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LETTER TO THE EDITOR

An analysis of the Monte Carlo diamond lattice calculation using an exact reduction relation

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Abstract. A reduction relation is noted which allows one to relate exactly, at any temperature T, two quantities for the Ising model on the diamond lattice: (i) the ratio, essentially, of the average neighbour–neighbour correlation function and the energy per spin, $P = T_2/U_2$ and (ii) a ratio of a certain pair of four-spin correlation functions $Q = T_4/U_4$. This relation is applied to Mouritsen's Monte Carlo determination of these quantities P_c and Q_c, at the critical point T_c. It is shown that the Monte Carlo values are severely inconsistent with the exact relation. A more reliable value of the neighbour–neighbour correlation function, $\langle\sigma_1\sigma_2\rangle \simeq 0.283$, is calculated from the Monte Carlo data.

In his paper on the phase transition and critical correlation functions in the spin-$\frac{1}{2}$ Ising model on a diamond lattice, Mouritsen (1980) calculated, using the Monte Carlo (MC) technique, certain ratios P and Q of two- and four-spin correlation functions, respectively. These had been assumed in an early theory of Frank and Mitran (1978) to be unity. Mouritsen showed (using up to 16 384 lattice points) that this assumption was, although a good approximation, not exact, as he obtained $P_{MC} = 0.978 \pm 0.002$, $Q_{MC} = 1.0935 \pm 0.0005$. Since then, progress has been made in the difference-equation approach to critical phenomena (see, e.g., Frank and Cheung 1984), and a re-examination of the numerical results of Mouritsen (1980) revealed significant quantitative discrepancies with the new theory. It is well known that MC calculations can sometimes give misleading results, as for example in the calculation (using $N = 128$ lattice points; Mouritsen *et al* 1981) of the critical temperature for the FCC Ising lattice with pure four-spin interactions. (The discrepancy of approximately 17% compared with the correct self-dual Onsager temperature was resolved by Mouritsen *et al* (1983) in a re-analysis using $N = 1024$ and $N = 2000$ lattice points.) Therefore, a method was sought whereby the results of Mouritsen (1980) could be checked for self-consistency.

In this work, an exact equation is derived for the diamond lattice, which connects P and Q for any given temperature T. The degree of consistency of Mouritsen's (1980) (P, Q) result with this equation is demonstrated, and implications for the critical value of the neighbour–neighbour correlation function are shown.

For the diamond lattice with Hamiltonian

$$H = -\sum_{i<j} J_{ij}\sigma_i\sigma_j \qquad (\sigma_i, \sigma_j = \pm 1) \tag{1}$$

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the Suzuki–Callen relations (Suzuki 1965, Callen 1963) read as follows:

$$\langle \sigma_i \{\overline{\sigma_i}\} \rangle = \langle \{\overline{\sigma_i}\} \tanh(2\beta J \theta_i) \rangle \tag{2}$$

where $\{\overline{\sigma_i}\}$ does not involve spin σ_i, $\theta_i = \frac{1}{4}(\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4)$, where $\sigma_1, \ldots, \sigma_4$ are the four nearest-neighbour spins of σ_i, and $\beta = 1/k_B T$. Choosing $\{\overline{\sigma_i}\} = \theta_i$ and then $\{\overline{\sigma_i}\} = \theta_i^3$, one obtains the two exact relations:

$$U_2 \equiv \langle \sigma_i \theta_i \rangle = \langle \theta_i \tanh(2\beta J \theta_i) \rangle \tag{3}$$

$$U_4 \equiv \langle \sigma_i \theta_i^3 \rangle = \langle \theta_i^3 \tanh(2\beta J \theta_i) \rangle. \tag{4}$$

Since θ_i may take on only the values 1, $\frac{1}{2}$, 0, $-\frac{1}{2}$, -1, there exists a reduction relation for the θ_i operators:

$$\theta_i(\theta_i^2 - 1^2)(\theta_i^2 - (\tfrac{1}{2})^2) = 0. \tag{5}$$

Thus, any even function of the θ_i may be written as

$$f_{\text{even}}(\theta_i) = C_0 + C_2 \theta_i^2 + C_4 \theta_i^4 \tag{6}$$

where

$$\begin{aligned} C_0 &= f_{\text{even}}(0) \\ C_2 &= \tfrac{1}{3}\left[-15 f_{\text{even}}(0) + 16 f_{\text{even}}(\tfrac{1}{2}) - f_{\text{even}}(1)\right] \\ C_4 &= \tfrac{1}{3}\left[12 f_{\text{even}}(0) - 16 f_{\text{even}}(\tfrac{1}{2}) + 4 f_{\text{even}}(1)\right] \end{aligned} \tag{7}$$

are obtained by substituting $\theta_i = 0$, $\frac{1}{2}$ and 1 into (6). The thermal average of (6)

$$\langle f_{\text{even}}(\theta_i) \rangle = C_0 + C_2 \langle \theta_i^2 \rangle + C_4 \langle \theta_i^4 \rangle \tag{8}$$

