Exact Isotherm for the F Model in Direct and Staggered Electric Fields

R. J. BAXTER*
Mathematics Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
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Both staggered and direct external fields are applied to the F model. At a particular temperature, the properties can be evaluated exactly. As the fields are varied, the system undergoes two transitions between states of zero, partial, and complete direct polarization.

THE F model of an antiferroelectric[1] has been solved exactly both with and without applied electric fields.[2] However, only low-temperature expansions[3] are as yet available when a staggered field (one alternating in sign on successive bonds) is applied. The application of such a field is of interest since it resolves the degeneracy of the ordered state and completes the description of the phase transition, playing a role similar to that of the magnetic field in the Ising model (see discussion on p. 2 of Ref. 3).

We obtain here the exact solution for the F model in both staggered and direct fields at the particular temperature[4] T given by

$$e^{2\epsilon/kT}=2, \tag{1}$$

and find the following behavior:

(a) For a nonzero staggered field, there is no direct polarization unless the direct fields are sufficiently large. Thus, although T lies above the critical temperature T_c of the zero-field F model, application of a staggered field makes the direct polarization behave similarly to the $T<T_c$ case.

(b) In zero fields the staggered susceptibility is infinite and correlations at large distances r decay only as r^{-2}, implying that the lattice is in an ordered state, even though $T>T_c$.

(c) Complete direct polarization, and zero staggered polarization, can be achieved by applying sufficiently strong, but finite, direct fields in both the horizontal and vertical directions. However, if one of these fields is zero, complete polarization is achieved only when the other is infinite.

The model can be interpreted as placing an arrow on each bond of an M-by-N two-dimensional rectangular lattice so that there are two arrows pointing in to each vertex, and then associating an interaction energy ϵ with the first four of the allowed vertex configurations shown in Fig. 1. Direct fields h and v are then applied in the horizontal and vertical directions, so that each horizontal arrow contributes an energy $-h$ $(+h)$ if it points to the right (left), while each vertical arrow contributes $-v$ $(+v)$ if it points upward (downward).

To apply the staggered field s, divide the vertices into two sets (sublattices) A and B such that each vertex in set A is joined by bonds only to vertices in set B, and vice versa. Then each horizontal (vertical) arrow further contributes an energy $-s$ $(+s)$ if it points from an A vertex to a B vertex, and an energy $+s$ $(-s)$ if it points from B to A. Noting that each arrow is shared by two vertices, all these energies can be absorbed into the configurational energies shown in Fig. 1, giving

$$\begin{aligned} &\epsilon_1=\epsilon-h-v, && \epsilon_2=\epsilon+h+v,\\ &\epsilon_3=\epsilon-h+v, && \epsilon_4=\epsilon+h-v.\\ &A\ \textit{vertex:} && \epsilon_5=2s, \quad \epsilon_6=-2s.\\ &B\ \textit{vertex:} && \epsilon_5=-2s, \quad \epsilon_6=2s. \end{aligned} \tag{2}$$

The partition function can now be calculated by representing the arrow configurations by lines, and then showing that these lines correspond to dimers on a decorated lattice. First consider a basic configuration in which all A vertices are in state 6 of Fig. 1, and all B vertices are in state 5. Any arrow configuration can then be represented by drawing lines on bonds where the arrow points oppositely to the basic configuration, and the six vertex states are represented by either no lines on the surrounding bonds, two lines at 90°, or four lines.

Now replace the original lattice L with a decorated lattice L' in which each vertex is replaced by a "city" of four internally connected points, as indicated in Figs. 2 and 3. Regarding lines on L as dimers on the external bonds of L', dimers can be added to the internal bonds so that L' is completely covered, giving the seven possible dimer coverings of a city shown in Fig. 2. On an A (B) vertex, the arrow configurations 1, 2, 3, 4, 5 (2,1,4,3,6) of Fig. 1 then correspond, respectively, to the

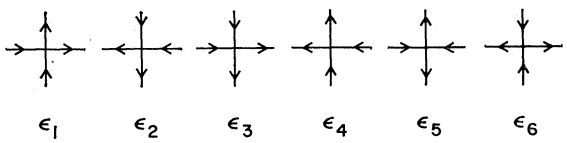

FIG. 1. Six possible vertex configurations with associated energies.

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[1] F. Rys, Helv. Phys. Acta **36**, 537 (1963).

