$6\gamma_4(w_{25}+w_{27}-w_{29})+6\gamma_5(w_{26}+w_{28}-w_{29}-w_{211})+6\gamma_6(w_{27}-w_{210})+6\gamma_7(w_{28}-w_{210}-w_{212}) +6\gamma_9(w_{214}-w_{213}-w_{215}) \quad . \tag{B1}$$

Parameters β are used for constraints between the w_2's and w_3's as follows:

$$6\beta_4(w_{29}-w_{311}-w_{312})+6\beta_5(w_{26}+w_{28}-w_{312}-w_{314})+6\beta_6(w_{27}-w_{313}-w_{315})+6\beta_7(w_{28}-w_{315}-w_{316}) +6\beta_8(w_{213}-w_{311}-w_{313}-w_{317}-w_{318})+6\beta_9(w_{214}-w_{312}-w_{315}-w_{318}-w_{319}) +6\beta_{10}(w_{214}+w_{216}-w_{314}-w_{316}-w_{319}-w_{320}) \quad . \tag{B2}$$

Parameters α are used to add in terms for constraints between w_1's and w_2's:

$$6\alpha_1[w_{11}+w_{12}-w_{25}-w_{26}]+6\alpha_2[w_{12}-w_{27}-w_{28}]+6\alpha_3[w_{13}-w_{29}-w_{210}-w_{213}-w_{214}] +6\alpha_4[w_{13}+w_{14}-w_{211}-w_{212}-w_{215}-w_{216}] \quad . \tag{B3}$$

The three normalizations may be written as additive terms

$$\lambda_1(1-w_{11}-3w_{12}-3w_{13}-w_{14}) +3\lambda_2(1-w_{25}-w_{26}-2w_{27}-2w_{28}-2w_{29}-2w_{210}-w_{211}-w_{212}-2w_{213}-2w_{214}-w_{215}-w_{216}) +2\lambda_3(1-3w_{311}-6w_{312}-3w_{313}-3w_{314}-6w_{315}-3w_{316}-w_{317}-3w_{318}-3w_{319}-w_{320}) \quad . \tag{B4}$$

Then by noting for example what factor one must divide through by to obtain the factor $e^{-\lambda_2}$ in every w_2 expression by examining terms (B4) above and dividing through all other added constraint terms by this factor one finds for maximizing $F(t,K_1)/N$, for example,

$$w_{26} = e^{-\lambda_2}\hat{w}_{26}\exp(-2\alpha_1+2\gamma_5+2\beta_5) \quad ,$$

$$w_{27} = e^{-\lambda_2}\hat{w}_{27}\exp(-\alpha_2+\gamma_4+\gamma_6+\beta_6) \quad ,$$

etc.

Since the three normalizations in (B4) are not all independent, two of the parameters may be chosen as zero, namely,

$$\alpha_4=\beta_{10}=0 \quad .$$

Then there will be 14 Lagrangian parameters to deal with in every minor iteration.

The special constraint that fraction t of the cells is positive is handled by adding the one final term

$$6\mu(w_{11}+3w_{12}-t) \tag{B5}$$

such that when convergence is obtained the free-energy function is

$$\frac{F(t,K_1)}{N} = \lambda_1+3\lambda_2+2\lambda_3-6\mu t-\frac{S^{(2)}}{Nk_B} \tag{B6}$$

with the last term given by Eq. (2.11).

The determination of μ proceeded as follows. Since μ enters only in connection with w_{11} and w_{12} and we have

$$w_{11} = e^{-\lambda_1}\hat{w}_{11}e^{6\alpha_1} \quad ,$$
$$\hat{w}_{11} = \frac{(y_{11}^3)^{1/2}\exp(\frac{3}{2}K_1+6\mu)}{(x_{11}^3)^{1/6}} \quad , \tag{B7}$$
$$w_{12} = e^{-\lambda_1}\hat{w}_{12}e^{2\alpha_1+2\alpha_2} \quad ,$$
$$\hat{w}_{12} = \frac{(y_{11}y_{12}^2)^{1/2}e^{-K_1/2+6\mu}}{(x_1^2x_2)^{1/6}} \quad ,$$

after starting from a judicious guess for μ (aimed at achieving a particular value, t_0 for t) at the end of each major iteration step a new μ value is calculated from

$$\mu = \frac{1}{6}\ln\left(\frac{t_0}{F_1+F_2}\right) \tag{B8}$$

in which

$$F_1=\frac{(y_{11}^3)^{1/2}e^{3K_1/2}e^{-\lambda_1+6\alpha_1}}{(x_1^3)^{1/6}}$$

and

$$F_2=3\frac{(y_{11}y_{12}^2)^{1/2}e^{-K_1/2}\exp(-\lambda_1+2\alpha_1+2\alpha_2)}{(x_1^2x_2)^{1/6}} .$$

The overall calculation proceeds until for the nth major iteration,

$$\Delta=\sum_j|\ln w_{1j}^{(n)}-\ln w_{1j}^{(n-1)}|+\sum_j|\ln w_{2j}^{(n)}-\ln w_{2j}^{(n-1)}| + \sum_j|\ln w_{3j}^{(n)}-\ln w_{3j}^{(n-1)}|+|t-t_0| ,$$

is less than some small quantity. To obtain convergence it is necessary to start with Δ fairly large so as to fine tune the μ value needed to force $t=t_0$. For $K_1=0$ to force t to assume values in the range 0 to 0.32 (to seven decimal places) it is sufficient for μ to range from -2 to $+2$, respectively. However to achieve $t=\frac{1}{3}$ (to comparable precision) μ had to be chosen greater than 15.

We list finally the simplest set of relations used at the end of each major iteration to generate x's and y's for the next step:

$$\begin{aligned}
&x_1=w_{11}+2w_{12},\quad y_{11}=w_{11}+w_{12} ,\\
&x_2=w_{12},\quad y_{12}=w_{12} ,\\
&x_3=w_{13},\quad y_{13}=w_{13} ,\\
&x_4=w_{14}+2w_{13},\quad y_{14}=w_{13}+w_{14} ,\\
&y_{24}=w_{29},\quad y_{28}=w_{213} ,\\
&y_{25}=w_{26}+w_{28},\quad y_{29}=w_{214} ,\\
&y_{26}=w_{27},\quad y_{210}=w_{214}+w_{216} ,\\
&y_{27}=w_{28} .
\end{aligned} \tag{B9}$$

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