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Generalization of Conditions due to Domb for Reducing the Number of Unknown Terms in the Ising Fugacity Expansion*

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The derivation of low-temperature series for the Ising model is simplified by a high-temperature symmetry condition, a general proof of which does not exist in the open literature. The magnetic linked-cluster expansion provides an elementary and general proof.

BACKGROUND

We present the proof in detail for the free energy F of the nearest-neighbor $S=\frac{1}{2}$ Ising model. The straightforward generalization to $S>\frac{1}{2}$, longer-range interactions, and physical quantities other than F is indicated in conclusion. The Hamiltonian of the model is

$$-\beta\mathcal{H}=v\sum_{\langle ij\rangle}\sigma_i\sigma_j+h\sum_i\sigma_i, \qquad (1)$$

where $\sigma_i=1\,(-1)$ for spin up (down), the indices range over lattice sites, and the sum in the first term is over nearest-neighbor pairs. The free energy is given by $-\beta F=\ln \mathrm{Tr}e^{-\beta\mathcal{H}}$.

At low temperatures (1) can usefully be rewritten in terms of operators measuring the deviation from complete alignment, $n_i\equiv\frac{1}{2}(1-\sigma_i)$,

$$-\beta\mathcal{H}=N(\tfrac{1}{2}qv+h)+4v\sum_{\langle ij\rangle}n_in_j-2(h+qv)\sum_i n_i, \qquad (2)$$

where q is the number of nearest neighbors. The low-temperature (high-field) series for F is[1] just the Yvon-Mayer expansion with chemical potential $-2(h+qv)$. The free energy can be written as

$$-\frac{\beta F}{N}=\tfrac{1}{2}qv+h+\sum_{n=1}^{\infty}\mu^n L_n(u), \qquad (3)$$

where $\mu=e^{-2h}$, $u=e^{-4v}$, and the $L_n(u)$ are finite polynomials[2] in u,

$$L_n(u)=u^{nq/2}\sum_{r=0}^{\frac{1}{2}n(n-1)}[n,r]u^{-r}.$$

The coefficients $[n, r]$ may be determined from the Mayer graphs. The quantity $(1-u)$ is a high-temperature variable, so high-temperature series can be derived from (3),

$$-\frac{\beta F}{N}=\tfrac{1}{2}qv+h+\sum_{n=1}^{\infty}\sum_{r=0}^{\infty}(-1)^r\mu^n \times\frac{(1-u)^r}{r!}\frac{\partial^r L_n(u)}{\partial u^r}\bigg|_{u=1}. \qquad (4)$$

SYMMETRY CONDITION AND ITS USE

It is easy to see from (1) that the free energy F has the symmetry $F(v, h)=F(v, -h)$. This symmetry, which is explicit in the high-temperature series, is lost at low temperatures, where series converge only for $\mu\leq 1$. The high-temperature symmetry condition is

$$-\frac{\beta F}{N}=\tfrac{1}{2}qv+h+\ln(1+\mu)+\sum_{r=1}^{\infty}(1-u)^r\frac{\varphi_r(\mu)}{(1+\mu)^{2r}}, \qquad (5)$$

with the specification that

$$\varphi_r(\mu)\equiv\sum_{n=1}^{2r-1}\varphi_r^{(n)}\mu^n$$

is a finite polynomial having the symmetry $\varphi_r(\mu)=\mu^{2r}\varphi_r(1/\mu)$. Note that this incorporates invariance under $h\leftrightarrow -h$. Equation (5) was first conjectured by Domb[3] and has subsequently been proved for various cases.[4] To our knowledge there is no proof in the open literature which is applicable to close-packed lattices and spins greater than $\frac{1}{2}$.

