THEORY AND CALCULATIONS FOR A SPIN GLASS

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We obtain the properties of a mean-field spin-glass (in which the bonds connecting each spin to every other spin are "frozen-in" with random signs), by locating the zeros of the partition function in the complex T plane. For $N = 5$ and 9 spins, we obtain the relevant polynomials and zeros explicitly, and the resulting thermodynamic properties (free energy, specific heat, magnetic susceptibility, etc.). We then analyze the properties of such a system in the thermodynamic limit $N \to \infty$, where it is impossible to obtain the polynomials directly but where the presumed location of the zeros can be usefully construed. In this limit, the thermodynamic functions are obtainable as functions of the distribution functions of monopoles, quadrupoles, and possibly higher-order poles.

Despite a decade of activity in the subject, the topic of mean-field spin glasses is still very controversial. In a recent review, Chowdhury and Mookerjee [1] list some 750 papers on the topic, while commenting (p. 18): "In this field of research ... theory is lagging far behind experimental developments." In the present paper, we present details of an approach which, in our estimation, may remedy this situation. This approach is designed to provide a convenient basis for the theoretical understanding of a number of popular Ising-spin glass models, and in principle, can be readily generalized to obtain the statistical mechanics of many other systems with quenched-in disorder. We apply it here, to a variant of the Sherrington–Kirkpatrick [2,3] mean-field model of Ising-spin glasses (a model which is "canonically simple" yet has remained quite intractable). The outlines of our theory were previously drawn in quite general terms, in ref. [4] (denoted I) emphasizing the analogy between the free energy of a disordered system and the electrostatic potential of a continuous charge distribution in two dimensions. The present work (II) contains some (rigorous) calculations and observations on $N = 5$ and 9 spins, and a preliminary (speculative) treatment of the thermodynamic limit $N \to \infty$.

The method is based on the observation that in ordered systems (ordinary Ising models, for example) the partition function is a polynomial, the zeros of which lie predominantly on simple trajectories as they approach the real cut in the complex T plane; whereas in systems with quenched-in disorder, the zeros are generally distributed in areas near the real cut in the complex T plane. Each random ensemble is thus characterized by a quite specific two-dimensional distribution function, ρ, from which all thermodynamic properties may be calculated without Monte Carlo methods. Given the probability distribution characterizing a given random system, it becomes the task of theory to obtain ρ for this system. Unfortunately, ρ becomes continuous only in the thermodynamic limit. Thus, however detailed our numerical experiments on finite systems may seem, they still have to be complemented by conjectures relating to the appropriate behavior in the ultimate limit, $N \to \infty$.

Let us denote a particular frozen-in configuration of bonds α, and the relevant Sherrington–Kirkpatrick-

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type hamiltonian H_α:

$$H_\alpha = -(J/2N^{1/2}) \sum_{i}^{N}\sum_{j=1}^{N} \epsilon_{ij} S_i S_j$$

$$(\text{each } S_i = \pm 1, \text{ each } \epsilon_{ij} = \pm 1). \qquad (1)$$

As there are $N(N-1)/2$ bonds, there are $2^{N(N-1)/2}$ distinct configurations in the set $\{\alpha\}$ [‡1]. We denote an average over these by $\langle\ \rangle_\alpha$. The free energy is just:

$$F = \langle F_\alpha \rangle_\alpha , \qquad (2)$$

where, with $\beta = 1/T$ in the units $k = 1$ and $F^{(0)}$ common to all α,

$$F_\alpha \equiv -T \ln(\mathrm{Tr}\{\exp -\beta H_\alpha\}) = F^{(0)} + F_\alpha^{(1)}$$

$$= -NT \ln 2 - N(N-1)(T/2)$$

$$\times \ln[\cosh(\beta J/N^{1/2})] + F_\alpha^{(1)} , \qquad (3)$$

with $F_\alpha^{(1)} \equiv -T \ln P_\alpha(t)$ the nontrivial contribution. The polynomial P_α can be evaluated as follows:

