SOME RIGOROUS INEQUALITIES SATISFIED BY THE FERROMAGNETIC ISING MODEL IN A MAGNETIC FIELD*

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We show in this Letter that for the ferromagnetic Ising model, a function closely related to the magnetization, when considered as a function of the hyperbolic tangent of the magnetic field, has a very special structure. This structure enables us to prove two sorts of related inequalities. One type, Eq. (11), of interest to theorists, shows that the critical-index gap parameters, Δ_i, form a nondecreasing sequence. The other type, of interest to experimentalists, is that every difference (not derivative) of the function we introduce has a fixed sign as a function of magnetic field. We have also checked these relations on all the available data for the spin-$\frac{1}{2}$ Heisenberg model and find agreement.

Our starting point is a recent rearrangement[1] of the results of Yang and Lee[2] for the free energy F of the ferromagnetic Ising model:

$$F/kT=-mH/kT-\int_0^1\ln[(1-\mu)^2+4\mu y]d\varphi(y), \quad (1)$$

where $d\varphi(y)\geqslant 0$, m is the magnetic moment per spin, H the magnetic field, k Boltzman's constant, T the absolute temperature, and

$$\mu=\exp(-2mH/kT). \quad (2)$$

We shall rewrite this expression in terms of

$$\tau=\tanh(mH/kT) \quad (3)$$

as

$$F/kT=\tfrac{1}{2}\ln[\tfrac{1}{4}(1-\tau^2)]-\int_0^1\ln[\tau^2(1-y)+y]d\varphi(y), \quad (4)$$

where[2] use is made of

$$\int_0^1 d\varphi(y)=\tfrac{1}{2}.$$

Now, if we substitute $\omega=y^{-1}-1$, we obtain

$$\frac{F}{kT}=\tfrac{1}{2}\ln[\tfrac{1}{4}(1-\tau^2)]-\int_0^1\ln y\,d\varphi(y)-\int_0^\infty\ln(1+\tau^2\omega)d\varphi\left(\frac{1}{1+\omega}\right). \quad (5)$$

Hence, differentiating with respect to the magnetic field, we obtain the reduced magnetization per spin as

$$\frac{I}{mN}=\tau+\int_0^\infty\frac{2\tau(1-\tau^2)\omega}{1+\tau^2\omega}d\varphi\left(\frac{1}{1+\omega}\right), \quad (6)$$

or the function

$$G(\tau^2)=\frac{(I/mN)-\tau}{\tau(1-\tau^2)}=\int_0^\infty\frac{d\psi(\omega)}{1+\tau^2\omega}, \quad (7)$$

where $d\psi\geqslant 0$. We remark that for $T>T_c$, the critical temperature, the upper limit of integration is less than infinity, but for $T\leqslant T_c$ it is infinite. We note that $G(0)=\infty$ for $T\leqslant T_c$.

The consequence of form (7) is that $G(\tau^2)$ is a series of Stieltjes.[3] This fact means that if we expand

$$G(\tau^2)=G_0(T)-G_1(T)\tau^2+G_2(T)\tau^4-\cdots, \quad (8)$$

then

$$D(m,n)=\begin{vmatrix} G_m & G_{m+1} & \cdots & G_{m+n} \\ G_{m+1} & G_{m+2} & & \vdots \\ \vdots & & \ddots & \\ G_{m+n} & & \cdots & G_{m+2n}\end{vmatrix}\geqslant 0. \quad (9)$$

It is easy to show that the divergence of the G_i at $T=T_c$ is the same as the corresponding (one power of τ or H higher) coefficients in the magnetization. Following the notation of Baker, Gilbert, Eve, and Rushbrooke[4] ($\gamma_i-\gamma_{i-1}=2\Delta$ in the notation of Fisher[5]),

$$G_m(\tau^2,T)\propto(T-T_c)^{-\gamma_m},\quad T\to T_c^{\,+}. \quad (10)$$

It follows at once from (9) for $n=1$ that the critical exponents obey

$$\gamma_{i+1}-2\gamma_i+\gamma_{i-1}\geqslant 0 \quad (11)$$

or that the γ_i increase at least linearly with i. These relations are obeyed in every known case within calculational error. See Fisher[5] for a review. The linear relation

$$\gamma_i=\gamma_0+2\Delta i \quad (12)$$

required by the scaling laws[6] is allowed by (11). We have also tested all available Heisenberg

Table I. The Heisenberg-model g_{mn} coefficients.

