HIGH-TEMPERATURE EXPANSIONS—THE CLASSICAL HEISENBERG MODEL

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In this Letter we point out that useful results may be obtained by calculating for the classical Heisenberg model[1] the high-temperature expansions in $1/T$ of the susceptibility χ and the specific heat C. Moreover, we prove that to extend the high-T expansion by several orders classically, one need treat less than one-tenth as many diagrams as for the quantum-mechanical model. We further note that the treatment of each of the remaining diagrams is extraordinarily simplified.

The extension of the high-temperature expansion for the Heisenberg model with arbitrary spin seems to be highly impractical because of the enormous labor involved.[2] Nevertheless, there exists a considerable need for more terms in order to study several unresolved problems. For simple lattices with nearest-neighbor interactions only—for which the number of known terms[3] in the series for χ and C is six and five, respectively—there is a need for more terms in order to treat the singular behavior of both χ and C.[4] For ferromagnetic spinels with B-B interactions only, there is a large uncertainty in the estimate of the critical temperature[5] T_c and the form of the singularity in χ (a "$\frac{4}{3}$-power law"?), as obtained by extrapolation of the known terms.[6] Unanswered questions for spinels with both A-B and B-B interactions, for which only four terms in χ are known,[7] concern which type[7] of long-range magnetic ordering occurs at T_c, and which of the several varieties of susceptibility (ordinary, "staggered," $\cdots$) provides a reliable estimate of T_c.[8]

Now many properties of the Heisenberg model are rather insensitive to the value of S. For example, the unresolved problems discussed in the previous paragraph persist in the limit of large S. Moreover, it was proposed[9] that for the simple lattices, the celebrated form $(T-T_c)^{-4/3}$ of the divergence of χ is independent of S. Furthermore, Rushbrooke and Wood[3] (RW) found that the normalized critical temperature $T_c/S(S+1)$ is nearly proportional to $11-1/S(S+1)$, so that the error in using the $S=\infty$ value is small and decreases rapidly with increasing spin—it is ~13% for $S=\frac{1}{2}$ and only ~2% for $S=\frac{3}{2}$. Recently several additional terms have been obtained by methods which are restricted to spin $S=\frac{1}{2}, 1$.[10] Thus a corresponding extension of the classical calculation may be expected to complement ideally this recent advance for the $S=\frac{1}{2}, 1$ cases.

All pertinent information can be obtained[11] from the zero-field spin-correlation function

$$\frac{\mathrm{tr}\vec{\mathfrak{S}}_f\cdot\vec{\mathfrak{S}}_g e^{-\beta\mathfrak{H}}}{\mathrm{tr}e^{-\beta\mathfrak{H}}}=\sum_{l=0}^{\infty}\frac{(-1)^l}{l!}\alpha_l\beta^l \tag{1}$$

between spins $\vec{\mathfrak{S}}_f$ and $\vec{\mathfrak{S}}_g$ localized on the sites f, g; $\beta=1/kT$, and $\mathfrak{H}$ is the spin Hamiltonian for zero magnetic field. The α_l satisfy[12] (for $l\geq 2$)

$$\alpha_l=\nu_l-\sum_{k=1}^{l-1}\binom{l}{k}\alpha_k\mu_{l-k}, \tag{2}$$

where $\nu_m=\langle\vec{\mathfrak{S}}_f\cdot\vec{\mathfrak{S}}_g\mathfrak{H}^m\rangle$, $\mu_m=\langle\mathfrak{H}^m\rangle$, and $\langle\mathfrak{O}\rangle=\mathrm{tr}\mathfrak{O}/\mathrm{tr}1$ denotes the $\beta=0$ thermal average of the operator $\mathfrak{O}$.

The RW diagrammatic representation of μ_l comes naturally from the fact that $\mathfrak{H}=\sum J_{ij}\vec{\mathfrak{S}}_i\cdot\vec{\mathfrak{S}}_j\equiv\sum_{ij}O_{ij}$; hence $\mathfrak{H}^l$ is a sum of products $\prod O_{ij}$, and each product contains l factors O_{ij}. For each of the l factors O_{ij} in the product, one draws a straight line connecting sites i and j; the collection of these l lines corresponding to the entire product is the diagram associated with that product. Thus one can write $\mu_l=\sum_d\mu_l(d)=\sum_d P(d)\langle d\rangle$, where $P(d)$ is the number of permutations of the l lines in a diagram d, and $\langle d\rangle=P(d)^{-1}\sum\langle\mathcal{P}(\cdots O_{ij}\cdots)\rangle$, the sum going over all permutations of the factors O_{ij}. Similarly, we indicate a diagram $\bar{d}$ corresponding to one of the products in $\nu_l=\langle\vec{\mathfrak{S}}_f\cdot\vec{\mathfrak{S}}_g\mathfrak{H}^l\rangle$ by

