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Exact expressions for diagonal correlation functions in the $d=2$ Ising model

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We present exact explicit expressions for the diagonal spin-spin correlation functions $\langle \sigma_{00}\sigma_{nn} \rangle$ in the $d=2$ Ising model, in terms of elliptic integrals, for n up to 6. We also give a general structural formula for $\langle \sigma_{00}\sigma_{nn} \rangle$ and discuss its properties.

The two-dimensional Ising model remains of great importance as an interacting many-body system which is exactly soluble. Although the free energy, magnetization, and certain other thermodynamic quantities were calculated in classic papers long ago,[1-3] there remain a number of quantities which are not yet completely determined. Among the interesting objects of study in this model are the (static) spin-spin correlation functions $\langle \sigma_{00}\sigma_{mn} \rangle$.[4-6] Recently, we presented a new method for calculating high- and low-temperature series expansions for the diagonal correlation functions $S_n=\langle \sigma_{00}\sigma_{nn} \rangle$.[7] In the course of this work we found that explicit analytic expressions for these correlation functions had not been published, except for the case $n=1$.[3-5] Thus S_2 was recently calculated.[7,9]

Here we present a general structural formula for the S_n expressed directly in terms of elliptic integrals. We also give explicit expressions for the S_n, for $n \le 6$.[8] The method of calculation is based on the formulation of these correlation functions in terms of Toeplitz determinants.[1,3,5]

To fix conventions for the exchange constants $J_{1,2}$ we exhibit our form for the Hamiltonian of the $d=2$ Ising model:

$$H=-\sum_{(j,k)\in \mathbb{Z}^2}(J_1\sigma_{j,k}\sigma_{j+1,k}+J_2\sigma_{j,k}\sigma_{j,k+1}) \tag{1}$$

Further, let $\beta=(k_BT)^{-1}$ and define

$$k_> = \sinh(2\beta J_1)\sinh(2\beta J_2) \tag{2}$$

applicable for $T>T_c$, and

$$k_< = k_>^{-1} \tag{3}$$

applicable for $T<T_c$, where T_c is the critical temperature of the model, given by

$$k_>(\beta_c)=k_<(\beta_c)=1 \; . \tag{4}$$

Since the S_n have different expressions for $T>T_c$ and $T<T_c$, it is convenient to use the notation $S_{n,+}$ and $S_{n,-}$ for these two respective temperature regimes.

Since $\langle \sigma_{00},\sigma_{m,n} \rangle = \langle \sigma_{00}\sigma_{-m,-n} \rangle$, we can take $n \ge 0$ in $\langle \sigma_{00}\sigma_{nn} \rangle$ with no loss of generality and will do so henceforth. Recall that $S_0=1$. For $n>1$, S_n can be expressed in terms of a Toeplitz determinant as[1,3,5]

$$S_n=\begin{vmatrix} a_0 & a_{-1} & \cdots & a_{-n+1} \\ a_1 & a_0 & \cdots & a_{-n+2} \\ \vdots & & & \\ a_{n-1} & & \cdots & a_0 \end{vmatrix} \, , \tag{5}$$

where

$$a_n=\frac{1}{2\pi}\int_0^{2\pi} d\theta\, e^{-in\theta}\varphi(\theta) \tag{6}$$

and

$$\varphi(\theta)=\left[\frac{k_>-e^{-i\theta}}{k_>-e^{i\theta}}\right]^{1/2} . \tag{7}$$

The point of our analysis is to use (5)—essentially a sum of products of integral representations—to calculate explicit expressions for the S_n, and then to determine the general structural form of these expressions.

We find that the S_n have the following general form

$$S_{n,\pm}=A_n\pi^{-n}k^{\{-2p_n-[1-(-1)^n]\Theta(T-T_c)/2\}} \times \sum_{l=0}^{n}\mathscr{P}^{(n,\pm)}_{n-l,l}(k^2-1)^{[l+\delta_{l,1}\Theta(T_c-T)]} \times [E(k)]^{n-l}[K(k)]^l \, , \tag{8}$$

where $k=k_>$ and $k=k_<$ for $S_{n,+}$ and $S_{n,-}$, respectively; $\Theta(x)=0$ for $x\le 0$ and 1 for $x>0$; $\delta_{i,j}$ is the Kronecker delta function; and $K(k)$ and $E(k)$ are the complete elliptic integrals of the first and second kinds, respectively. In (8), $A_n\in\mathbb{Q}$, p_n is a positive-semidefinite integer, and $\mathscr{P}^{(n,\pm)}_{n-l,l}$ is a polynomial in k^2. Since $K(k)$ and $E(k)$ also depend only on k^2, the summand in (8) is a function only of k^2. It follows that $S_{n,+}$ is an even (odd) function of $k_>$ for even (odd) n, whereas $S_{n,-}$ is an even function of $k_<$ for all n.