Equation (5) allows information about the symmetry to be incorporated into the low-temperature series: Knowledge of the first $(s-1)$ L_n's determines the φ_r's through φ_{s-1}. This information [via (4)] puts s conditions on $L_s(\mu)$, thus reducing the number of coefficients $[s, r]$ which must be independently computed, a labor-saving device of considerable practical importance.[2]

PROOF

The linked-cluster theorem allows the free energy to be expanded at high temperatures,

$$-\frac{\beta(F-F_0)}{N}=\sum_{n=1}^{\infty}C_n(h)v^n, \qquad (6)$$

where the nth-order coefficient $C_n(h)$ is the sum of contributions from all n-line graphs. F_0 is the free energy when $v\equiv 0$,

$$-\beta F_0/N=\ln(\mu^{1/2}+\mu^{-1/2})=h+\ln(1+\mu), \qquad (7)$$

and it is useful to introduce the semi-invariants

$$\begin{aligned}M_n{}^0(\mu)&\equiv(d^n/dh^n)(-\beta F_0/N)\\&=(-1)^nM_n{}^0(1/\mu)\\&\equiv p_n(\mu)/(1+\mu)^n, \qquad (8)\end{aligned}$$

where

$$p_n(\mu)\equiv\sum_{r=0}^{n}p_n(r)\mu^r=(-1)^n\mu^np_n(1/\mu)$$

and

$$p_n{}^{(0)}=p_n{}^{(n)}=0 \quad \text{for} \quad n>1.$$

Each graph G_n in the expansion for $C_n(h)$ carries[5] a factor

$$X[G_n,\mu]=\prod_{G_n}M_s{}^0$$

consisting of one factor of $M_s{}^0$ for each vertex in G_n with s impinging lines, which expresses the entire magnetic field dependence of G_n. There are $2n$ line ends in G_n, so it is clear that $X[G_n, \mu]$ and, therefore, $C_n(h)$ have $(1+\mu)^{2n}$ as denominator and the symmetrical numerator required. The term $\frac{1}{2}qv$ appearing in (4) and (5) comes from the contribution to $C_1(h)$ of the graph consisting of a single bond. We have now shown that

$$-\frac{\beta F}{N}=\tfrac{1}{2}qv+h+\ln(1+\mu)+\sum_{n=1}^{\infty}v^n\frac{\Phi_n(\mu)}{(1+\mu)^{2n}}, \qquad (9)$$

where

$$\Phi_n(\mu)=\sum_{r=1}^{2u-1}\Phi_n{}^{(r)}\mu^r=\mu^{2n}\Phi_n(1/\mu). \qquad (10)$$

Finally, $u=e^{-4v}$ can be inverted, giving v as a power series in $(1-u)$, so (9) implies (5).[6]

The proof depended only on the graph weights [via the simple properties (8) of the semi-invariants] and not on their embeddings. It is therefore lattice independent.

GENERALIZATIONS

Generalization to higher-spin and longer-range interactions is straightforward. To treat a spin variable ranging $\sigma=2S, 2S-2, \ldots, -2S$, one must in (7)–(9) replace the combination $(1+\mu)$ by

$$Z_0(S)=\sum_{n=0}^{2S}\mu^n.$$

Equation (9) then becomes

$$-\beta F/N=(2S)^2\tfrac{1}{2}qv+2Sh+\ln Z_0(S)+\sum_{n=1}^{\infty}v^n\frac{{}_S\Phi_n(\mu)}{Z_0{}^{2n}(S)}, \qquad (11)$$

where the polynomial

$${}_S\Phi_n(\mu)=\sum_{r=1}^{4nS-1}{}_S\Phi_n{}^{(r)}\mu^r=\mu^{4nS}{}_S\Phi_n(1/\mu).$$

The corresponding generalization of (5) is immediate.

The semi-invariants $M_n{}^0$ are interaction independent, so, when longer-range interactions are present (e.g., a second-neighbor interaction w), the generalization of (9) is

$$-\beta F/N=\tfrac{1}{2}(q_1v+q_2w)+h+\ln(1+\mu)+\sum_{n,m;\,n+m\geq 1}^{\infty}v^nw^m\frac{\Phi_{n,m}(\mu)}{(1+\mu)^{2(n+m)}}, \qquad (12)$$

where

$$\Phi_{n,m}(\mu)=\sum_{r=1}^{2(n+m)-1}\Phi_{n,m}{}^{(r)}\mu^r=\mu^{2(n+m)}\Phi_{n,m}(1/\mu),$$

and q_1 and q_2 are the number of nearest and next nearest neighbors, respectively.

Equivalent expressions for other thermodynamic and correlation functions may be written down by inspection from the linked-cluster expansion.

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