l straight lines (arising from $\mathcal{K}^l$) and a wavy line connecting f and g. Writing $\nu_l = \sum_{\bar{d}} \nu_l(\bar{d})$, where all $\bar{d}$ in the sum include the fixed points f and g, we have $\alpha_l = \sum_{\bar{d}} \alpha_l(\bar{d})$, with

$$\alpha_l(\bar{d}) = \nu_l(\bar{d}) - \sum_{k=1}^{l-1} \binom{l}{k} \sum_{\bar{d}_a, d_b}{}' \alpha_k(\bar{d}_a)\mu_{l-k}(d_b), \quad (3)$$

as may be proved from (2) by induction. The restricted summation $\sum'$ is over all partitions of $\bar{d}$ into diagrams $\bar{d}_a, d_b$ such that the sum $\bar{d}_a + d_b = \bar{d}$. Equations (2) and (3) are of general validity and, to the best of our knowledge, are new. Henceforth, we specialize to the classical Heisenberg model.

There are three simplifying aspects to the classical calculation.

(i) The requisite traces[3] (or averages) become integrals and may be evaluated in a tractable closed form.

(ii) The number of diagrams is reduced by roughly an order of magnitude,[13] for one can ignore all noncontinuous paths[14] and trees. By standard definition a tree, $\bar{d} = \bar{d}_1 + d_2$, may be partitioned into two diagrams $\bar{d}_1$ and d_2 connected to each other only at one vertex, an "articulation point" (see Fig. 1). Now by induction one can prove from (3) that $\alpha_l(\bar{d}) = 0$ for trees and disconnected diagrams $\bar{d}$, provided we first show that $\langle \bar{d} \rangle = \langle \bar{d}_1 \rangle \langle d_2 \rangle$.[15] This "factorization" is apparent for $\bar{d}$ disconnected; for trees a proof is required. Let vertices $1, \cdots, p_1$ be in $\bar{d}_1$; $p_1+1, \cdots, p_1+p_2$ be in d_2; and vertex o be the articulation point which is common to both. We then have

$$\langle \bar{d} \rangle = \int \frac{d\Omega_o}{4\pi} \frac{d\Omega_1}{4\pi} \cdots \frac{d\Omega_{p_1+p_2}}{4\pi} I(\{\vec{S}_i \cdot \vec{S}_j\}),$$

where $I(\{\vec{S}_i \cdot \vec{S}_j\})$ is a product with the appropriate $\vec{S}_i \cdot \vec{S}_j$ as factors and i, j are either both in $\bar{d}_1$ or both in d_2. Hence $I = I_1 I_2$, where I_1 and I_2 represent the same integrands as in $\langle \bar{d}_1 \rangle$ and $\langle d_2 \rangle$, respectively. Finally, because of isotropy, the integral over all spins $\vec{S}_i$ except $\vec{S}_o$ is independent of the orientation of $\vec{S}_o$. Therefore the above integral factors into $\langle \bar{d}_1 \rangle \langle d_2 \rangle$. This simplification of being able to ignore the trees does not exist for the general spin Ising model ($S > \frac{1}{2}$) so that commutativity alone is not sufficient.[16]

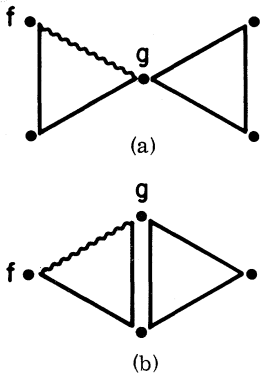

FIG. 1. Diagram (a) is a tree; diagram (b) is not. Both are continuous paths.

(iii) All of the different products ΠO_{ij} corresponding to the same diagram are equal, so that the summation over all permutations of the O_{ij} may be replaced by a simple multiplicative factor, $P(d)$. To illustrate the import of this simplification, we note that 10-line diagrams (which are necessary to extend the calculation by three terms) give rise to as many as 350 000 separate averages—each of which would have to be evaluated individually for the RW quantum-mechanical calculation!