applied to the RHS of (3) and (4) yields, with the notation $T_2 = \langle \theta_i^2 \rangle$ and $T_4 = \langle \theta_i^4 \rangle$,

$$U_2 = A_2 T_2 + A_4 T_4 \tag{9}$$

$$U_4 = B_2 T_2 + B_4 T_4 \tag{10}$$

where

$$\begin{aligned} A_2 &= \tfrac{1}{3}[8\tanh(\beta J) - \tanh(2\beta J)] & B_2 &= \tfrac{1}{3}[2\tanh(\beta J) - \tanh(2\beta J)] \\ A_4 &= \tfrac{4}{3}[-2\tanh(\beta J) + \tanh(2\beta J)] & B_4 &= \tfrac{2}{3}[-\tanh(\beta J) + 2\tanh(2\beta J)]. \end{aligned} \tag{11}$$

Dividing (9) by T_2 and (10) by T_4 and eliminating T_2/T_4 from the resulting equations, one obtains

$$(1/P - A_2)(1/Q - B_4) = A_4 B_2 \tag{12}$$

where P, Q are, respectively, the ratios T_2/U_2 and T_4/U_4. For a given T, the As and Bs are determined, and P and Q are related in a one-to-one fashion. The critical temperature of the Monte Carlo calculation $T_c = (2.705 \pm 0.005) J/k_B$ (Mouritsen 1980) is consistent with

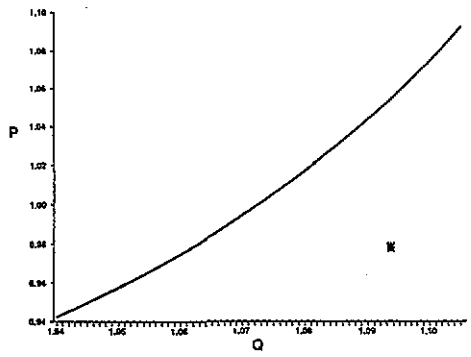

Figure 1. Exact P versus Q curve for $T = T_c = 2.705J/k_B$ for the diamond Ising lattice, from (12). The $*$ denotes $(Q, P)_{MC}$.

the result (2.7043 ± 0.0002) from high-temperature series calculations (Gaunt and Sykes 1973), and so may be taken to be correct. In figure 1, we plot P versus Q, from (12) at this temperature (the error bars for both series and MC are vanishingly small on the scale of this figure). It is seen that the $(Q, P)_{MC}$ point, denoted by $*$ in the figure, is not consistent with (12) at the accepted critical temperature. If $Q_{MC} = 1.0935 \pm 0.0005$ is correct, then the inconsistency in P_{MC} is $\simeq 7\%$.

It can be shown, moreover, that the inconsistency in the neighbour–neighbour correlation function $\langle\sigma_1\sigma_2\rangle$ is as high as 17%. One invokes the identity (see, e.g., (1.3) of Mouritsen 1980)

$$P = \big(1 + 3\langle\sigma_1\sigma_2\rangle\big)/4\langle\sigma_i\sigma_1\rangle \tag{13}$$

to eliminate P from (12) in favour of $\langle\sigma_1\sigma_2\rangle$ and $\langle\sigma_i\sigma_1\rangle$. Thus, one obtains the exact equation

$$\langle\sigma_1\sigma_2\rangle = \tfrac{1}{3}\big\{4\big(1 - B_4Q\big)\langle\sigma_i\sigma_1\rangle/\big[A_2 + \big(A_4B_2 - A_2B_4\big)Q\big] - 1\big\} \tag{14}$$

relating $\langle\sigma_1\sigma_2\rangle$ to $\langle\sigma_i\sigma_1\rangle$ and Q at any value of T. If, then, one substitutes at $T_{c,MC} = 2.705J/k_B$, the values $Q_{MC} = 1.0935$ and $\langle\sigma_i\sigma_1\rangle_{MC} = 0.439$ one obtains $\langle\sigma_1\sigma_2\rangle = 0.283$ which is $\simeq 17\%$ higher than the MC value, $\langle\sigma_1\sigma_2\rangle_{MC} = 0.235 \pm 0.002$, of Mouritsen (1980).

One would like to have an accurate value of $\langle\sigma_1\sigma_2\rangle$ at T_c. Unfortunately, a series calculation of the critical value of $\langle\sigma_1\sigma_2\rangle$ is not available. We believe the value of $\langle\sigma_1\sigma_2\rangle = 0.283$ calculated above to be reasonably accurate for two reasons: (i) the values of T_c and $\langle\sigma_i\sigma_1\rangle_{MC}$ used on the RHS of (14) are consistent with the values obtained from series calculations ($T_{c,series} = (2.7043 \pm 0.0002)J/k_B$, Gaunt and Sykes 1973; $\langle\sigma_i\sigma_1\rangle_{series} = 0.437 \pm 0.003$, Domb 1974), and (ii) the value of $Q_{MC} = 1.0935 \pm 0.0005$ used on the RHS of (14) is close to the value $Q = 1.0898$ which we have calculated using the theory of Frank and Cheung (1984). It would be of interest to have this verified by either a series calculation or an improved Monte Carlo calculation.

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