$$P_\alpha(t) = \langle 0 | \Pi(1 + t\epsilon_{ij} S_i^x S_j^x) | 0 \rangle$$

$$= 1 + t^3 \sum\sum\sum \epsilon_{ij}\epsilon_{jk}\epsilon_{ki} + \ldots = \sum a_n t^n , \qquad (4)$$

where $|0\rangle$ is the state of all spins "up" and $S_i^x = S_i^+ + S_i^-$ is a Pauli matrix. The variable $t = \tanh(\beta J/N^{1/2})$ is real, and ranges from 1 (at $T = 0$) to 0 (as $T \to \infty$.) We also wish to consider a variable $z \equiv t + iy = r \exp i\theta$, and $N(N-1)/2$ zeros of the polynomial (4), which lie at the points $z_j^{(\alpha)}$ (not necessarily all distinct) in the z-plane. In terms of such zeros, $\ln P_\alpha$ can conveniently be written:

$$\ln P_\alpha(t) = \sum_{j=1}^{N(N-1)/2} \ln(z_j^{(\alpha)} - t)$$

$$= \sum_{j=1}^{N(N-1)/2} \ln(1 - t/z_j^{(\alpha)}) . \qquad (5)$$

We note that $a_0 = 1$ in ( ), hence $\Pi z_j^{(\alpha)} = 1$, for any α. Other properties which can be inferred from (4), which are satisfied by the z_j for any α, include the fact that roots occur in complex pairs z_j and z_j^* and never lie on the real cut $y = 0$, $0 \leqslant t < 1$; as well as the sum rules:

$$a_1 = 0 \Rightarrow \sum_j 1/z_j = 0,$$

$$a_2 = 0 \Rightarrow \sum\sum_{j<k} 1/z_j z_k = 0 . \qquad (6)$$

In fact, the systematic evaluation of (4) is highly nontrivial when $N \gg 1$. Each coefficient can be expressed graphically. The numerical evaluation of the relevant graphs involves the concept of even graphs [5] and of signed graphs [6]. For 5 spins, the 1024 possible polynomials reduce to 7 distinct equivalence classes. We give the coefficients a_n and also indicate the symmetry class and weight (W) of each, in table 1. The first polynomial (labeled F) results from the purely ferromagnetic case, all $\epsilon = +1$, and from 15 other arrangements which can be transformed into the ferromagnet by "gauge" transformations of some $S_i \to -S_i$

[‡1] If we adopted a gaussian distribution of ϵ's instead, the number of configurations would always be ∞, regardless of N.

Table 1
5 spins, 1024 polynomials. The label indicates special cases: F, AF, and SR (see text for definitions); W (weight) indicates the number (out of 1024) of equivalent polynomials.

a_0	a_1	a_2	a_3	a_4	a_5	a_6	a_7	a_8	a_9	a_{10}	W	label
1	0	0	10	15	12	15	10	0	0	1	16	F
1	0	0	−10	15	−12	15	−10	0	0	1	16	AF
1	0	0	4	3	0	−3	−4	0	0	−1	160	–
1	0	0	−4	3	0	−3	4	0	0	−1	160	–
1	0	0	2	−1	−4	−1	2	0	0	1	240	–
1	0	0	−2	−1	4	−1	−2	0	0	1	240	–
1	0	0	0	−5	0	5	0	0	0	−1	192	SR

(N.B.: in the absence of external fields, gauge transformations cannot affect the partition function, which involves taking traces over all the spins); it therefore has weight 16. The second, (AF), consists of all antiferromagnetic bonds (plus the 15 configurations which differ from this by gauge transformations.)

The particular configurations of all $\epsilon > 0$ (long-range ferromagnet) or all $\epsilon < 0$ ("fully-frustrated long-ranged model") have previously been studied in some detail, in a precursor work [7]. The weight of the AF polynomial is also 16, as indicated in table 1.