In summary, then, we have seen that the actual effort to extend the high-temperature expansion for general spin is enormously simplified in going to the classical model. Indeed, the classical calculation for the simple models through order six required only a few days, as compared to the several years which were necessary for the corresponding quantum-mechanical calculation. Nonetheless, the labor in adding just one more term to the classical series is still considerably greater than the work in calculating all the previous terms. We have begun extending the calculation of both χ and C for the simple lattices and the results, together with their analysis, will be published elsewhere.

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[1]The classical Heisenberg magnet has been defined by H. A. Brown and J. M. Luttinger [Phys. Rev. 100, 685 (1955)] as the one for which the spin operators in the Heisenberg model are replaced by classical vectors of length $[S(S+1)]^{1/2}$. They observed that the coefficients in the high-T expansion for this classical model can be obtained asymptotically as $S \to \infty$ in the quantum-mechanical model.

[2]"The labour of calculating just one more term in the series is considerably greater than the labour of calcu-

lating all the previous terms." P. J. Wood, thesis, King's College, Newcastle-upon-Tyne, 1958 (unpublished).

[3]G. S. Rushbrooke and P. J. Wood, Mol. Phys. 1, 257 (1958), hereafter referred to as RW.

[4]J. Gammel, W. Marshall, and L. Morgan, Proc. Roy. Soc. (London) 275, 257 (1963).

[5]N. Menyuk, K. Dwight, R. J. Arnott, and A. Wold, J. Appl. Phys. 37, 1387 (1966).

[6]Six terms in χ were calculated using Ref. 3 by K. Dwight, N. Menyuk, and H. E. Stanley (unpublished), and by P. J. Wojtowicz [see P. K. Baltzer, H. W. Lehmann, and M. Robbins, Phys. Rev. Letters 15, 531 (1965)].

[7]T. A. Kaplan, H. E. Stanley, K. Dwight, and N. Menyuk, J. Appl. Phys. 36, 1129 (1965); and unpublished.

[8]K. Dwight, T. A. Kaplan, H. E. Stanley, and N. Menyuk, MIT Lincoln Laboratory Solid State Research Report No. 4, 1964 (unpublished); and unpublished.

[9]C. Domb and M. F. Sykes, Phys. Rev. 128, 168 (1962).

[10]G. A. Baker, H. E. Gilbert, J. Eve, and G. S. Rushbrooke, Phys. Letters 20, 146 (1966), and references contained therein.

[11]The zero-field thermodynamic functions (e.g., free energy, entropy, C and χ) follow directly from the correlation function. One advantage (over the RW method) of the formulation in terms of the correlation function is that both C and χ can be obtained from the same diagrammatic calculation. Furthermore there is additional physical information contained in the correlation function (see, e.g., Ref. 7).

[12]This is simply proved by multiplying both sides of (1) by $\mathrm{tr}\exp(-\beta\mathcal{H})$ and expanding everything in powers of β. The "recursion relation" (2) was first pointed out by K. Dwight (private communication).

[13]For example, there are only 1,1,2,2,5,7,17,27 classical diagrams of l straight lines ($l=2,3,\cdots,9$, respectively) as against 1,2,4,8,23,53,>150,>450 corresponding quantum-mechanical diagrams. Furthermore, RW required correspondingly 1,2,5,10,31,71, >200,>600 diagrams, because disconnected diagrams contribute to their moment expansion, and not to our Eq. (3); see Ref. 15.

[14]A continuous path is one which can be entirely traced out (using every straight line exactly once) from vertex f to vertex g without lifting one's pencil from the paper. This implies that a noncontinuous path has at least one "odd vertex"—i.e., a vertex at which an odd number of lines meet. The odd vertex will contribute an odd number of spin vectors to the integrand of $\nu_l(\vec{d})$, so that $\nu_l(\vec{d})=0$. Similarly, $\mu_l(d)=0$ for d noncontinuous, so that from (3) it is easy to see that $\alpha_l(\vec{d})=0$.

[15]Since even quantum-mechanically the factorization $\langle\vec{d}\rangle=\langle\vec{d}_1\rangle\langle d_2\rangle$ occurs for $\vec{d}$ disconnected, we have used the same inductive argument to prove for the quantum-mechanical Heisenberg model the "linked cluster" theorem, $\alpha_l(\vec{d})=0$ for disconnected $\vec{d}$. (A disconnected diagram is a diagram which has parts not connected to each other by any lines.)

[16]That trees can be ignored classically may appear to be merely a special case of F. Englert's result [Phys. Rev. 129, 567 (1963)] that trees ("reducible diagrams") may also be ignored for the quantum-mechanical calculation and for the general spin Ising model. However, our diagrammatic representation (which is more akin to that of RW) is essentially different from Englert's.