We shall now derive some general properties of (8). First, as $T\to\infty$, the system becomes completely disordered and $\langle \sigma_{00}\sigma_{mn} \rangle \to \delta_{m,0}\delta_{n,0}$. Since $S_{n,+}\sim O(k_>^n)$ in this limit, the summand in (8) must vanish like $k_>^{\{n+2p_n+(1/2)[1-(-1)^n]\}}$ as $T\to\infty$. It follows, in particular, that

$$\sum_{l=0}^{n}(-1)^l\mathscr{P}_{n-l,l}^{(n,+)}(0)=0 \tag{9}$$

Next as $T\to 0$, the lattice becomes completely ordered and $\langle\sigma_{00}\sigma_{mn}\rangle\to 1$. Consequently the summand of (8) must vanish like $k_<^{2p_n}$ and hence, in particular,

$$\sum_{l=0}^{n}(-1)^{l+\delta_{l,1}}\mathscr{P}_{n-l,l}^{(n,-)}(0)=0 \tag{10}$$

Finally, as $T\to T_c$, since $\langle\sigma_{00}\sigma_{mn}\rangle$ is a continuous function of T,

$$S_{n,+}(k_>=1)=S_{n,-}(k_<=1)\ , \tag{11}$$

which implies that

$$\mathscr{P}_{n,0}^{(n,+)}(1)=\mathscr{P}_{n,0}^{(n,-)}(1) \tag{12}$$

There is, of course, no analogous equality between $\mathscr{P}_{n-l,l}^{(n,+)}(1)$ and $\mathscr{P}_{n-l,l}^{(n,-)}(1)$ for $l\neq 0$, because these terms are annihilated by the $(k^2-1)^{[l+\delta_{l,1}\Theta(T_c-T)]}$ factor.] Writing

$$\left.\begin{matrix}\mathscr{P}_{n,0}^{(n,+)}\\ \mathscr{P}_{n,0}^{(n,-)}\end{matrix}\right\}=\sum_{j=0}^{j_{\max}(n)}\left\{\begin{matrix}c_j^{(n,+)}k_>^{2j}\\ c_j^{(n,-)}k_<^{2j}\end{matrix}\right. , \tag{13}$$

we find that

$$c_j^{(n,+)}=c_{j_{\max}(n)-j}^{(n,-)} \tag{14}$$

so that the equality equivalent to (12) and (13),

$$\sum_{j=0}^{j_{\max}(n)}c_j^{(n,+)}=\sum_{j=0}^{j_{\max}(n)}c_j^{(n,-1)}\ , \tag{15}$$

is actually met in the special manner implied by (14), i.e., there is a one-to-one equality between the individual terms on the left-hand side of (15) and the reordered terms in the right-hand side of (15). Further, using the known value

$$S_n(T_c)=\left[\frac{2}{\pi}\right]^n\prod_{l=1}^{n}\left[1-\frac{1}{4l^2}\right]^{l-n}\ ,\quad n\geq 1 \tag{16}$$

we find that

$$A_n\mathscr{P}_{n,0}^{(n,\pm)}(1)=2^n\prod_{l=1}^{n}\left[1-\frac{1}{4l^2}\right]^{l-n}\ ,\quad n\geq 1\ . \tag{17}$$

An interesting feature of S_n is that although it is continuous for all T, its derivative with respect to temperature is logarithmically divergent at $T=T_c$. Thus, one knows that

$$S_n(T)\to S_n(T_c)+b_n(T-T_c)\ln|T-T_c|\quad\text{as } T\to T_c \tag{18}$$

plus higher order terms, where $b_n>0$ from the general inequality

$$S_n(T_1)<S_n(T_2)\ \text{ if and only if } T_1>T_2\ . \tag{19}$$

To our knowledge, the value of b_n has not previously been calculated. From (8), we find that it is actually proportional to $S_n(T_c)$:

TABLE I. Values of the A_n for $1\leq n\leq 6$.

n	A_n
1	2
2	$\frac{2^2}{3}$
3	$\frac{2^5}{3^3\times 5}$
4	$\frac{2^8}{3^4\times 5^3\times 7}$
5	$\frac{2^{13}}{3^6\times 5^5\times 7^3}$
6	$\frac{2^{18}}{3^9\times 5^6\times 7^5\times 11}$

$$b_n=n\beta_c^2[J_1\coth(2\beta_cJ_1)+J_2\coth(2\beta_cJ_2)]\,k_BS_n(T_c)\ . \tag{20}$$

Further, we find that the leading singular corrections to (18) are of the form

$$(T-T_c)^2\ln^2|T-T_c|+\cdots\ ,$$

so that, for example, the curvature $d^2S_n(T)/dT^2$ diverges like $-b_n/(T-T_c)$ as $T\to T_c$.