The last, or SR (special random) configurations, are microscopically – archetypally – spin glasses. In an SR model, precisely half the bonds connecting each spin to the others are +, and half are –. Counting all configurations which are related to the SR model by a gauge transformation, there are 192 SR configurations (or configurations which differ from the SR type by a gauge transformation), comprising roughly 1/5 of the total 1024 configurations. The remaining 4 equivalence classes in table 1 are nondescript, and unlabeled.

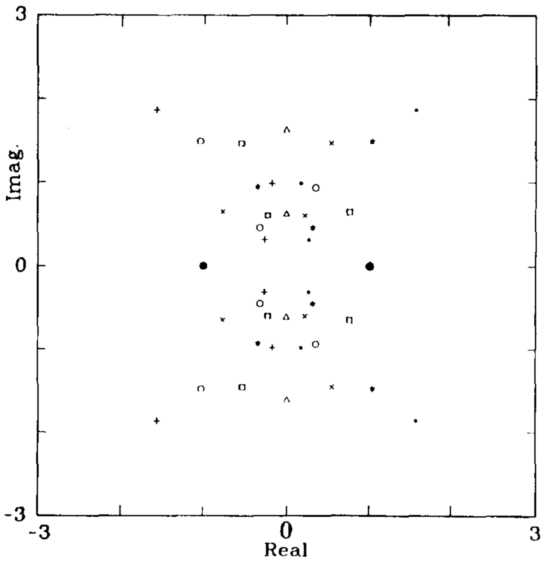

Fig. 1. $N = 5$, all configurations, "complex t plane". The origins of the 70 zeros as shown: • F (first polynomial in table 1), + AF (second polynomial), * third polynomial, o fourth polyn., X fifth polyn., □ sixth polyn., Δ SR (last polyn.). The zeros at $z = \pm 1$ ("delta points") are shown as ●. Note: taken as a whole, the zeros are distributed symmetrically about the real and imaginary axes; this is also a property of the zeros of the seventh polynomial (SR model) alone.

With 10 roots each, the 7 distinct polynomials generate 70 zeros. However, not all are distinct. Two important points of accumulation are $y = 0$, $t = \pm 1$, which we denote the "delta points". The location of zeros is shown in fig. 1.

We now turn to $N = 9$ spins. The total number of configurations is large, $2^{36} \approx 10^{11}$, although the number of distinct equivalence classes, or polynomials, is surely far smaller. We have found it possible to obtain all the polynomials corresponding to the 16 distinct SR classes. They are reproduced in table 2.

As the relative weights of all 16 SR polynomials are equal, they are not indicated in the table. Of 36 X 16 = 576 zeros, not all are distinct, with 320 accumulating at the delta points (the remainder being distributed as in fig. 2). The polynomials for configurations which do not satisfy the SR condition are more numerous and more difficult to obtain. But it seems reasonable that the relative fluctuations in the number of ± bonds at each spin, which when averaged over all conceivable configurations are $O((N-1)^{-1/2})$, become irrelevant for $N \gg 9$, so that the SR model is representative of all variants of the Sherrington–

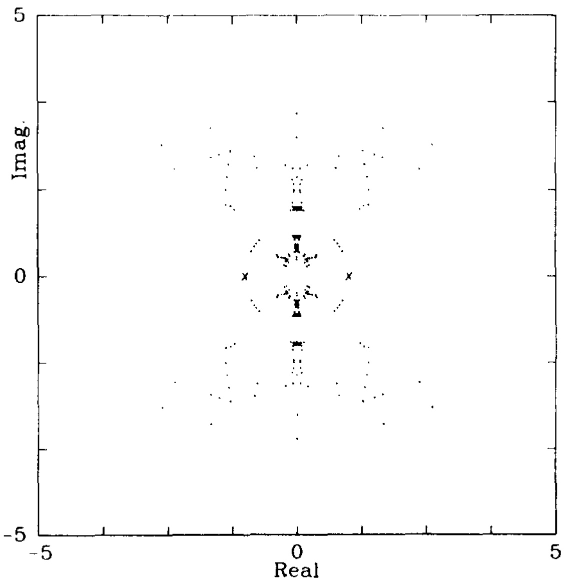

Fig. 2. $N = 9$, 576 zeros of SR model (accumulations at $z = \pm 1$ shown as X) Note: (a) a number of points are precisely on unit circle; (b) each point z_j within unit circle is matched by a point $1/z_j$ outside; (c) symmetry of distribution about real and imaginary axes.