[2] E. H. Lieb, Phys. Rev. Letters **18**, 1046 (1967); J. Phys. Soc. Japan **26**, 94 (1969); C. P. Yang, Phys. Rev. Letters **19**, 586 (1967); B. Sutherland, C. N. Yang, and C. P. Yang, *ibid.* 588 (1967).

[3] J. F. Nagle, J. Chem. Phys. **50**, 2813 (1969).

[4] F. Y. Wu has pointed out that the F model in zero staggered field can be solved combinatorially at this temperature (cf. first reference of Ref. 2).

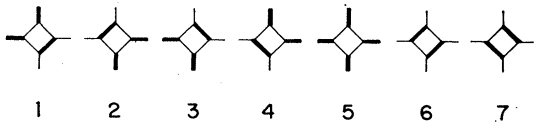

FIG. 2. Possible dimer coverings of a "city" of the decorated lattice L', corresponding to arrow configurations at a vertex of L.

dimer coverings 1, 2, 3, 4, 5 of Fig. 2, while the sixth (fifth) arrow configuration corresponds to both the sixth and seventh dimer coverings.

Associating activities u, v_1, v_2, w_1, w_2 with dimers on bonds as indicated in Fig. 3, one can regard the configurations of Fig. 2 as having weights equal to the product of the activities of dimers on internal bonds and the square root of the activities of dimers on external bonds (remembering that a dimer on an external bond is shared by two cities). Equating these to the vertex weights $\omega_i=e^{-\epsilon_i/kT}$ of the corresponding arrow configurations, one obtains from both A and B vertices the six equations

$$\begin{aligned} &\omega_1^2=u^2v_1w_1, \qquad \omega_2^2=u^2v_2w_2,\\ &\omega_3^2=u^2v_1w_2, \qquad \omega_4^2=u^2v_2w_1,\\ &e^{-S}=v_1v_2w_1w_2, \quad e^{S/2}=2u^2, \end{aligned} \tag{3}$$

where $S=4s/kT$. Using (2), these equations can be solved for u, v_1, v_2, w_1, w_2 only if the condition (1) is satisfied, in which case they can be chosen so that

$$\begin{aligned} &u=2^{-1/2}e^{S/4},\\ &v_1=e^{H-S/4}, \quad v_2=e^{-H-S/4},\\ &w_1=e^{V-S/4}, \quad w_2=e^{-V-S/4}, \end{aligned} \tag{4}$$

where $H=2h/kT$ and $V=2v/kT$.

At the temperature given by (1) the model is thus equivalent to a close-packed dimer problem on the planar lattice L', and hence the partition function Z and correlations can be calculated by Pfaffians.[5] In Appendix A it is shown that in the limit of M and N large the quantity $\psi=(MN)^{-1}\ln Z$, which is proportional to the free energy per vertex, is given by

$$\psi=\frac{1}{8\pi^2}\int_{-\pi}^{\pi}\int d\theta d\phi\,\ln[2\cosh S - 2\cos(\theta+iH)\cos(\phi+iV)]. \tag{5}$$

The staggered and direct polarizations P_S, P_H, P_V can be defined as the derivatives of ψ with respect to S, H, and V.

As is shown in Appendix B, the integral (5) has a different analytic behavior according as whether the branch points of the integrand in the complex ϕ plane lie on both sides of the real axis for all real θ, some real θ, or no real θ. These three cases are summarized below.

(i) $\cosh H\cosh V<\cosh S$: In this case the lattice is in a disordered state (i.e., correlations decay exponentially with distance) and ψ is found to be independent of H and V. Thus, both direct polarizations P_H and P_V are zero, and ψ is given by (5) with H and V replaced by zero.

(ii) $|\sinh H\sinh V|<\cosh S<\cosh H\cosh V$: The integrand of (5) has branch points at the *real* values $\theta=\theta_0$, $\phi=\phi_0$, where θ_0, ϕ_0 are defined by the complex equation $\cos(\theta_0+iH)\cos(\phi_0+iV)=\cosh S$. If H and V are positive, this equation has a solution such that $0<\theta_0<\frac{1}{2}\pi$ and $-\frac{1}{2}\pi<\phi_0<0$, and it is found that $P_H=-\phi_0/\pi$, $P_V=\theta_0/\pi$. Thus the lattice is partially polarized. It is also ordered in the sense that at large distances r correlations decay only as an oscillatory factor divided by r^2. When $H=V$, the equation for θ_0, ϕ_0 simplifies, giving

$$P_H=P_V=(2\pi)^{-1}\cos^{-1}[2\cosh S-\cosh 2H]. \tag{6}$$

(iii) $\cosh S<|\sinh H\sinh V|$: In this case $\psi=\frac{1}{2}[|H|+|V|-\ln 2]$ and the lattice is completely ordered, having complete direct polarization and zero staggered polarization. Note that this can occur only if H and V are both nonzero.