In passing, we recall that one might be tempted, *a priori*, to think that as $n\to\infty$, the behavior of S_n near T_c would be the same as that of the square of the magnetization, since

$$M^2=\lim_{m^2+n^2\to\infty}\langle\sigma_{00}\sigma_{mn}\rangle\ . \tag{21}$$

One would thus be led to conclude falsely that M vanishes at T_c with a critical exponent $\beta=\frac{1}{2}$ (the mean-field-theory value). The correct exponent is[2] $\beta=\frac{1}{8}$, and the fallacy in the naive approach alluded to above is that it implicitly assumes that the limits $n\to\infty$ and $T\to T_c$ commute, whereas in fact, they do not. In contrast, as was noted in Ref. 7, the low-temperature expansion for $S_{n,-}$ has a universal part up to order n in $k_<^2$, so that as $n\to\infty$, it becomes independent of n and is precisely the expansion of $(1-k_<^2)^{1/4}$. In this case one could justifiably infer the exact result for M^2 from the $n\to\infty$ form of the low-temperature expansion since the limits $n\to\infty$ and $T\to 0$ commute.

TABLE II. Values of the p_n for $1\leq n\leq 6$.

n	p_n
1	0
2	1
3	2
4	4
5	6
6	9

We proceed to give the explicit expressions for the $S_{n,\pm}$ for $n \le 4$. For completeness, the previously calculated $n=1$ and 2 cases are included. The values of A_n and p_n are listed in Tables I and II, respectively. It is convenient to define the variables

$$y_> = k_>^2 , \quad y_< = k_<^2 . \tag{22}$$

We then have the following.

$n=1$, $T>T_c$:

$$\mathscr{P}_{1,0}^{(1,+)} = 1 ,$$
$$\mathscr{P}_{0,1}^{(1,+)} = 1 ,$$

$n=1$, $T<T_c$:

$$\mathscr{P}_{1,0}^{(1,-)} = 1 ,$$
$$\mathscr{P}_{0,1}^{(1,-)} = 0 .$$

$n=2$, $T>T_c$:

$$\mathscr{P}_{2,0}^{(2,+)} = -y_> + 5 ,$$
$$\mathscr{P}_{1,1}^{(2,+)} = 8 ,$$
$$\mathscr{P}_{0,2}^{(2,+)} = 3 ,$$

$n=2$, $T<T_c$:

$$\mathscr{P}_{2,0}^{(2,-)} = 5y_< - 1 ,$$
$$\mathscr{P}_{1,1}^{(2,-)} = 2 ,$$
$$\mathscr{P}_{0,2}^{(2,-)} = -1 ;$$

$n=3$, $T>T_c$:

$$\mathscr{P}_{3,0}^{(3,+)} = -10y_>^3 - 21y_>^2 + 96y_> - 1 ,$$
$$\mathscr{P}_{2,1}^{(3,+)} = -3(y_>^3 + 3y_>^2 - 69y_> + 1) ,$$
$$\mathscr{P}_{1,2}^{(3,+)} = 3(y_>^2 + 48y_> - 1) ,$$
$$\mathscr{P}_{0,3}^{(3,+)} = 33y_> - 1 ,$$

$n=3$, $T<T_c$:

$$\mathscr{P}_{3,0}^{(3,-)} = -y_<^3 + 96y_<^2 - 21y_< - 10 ,$$
$$\mathscr{P}_{2,1}^{(3,-)} = 27(3y_< + 1) ,$$
$$\mathscr{P}_{1,2}^{(3,-)} = 6(3y_<^2 - 7y_< - 4) ,$$
$$\mathscr{P}_{0,3}^{(3,-)} = -9y_< - 7 .$$