Table 2
9 spins, SR model; 16 distinct polynomials. Coefficients listed in order: $a_0, ..., a_{18}$; ($a_{36-n} = a_n$ here).

(1)	1	0	0	−32	74	−160	562	−992	607	928
	−4588	8672	−5091	−7328	17902	−20192	8505	19104	−35944	
(2)	1	0	0	0	42	0	−270	0	255	0
	1428	0	−3843	0	1326	0	7641	0	−13160	
(3)	1	0	0	−8	18	24	−126	72	−9	−408
	1332	504	−2907	408	414	−1528	6993	936	−11432	
(4)	1	0	0	−16	42	−80	242	−496	255	464
	−1644	4336	−3843	−3664	9006	−10096	7641	9552	−23400	
(5)	1	0	0	−16	−6	48	18	144	−273	−816
	1236	1008	−1971	816	−498	−3056	6345	1872	−9704	
(6)	1	0	0	−24	18	72	−126	216	−9	−1224
	1332	1512	−2907	1224	414	−4584	6993	2808	−11432	
(7)	1	0	0	−8	2	24	−30	72	−185	−408
	1268	504	−2283	408	−194	−1528	6561	936	−10280	
(8)	1	0	0	0	10	0	−78	0	−97	0
	1300	0	−2595	0	110	0	6777	0	−10856	
(9)	1	0	0	8	18	−24	−126	−72	−9	408
	1332	−504	−2907	−408	414	1528	6993	−936	−11432	
(10)	1	0	0	8	2	−24	−30	−72	−185	408
	1268	−504	−2283	−408	−194	1528	6561	−936	−10280	
(11)	1	0	0	0	−22	0	114	0	−449	0
	1172	0	−1347	0	−1106	0	5913	0	−8552	
(12)	1	0	0	16	42	80	242	496	255	−464
	−1644	−4336	−3843	3664	9006	10096	7641	−9552	−23400	
(13)	1	0	0	32	74	160	562	992	607	−928
	−4588	−8672	−5091	7328	17902	20192	8505	−19104	−35944	
(14)	1	0	0	0	−54	0	306	0	−801	0
	1044	0	−99	0	−2322	0	5049	0	−6248	
(15)	1	0	0	16	−6	−48	18	−144	−273	816
	1236	−1008	−1971	−816	−498	3056	6345	−1872	−9704	
(16)	1	0	0	24	18	−72	−126	−216	−9	1224
	1332	−1512	−2907	−1224	414	4584	6993	−2808	−11432	

Kirkpatrick mean-field model. Assuming that *is* the archetype spin glass, we are presently preparing for the (nontrivial) study of 13 spins in the SR model (involving already O(100) distinct polynomials, each with 78 roots).

Fig. 3 is a very sensitive test of convergence, as it involves a second derivative of F. It shows the specific heat obtained after averaging on all configurations ($N = 5$) and in the SR model ($N = 5$ and 9).

Fig. 4 shows the convergence of the harmonic series introduced in our earlier paper [4]. Calculated with the help of the polynomials in table 2 for 9 spins, it shows the contribution of the high-temperature terms $F^{(0)}$, of the delta-points, and of the $m = 0$ and $m = 2$ harmonics to the total free energy. Our numerical studies suggest that the individual contributions of $m = 4, 6, ...$ are all small and tend to cancel. If this trend persisted at large N, we would need know only the fraction of zeros at the delta-points and the distribution functions $R_0(r)$ and $R_2(r)$ in order to have com-