n \ m	0	1	2	3
		Simple Cubic Lattice		
1	3.0	0	0	0
2	6.0	16.5	0	0
3	11.0	93.5	109.5	0
4	20.625	364.5	1085.625	797.625
5	39.025	1201.75	6631.5	11514.75
6	68.777083333	3575.7125	31861.49375	96787.8125
7	119.42976190	9860.1833333	131563.225	615203.4375
8	216.16227679	25661.864211	487668.51942	3265575.2925
9	387.19383267			
10	658.34153977			
		Body-Centered Cubic Lattice		
1	4.0	0	0	0
2	12.0	30.0	0	0
3	34.666666667	250.0	274.0	0
4	95.833333333	1460.6666667	3970.5	2759.5
5	262.7	7193.0	35853.0	58041.0
6	708.04166667	31871.133333	255427.325	716544.91667
7	1893.2896825	131144.06111	1565813.8833	6716153.4833
8	5012.1086310	510344.67827	8627298.6205	52696392.526
9	13235.513272			
10	34737.965232			
		Face-Centered Cubic Lattice		
1	6.0	0	0	0
2	30.0	69.0	0	0
3	138.0	931.0	969.0	0
4	611.25	8736.0	22529.25	15015.75
5	2658.55	68948.5	325798.5	504508.5
6	11432.5125	488853.18333	3714828.2375	9949385.625
7	48726.726190	3215606.1083	36427972.0	148992174.07
8	206142.36741	19994641.556	320929521.10	1867849644.0
9	866895.50635			
		Square Lattice		
1	2.0	0	0	0
2	2.0	7.0	0	0
3	1.3333333333	21.0	29.0	0
4	1.0833333333	38.666666667	153.75	130.25
5	1.1833333333	57.5	468.5	1007.5
6	0.50972222222	77.544444444	1074.9125	4318.0416667
7	-0.32182539683	93.741666667	2070.7833333	13500.325
8	0.40739087302	97.905307540	3509.2290179	34373.307794
9	1.0672839506			
10	-0.69281883818			
		Triangular Lattice		
1	3.0	0	0	0
2	6.0	16.5	0	0
3	8.5	90.5	108.0	0
4	9.375	312.0	1020.375	767.625
5	11.025	839.25	5638.5	10455.75
6	16.964583333	1934.5	23391.21875	80023.9375
7	21.152678571	4022.1625	80285.9625	448375.7625
8	8.8058779762	7701.2694196	239966.59621	2039001.7915
9	-9.6784556878			

model data[4,7] to see if they seem valid there also. To this end we have computed the following (Table I):

$$G(\tau^2,T)=\sum_{m=0}^{\infty}\sum_{n=m+1}^{\infty}g_{m,n}(-\tau^2)^mK^n, \quad (13)$$

where $K=J/kT$ (with J the exchange integral) for square, triangular, simple cubic, bcc, and fcc lattices, to order τ^6 and K^9 or K^{10} for close- or loose-packed lattices, respectively, and (τ^0) and K^8 otherwise. Where comparison is possible, our results agree with those (as corrected) of Opechowski.[8] Except for the coefficient of τ^0 for the two-dimensional lattices, all the coefficients had the expected signs. All the coefficients of the determinants $D(0,1)$ and $D(1,1)$ were positive. Since the coefficient of τ^0 is reduced magnetic susceptibility minus unity and has been extensively studied,[9] there is little doubt that it is positive over the range $T>T_c$ (if any). Consequently, the inequalities which we have proved rigorously for the ferromagnetic Ising model appear to be valid for the ferromagnetic Heisenberg model as well.

Hence we propose that it may be worthwhile to test them experimentally. This test can be made by noting that form (7) implies that

$$(-1)^n\Delta^nG(\tau^2)\geqslant 0, \quad (14)$$

where Δ is the difference operator with respect to τ^2. That a difference is involved instead of a derivative allows the direct use of experimental data without the difficulty of trying to extract a derivative.

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INTRINSIC SURFACE STATES IN SEMICONDUCTORS*

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Experimentally well established features of semiconductor surface-state distributions are explained in terms of a realistic model calculation.

Calculations reported here for a model crystal surface provide a consistent explanation of the surface-state distributions observed in silicon and germanium, and a simple extension suggests reasons for trends observed in the distributions for III-V and II-VI compounds. These are believed to be the first detailed calculations based on a realistic potential.

A recent survey[1] of measurements on semiconductor-vacuum interfaces indicated two distinct types of behavior. In covalent semiconductors, such as silicon, the densities of surface states and surface atoms are comparable and the Fermi level lies in the lower part of the band gap. Markedly different are more ionic crystals, which exhibit much lower densities of states. A similar situation appears to exist at semiconductor-metal contacts,[2] though in this case the surface states must be interpreted as tails on the metal wave functions.[3,4]

Calculations of localized states for the (110) face of silicon are reported here. The model is similar to that also suggested by Chaves, Majlis, and Cardona[5] and is described elsewhere.[6] The bulk crystal potential is unaltered up to the surface plane, where it changes abruptly to the vacuum level, determined by work-function measurements. For this model, the calculation sep-