The states of zero, partial, and complete direct polarization are clearly shown in Fig. 4, where $P_H(=P_V)$ is plotted against H for the case $H=V$, $S=0.5$. It seems that in zero direct field the staggered field S "locks" the lattice into a disordered state, and a direct field of magnitude comparable to S is required to unlock it again.

It is also interesting to consider the lattice when $H=V=0$. In this case ψ is an analytic function of S for $S>0$ and $S<0$, but near $S=0$ the staggered susceptibility $-\partial^2\psi/\partial S^2$ diverges like $\ln|S|$. Thus the system undergoes a nonanalytic transition from positive to negative staggered field. Further, at $S=0$ the correlations at large distances r are found to decay only as r^{-2}, indicating that in zero fields the lattice is in an ordered

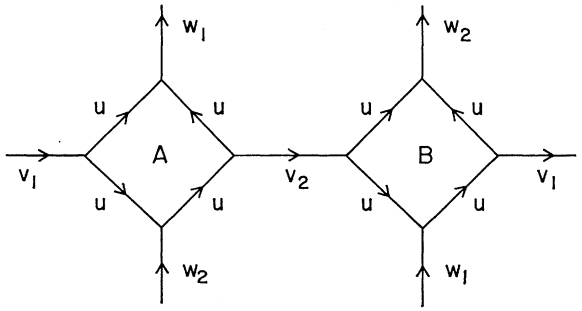

FIG. 3. Decorated lattice L' showing dimer activities and orientations associated with the bonds. The "cities" on the left and right correspond to A and B vertices of L, respectively.

[5] C. A. Hurst and H. S. Green, J. Chem. Phys. **33**, 1059 (1960); P. W. Kasteleyn, J. Math. Phys. **4**, 287 (1963); E. W. Montroll, in *Applied Combinatorial Mathematics*, edited by E. F. Beckenbach (John Wiley & Sons, Inc., New York, 1964).

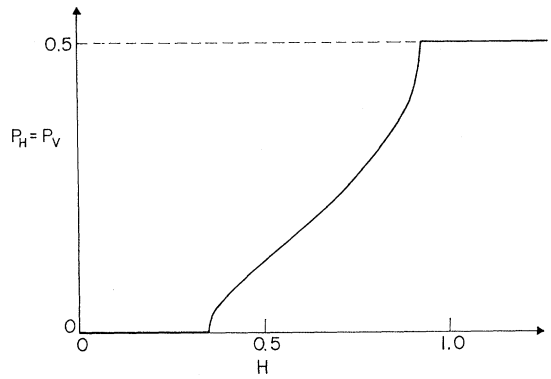

FIG. 4. Plot of direct polarization against field for the case $H=V$, $S=0.5$.

state, even though the temperature (1) lies above the critical temperature of the F model.

The author thanks Professor E. H. Lieb for numerous enlightening discussions.

APPENDIX A

Using the Pfaffian method,[5] one can see that an appropriate orientation of the bonds is that shown in Fig. 3. Supposing the vertices of L' to be labeled in some way as $\mathrm{I}=1, 2, \ldots, 4MN$, it follows that

$$Z^2=\det\mathbf{D}, \tag{A1}$$

where $\mathbf{D}$ is a $4MN$ by $4MN$ antisymmetric matrix with elements $D(I,I')$ such that

$$D(I,I')=-D(I',I)=u, v_1, v_2, w_1, w_2, \tag{A2a}$$

if the vertices I and I' are connected by a bond with associated activity u, v_1, v_2, w_1, w_2, oriented so as to point from I to I';

$$D(I,I')=0 \tag{A2b}$$

if I and I' are not connected by a bond.

The determinant of $\mathbf{D}$ is of course the determinant of the coefficients of the $4MN$ linear equations.

$$\sum_{I'} D(I,I')x(I')=0, \tag{A3}$$

where $x(I)$ is an unknown variable associated with the Ith vertex of L'. These variables can be written as $a_{m,n}$, $b_{m,n}$, $c_{m,n}$, $d_{m,n}$, corresponding, respectively, to the upper, lower, left, and right vertices of the city in the mth row and nth column of the lattice. Supposing that cities of type-A have $m+n$ even, the Eqs. (A3) can then be written explicitly as

$$\begin{aligned}
ua_{m,n} \quad &+ub_{m,n} \quad -v_1d_{m-1,n}=0,\\
ua_{m,n} \quad &-ub_{m,n} \quad +v_2c_{m+1,n}=0,\\
w_2b_{m+1,n+1} &-uc_{m+1,n} -ud_{m+1,n}=0,\\
-w_1a_{m+1,n-1} &-uc_{m+1,n} +ud_{m+1,n}=0,
\end{aligned} \tag{A4}$$

when $m+n$ is even.