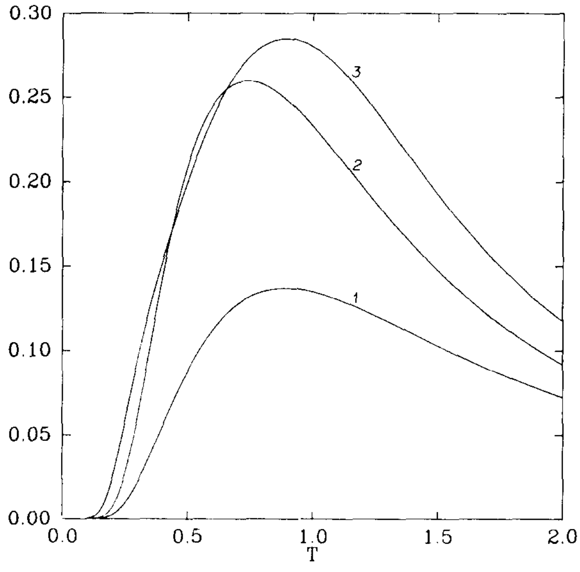

Fig. 3. Specific heat (C/Nk) versus T (in units of J). Curve 1 is $N = 5$, SR model; curve 2 $N = 5$, all configurations; curve 3, $N = 9$ SR model.

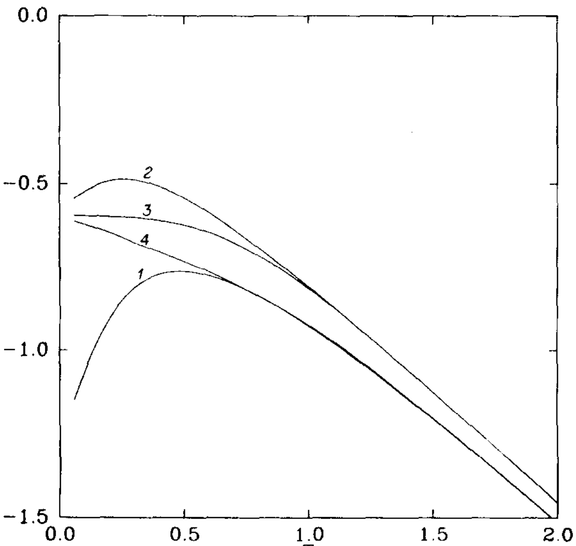

Fig. 4. Free energy per spin (F/N) versus T (units of J), $N = 9$ SR model. Curve 1 is $F^{(0)}$, curve 2 is $F^{(0)} + F^{(\delta)}$, curve 3 includes monopoles, is $F^{(0)} + F^{(\delta)} + F_0^{(1)}$. Curve 4 includes quadrupole distribution as well, and is $F^{(0)} + F^{(\delta)} + F_0^{(1)} + F_2^{(1)}$. The exact F, as calculated with the aid of table 2, is indistinguishable from curve 4 on this scale, hence is not displayed separately.

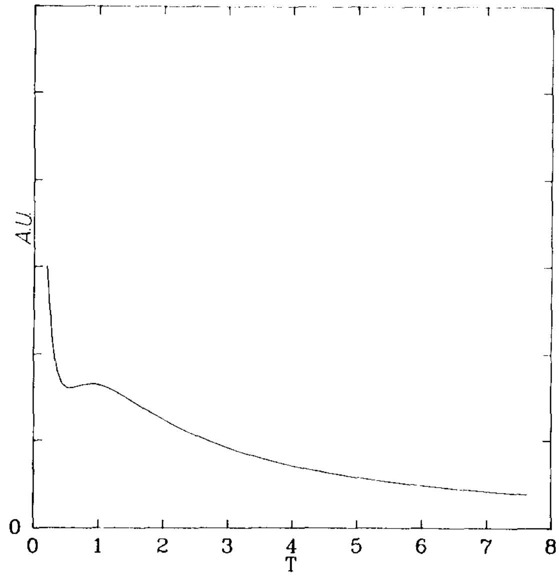

Fig. 5. Paramagnetic susceptibility χ_0 (au) versus T (units of J) in SR model, $N = 5$.

plete information concerning the spin glass in the absence of external fields. We return to these points below.

Fig. 5 shows the zero-field magnetic susceptibility χ_0 in the SR model, obtained for $N = 5$.

We now turn to some observations and conjectures on the thermodynamic limit. All $N(N-1)/2$ zeros lie between two concentric circles, one at $r = t_c$ (<1) and the other at $1/t_c$. A fraction f_δ of them are at the delta-points, half at $z = +1$ and half at -1, while the remainder are expected to become continuously distributed as $N \to \infty$. We therefore introduce a distribution function $\rho(z)$ (also denoted $\rho(r,\theta)$),

$$\rho(z) = (2/N^2) \langle \Sigma_j \delta(z - z_j^{(\alpha)}) \rangle_\alpha \,. \tag{7}$$

For purposes of normalization, the factor $(2/N^2)$ here differs from that chosen in 1. The two-dimensional character of ρ comes principally from $\langle\ \rangle_\alpha$ which superposes a great many distinct trajectories (or even areas) of zeros. Roots at the delta-points $z_j = \pm 1$ are specifically excluded from ρ, and are treated separately. We note that ρ contains all the information concerning the thermal properties at $T \leqslant T_c$ and the phase transition at T_c. We return to this point shortly.

The nontrivial part of the free energy has been defined as $F^{(1)}$,

$$F^{(1)} = -(N^2T/4)\int \mathrm{d}r\, r \int \mathrm{d}\theta\, \rho(r,\theta)$$
$$\times \ln[1 + (t/r)^2 - 2(t/r)\cos\theta] + F^{\delta}\,, \qquad (8)$$

with the vanishing of ρ outside the range $t_c \leqslant r \leqslant t_c^{-1}$ determining the range of integration. As in I, the multipole distribution functions are the coefficients in a Fourier series:

$$\rho(r,\theta) \equiv r^{-2}\left(R_0(r) + \sum_{m\geqslant 1} R_m(r)\cos m\theta\right)\,. \qquad (9)$$

At high temperature ($t < t_c$) the expansion (9) gives the following appearance to $F^{(1)}$:

$$F^{(1)} = (N^2T\pi/2)\sum_{m=0}^{\infty} C_m t^m$$
$$+ f_\delta N(N-1)T\ln[\cosh(\beta J/\sqrt{N})]\,, \qquad (10)$$

i.e.

$$F^{(1)} = \sum F_m^{(1)} + F^{(\delta)}\,,$$

with

$$C_0 = 0, \quad C_m = (1/m)\int \mathrm{d}r\, r^{-(m+1)}R_m(r)\,, \qquad (11)$$

the integration being from t_c to $1/t_c$. In the absence of ferromagnetic or antiferromagnetic bias ρ is an even function of J, hence all odd harmonics vanish ($R_{2n+1} \equiv 0$). As R_0 does not even appear in the high-temperature expansion (thus, $C_0 \equiv 0$), the series in (10) effectively starts at $m = 2$ and contains only even harmonics $m = 4, 6, \ldots$. The aspect of $F_4^{(1)}$ is typical of all $m > 2$:

$$F_4^{(1)} = [(\pi/2)N^2Tt^4]\,C_4\,. \qquad (12)$$

If C_4 is $O(1)$, $F_4^{(1)}$ will fail to be extensive. There is reason to believe this is the case, using arguments which are extraneous to the present theory: the replica method used in the original treatments of the method yielded an exact high-temperature result, which coincides precisely with the present $F^{(0)}$ [3] implying $F^{(1)} \equiv 0$ for $T > T_c$. The cumulant expansion offers an independent means of expressing the free energy directly [8,9]. Upon averaging over configurations, it too yields a result which coincides perfectly with $F^{(0)}$ in the thermodynamic limit ‡2. Thus, above T_c the coefficients of all powers of T in the expansion of $F^{(1)}$ must vanish $O(N)$, and $F_m^{(1)} \equiv 0$ for $m > 2$. At $m = 2$, this requires a cancellation between $F_2^{(1)}$ and $F^{(\delta)}$:

$$F_2^{(1)} + F^{(\delta)} = 0\,, \quad \text{i.e.} \quad \pi C_2 + f_\delta = 0\,. \qquad (13)$$

As R_0 is the angular average of a nonnegative quantity, it too must be nonnegative. On the other hand, (13) requires C_2 to be negative, so that $R_2(r)$ must be negative over some range of r ‡3.