When $m+n$ is odd, v_1, w_1 should be interchanged with v_2, w_2 in Eqs. (A4). Notice however that these two sets of equations are independent, the first (second) relating variables $a_{m,n}$ and $b_{m,n}$ for $m+n$ even (odd) with $c_{m,n}$ and $d_{m,n}$ for $m+n$ odd (even). Thus the determinant of the coefficients of all $4MN$ equations is the product of the determinants of the two separate sets. Further, if M and N are even and appropriate boundary conditions are imposed, these two determinants are the same.

It follows that $\det\mathbf{D}$ is equal to the determinant of the coefficients of the $4MN$ equations obtained from (A4) by letting m and n assume *all* values such that $1\leqslant m\leqslant M$ and $1\leqslant n\leqslant N$. When M and N are large we can impose cyclic boundary conditions[6] on the equations and make a similarity transformation to the variables $\bar{a}_{p,q}$, $\bar{b}_{p,q}$, $\bar{c}_{p,q}$, $\bar{d}_{p,q}$, where

$$\bar{a}_{p,q}=\sum_{m=1}^{M}\sum_{n=1}^{N} a_{m,n}\exp\{2\pi i(mp/M+nq/N)\} \tag{A5}$$

for $1\leqslant p\leqslant M$, $1\leqslant q\leqslant N$, and $\bar{b}_{p,q}$, $\bar{c}_{p,q}$, $\bar{d}_{p,q}$ are similarly defined in terms of $b_{m,n}$, $c_{m,n}$, $d_{m,n}$. In terms of these variables Eqs. (A4) break up into MN independent sets of four equations, giving

$$\det\mathbf{D}=\prod_{p=1}^{M}\prod_{q=1}^{N}\Delta_{p,q}, \tag{A6}$$

where $\Delta_{p,q}$ is the 4-by-4 determinant

$$\Delta_{p,q}=\begin{vmatrix} u & u & 0 & -v_1\alpha^{-p} \\ u & -u & v_2\alpha^{p} & 0 \\ 0 & w_2\beta^{q} & -u & -u \\ -w_1\beta^{-q} & 0 & -u & u \end{vmatrix}, \tag{A7}$$

α, β being defined by

$$\alpha=e^{2\pi i/M}, \quad \beta=e^{2\pi i/N}. \tag{A8}$$

From Eq. (4) it follows that

$$\begin{aligned}\Delta_{p,q}=2\cosh S-2\cos[2\pi p/M+iH]\\ \times\cos[2\pi q/N+iV].\end{aligned} \tag{A9}$$

Substituting this expression into (A6) and (A1), it is found that in the limit of M and N large

$$(MN)^{-1}\ln Z\rightarrow\psi, \tag{A10}$$

where

$$\begin{aligned}\psi=\frac{1}{8\pi^2}\int_{-\pi}^{\pi}\int d\theta d\phi\,\log[2\cosh S\\ -2\cos(\theta+iH)\cos(\phi+iV)].\end{aligned} \tag{A11}$$

This is the expression quoted above for the free energy.

[6] P. W. Kasteleyn, Physica **27**, 1209 (1961).

APPENDIX B

It can be seen from the reflection symmetries of the F model, or directly from Eq. (5), that ψ is an even function of S, H, and V. Hence without any loss of generality we can suppose that S, H, and V are all nonnegative.

The ϕ integration in (5) can be evaluated as a contour integral in the complex $z=e^{i\phi}$ plane. Let $\Phi_1(\theta)$ and $\Phi_2(\theta)$, or simply Φ_1 and Φ_2, be the two values of ϕ in the domain $-\pi<\mathrm{Re}(\phi)\leqslant\pi$ such that

$$\cos(\theta+iH)\cos(\phi+iV)=\cosh S. \tag{B1}$$

Then it can be seen that $\Phi_1+\Phi_2=-2iV$ and they can be ordered so that $\mathrm{Im}(\Phi_1)\geqslant -V\geqslant \mathrm{Im}(\Phi_2)$.