For $T \leqslant T_c$, the expansion of (8) yields $F^{(1)}$:

$$F^{(1)} = -TN^2\pi\int_{t_c}^{t} \mathrm{d}r\, r^{-1}R_0(r)\ln(t/r) + \sum_{m\geqslant 2}\Phi_m\,, \qquad (14)$$

where we have made use of (13) to eliminate $F^{(\delta)}$. The quantities Φ_m are the low-temperature versions of the $F_m^{(1)}$, and for $m \geqslant 2$, are given by:

$$\Phi_m = TN^2(\pi/2m)\int_{t_c}^{t} \mathrm{d}r\, r^{-1}R_m(r)\,[(r/t)^m - (t/r)^m]\,. \qquad (15)$$

We have made use of the additional information, $F_m^{(1)} \equiv 0$, and of (13), in deriving (15). We can now define Φ_0 by extension, as the integral involving R_0 in (14), and replace (14) by the somewhat more elegant form: $F^{(1)} = \Sigma\Phi_m$ (the sum now being over all $m \geqslant 0$). For each Φ_m, we need know the distribution function R_m only on the interval $t_c \leqslant r \leqslant t$ ‡4.

In summary: Although the calculation of thermodynamic data from the zeros of the partition function

‡2 This observation alone is tantamount to a proof that there is a phase transition at a finite T_c! The argument is as follows: $F^{(0)}$ is singular at low T, therefore F cannot be equal to $F^{(0)}$ at low T and $F^{(1)}$ must become nonzero at, or below some finite T, which we denote T_c. From this, it follows that F fails to be analytic at T_c, which locates the phase transition there. (Additionally, $F^{(1)}$ must have singularities which, at low T, cancel those of $F^{(0)}$ precisely.)

‡3 Our numerical results so far (9 spins, SR model) show R_0 to be positive and R_2 to be negative over the entire interval $t_c \leqslant r \leqslant 1/t_c$. R_4, R_6 ... are much smaller than the preceding, and oscillate in sign, while all odd moments vanish identically. These findings are in agreement with the general considerations in the text and with the rapid convergence of the harmonic series, exhibited in fig. 4.

‡4 Thus justifying the cryptic claim in I, that the zeros at $r > 1$ do not contribute to F. (Note that the r.h.s. of eq. (10a) of I should be multiplied by 2.)

in the complex T plane is unnecessarily complicated and impractical in problems where other methods work adequately (e.g. for the 2D nearest-neighbor Ising model), the study of the zeros seems quite appropriate in the study of random system. What appears to be the generic difficulty of random ensembles (that it is F_α and not Z_α which must be averaged over configurations α) is easily surmounted, upon noting that such averaging causes trajectories of zeros to be smeared, and then applying an appropriate analysis.

In future work (III) we intend to examine plausible forms of the R_m (compatible with the normalization implied by (7)) and their resulting low-temperature and critical properties.

The magnetic properties are obtainable by calculating the shift in the zeros in the presence of an external field. We shall wish to examine the motion of the zeros under arbitrary external fields. Weak-field results are, however, relatively simple. Writing $z_j(h) = z_j + g(h)\,\delta z_j$ and expanding the arguments of ln( ) in eq. (5) to lowest order in $g(h)$, one finds the shift in F. The calculated zero-field susceptibility χ_0 for 5 spins (SR model) is shown in fig. 5; we intend to discuss the general case in III.

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