With these conventions, it is found that

$$\psi=\frac{1}{4\pi}\int_{-\pi}^{\pi}d\theta\, F(\theta), \tag{B2}$$

where

$$F(\theta)=\ln[\cos(\theta+iH)e^{V}] \tag{B3a}$$

if

$$\mathrm{Im}[\Phi_1(\theta)]<0,$$

and

$$F(\theta)=\ln[\cos(\theta+iH)e^{V}]-i\Phi_1(\theta) \tag{B3b}$$

if

$$\mathrm{Im}[\Phi_1(\theta)]>0.$$

The three cases mentioned in the text can now be discussed.

(i) $\cosh H\cosh V<\cosh S$: In this case $\Phi_1(\theta)$ has a positive imaginary part for all real θ. Solving (B1) for $\phi=\Phi_1(\theta)$ and substituting the result into (B3b), it follows that

$$\psi=\frac{1}{4\pi}\int_{-\pi}^{\pi}d\theta\ln\{\cosh S+[\cosh^2 S-\cos^2(\theta+iH)]^{1/2}\}. \tag{B4}$$

The integrand in (B4) is an analytic function of θ in the domain $-H\leqslant\mathrm{Im}(\theta)\leqslant 0$, so the integration can be changed to the contour $\theta=-iH+\theta'$ (θ' real), giving

$$\psi=\frac{1}{4\pi}\int_{-\pi}^{\pi}d\theta'\ln\{\cosh S+[\cosh^2 S-\cos^2\theta']^{1/2}\}, \tag{B5}$$

from which it is apparent that ψ is independent of H and V.

(ii) $\sinh H\sinh V<\cosh S<\cosh H\cosh V$: In this case $\Phi_1(\theta)$ is real at the four points $-\pi+\theta_0$, $-\theta_0$, θ_0, $\pi-\theta_0$, where it has the values $\pi+\phi_0$, $-\phi_0$, ϕ_0, $-\pi-\phi_0$, respectively, and $0<\theta_0<\frac{1}{2}\pi$, $-\frac{1}{2}\pi<\phi_0<0$. The imaginary part of $\Phi_1(\theta)$ is positive in the domains $-\pi+\theta_0<\theta<-\theta_0$, $\theta_0<\theta<\pi-\theta_0$ and negative elsewhere. Thus from (B2) and (B3)

$$\psi=\frac{1}{4\pi}\int_{-\pi}^{\pi}d\theta\ln[\cos(\theta+iH)e^{V}]-\frac{i}{4\pi}\int_{\theta_0}^{\pi-\theta_0}d\theta[\Phi_1(\theta)+\Phi_1(-\theta)]. \tag{B6}$$

The first integration in this equation can be performed, giving

$$\psi=\tfrac{1}{2}[H+V-\ln 2]-\frac{i}{4\pi}\int_{\theta_0}^{\pi-\theta_0}d\theta[\Phi_1(\theta)+\Phi_1(-\theta)]. \tag{B7}$$

From the above values of $\Phi_1(\theta)$, the function $\Phi_1(\theta)+\Phi_1(-\theta)$ vanishes when $\theta=\theta_0$ or $\pi-\theta_0$. Thus on differentiating (B7) with respect to V or H the terms arising from differentiating the limits of integration in the right-hand side vanish. Noting also that $\Phi_1(\theta)=-iV+$ a function independent of V, it follows that

$$P_V=\partial\psi/\partial V=\theta_0/\pi. \tag{B8}$$

Similarly, noting that $\Phi_1(\theta)$ depends on θ and H only via the combination $\theta+iH$, differentiating (B7) with respect to H gives

$$P_H=\partial\psi/\partial H=\tfrac{1}{2}+\frac{1}{4\pi}\int_{\theta_0}^{\pi-\theta_0}d\theta[\Phi_1'(\theta)+\Phi_1'(-\theta)], \tag{B9}$$

where the primes denote derivatives. The integration in (B9) can be performed immediately, and using the above values of $\Phi_1(\theta)$ gives

$$P_H=-\phi_0/\pi. \tag{B10}$$

(iii) $\cosh S<\sinh H\sinh V$: The imaginary part of $\Phi_1(\theta)$ is negative for all values of θ, so $F(\theta)$ is given by Eq. (B3a). Substituting this into (B2) and performing the θ integration, it is found that

$$\psi=\tfrac{1}{2}[H+V-\ln 2]. \tag{B11}$$

Remembering that ψ is an even function of H and V, these are the results quoted in the text.