$n=4$, $T>T_c$:

$$\mathscr{P}_{4,0}^{(4,+)} = 3y_>^6 - 1549y_>^5 - 1977y_>^4 - 5366y_>^3 + 21\,773y_>^2 - 549y_> - 47 ,$$
$$\mathscr{P}_{3,1}^{(4,+)} = -8(129y_>^5 + 134y_>^4 + 658y_>^3 - 7332y_>^2 + 245y_> + 22) ,$$
$$\mathscr{P}_{2,2}^{(4,+)} = -6(30y_>^5 - 81y_>^4 + 70y_>^3 - 9704y_>^2 + 428y_> + 41) ,$$
$$\mathscr{P}_{1,3}^{(4,+)} = 4(45y_>^4 + 111y_>^3 + 6389y_>^2 - 363y_> - 38) ,$$
$$\mathscr{P}_{0,4}^{(4,+)} = -5(9y_>^3 - 843y_>^2 + 59y_> + 7) ,$$

$n=4$, $T<T_c$:

$$\mathscr{P}_{4,0}^{(4,-)} = -47y_<^6 - 549y_<^5 + 21\,773y_<^4 - 5366y_<^3 - 1977y_<^2 - 1549y_< + 3 ,$$
$$\mathscr{P}_{3,1}^{(4,-)} = -4(3y_<^5 + 62y_<^4 - 7047y_<^3 - 2997y_<^2 - 1288y_< + 3) ,$$
$$\mathscr{P}_{2,2}^{(4,-)} = 6(3y_<^5 + 2149y_<^4 - 2804y_<^3 - 1360y_<^2 - 1063y_< + 3) ,$$
$$\mathscr{P}_{1,3}^{(4,-)} = 4(504y_<^4 - 1739y_<^3 - 975y_<^2 - 865y_< + 3) ,$$
$$\mathscr{P}_{0,4}^{(4,-)} = -1011y_<^3 - 599y_<^2 - 697y_< + 3 .$$

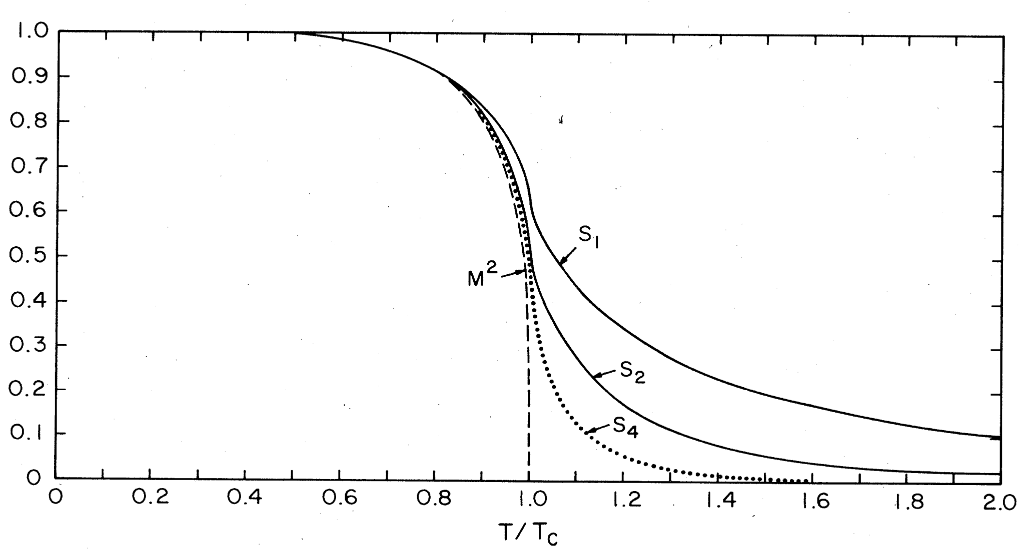

FIG. 1. Plot of the diagonal correlation functions S_1, S_2, and S_4, together with the squared magnetization M^2 as functions of T/T_c in the isotropic $d=2$ Ising model.

The $\mathscr{P}_{n-l,l}^{(n,\pm)}$ for $n=5$ are given in the Appendix. (Our results for $n=6$ are listed in Ref. 8.) Although the exsions are quite long, we believe that it is worthwhile to record them, since they are exact and are in an explicit form which can be used directly for analytical or numerical analysis.

In Fig. 1 we plot S_1,S_2,S_4, and the squared magnetization M^2 as functions of T/T_c. The elementary correlation inequalities (19) and

$$S_m(T) \geq S_n(T) \quad \text{if } m<n \tag{23}$$

(where the equality holds only at $T=0$ and $T=\infty$), and hence (with equality only at $T=0$)

$$S_n(T) \geq M^2(T) \quad \forall n \tag{24}$$

are evident in the graph. One can also discern the infinite slopes in the S_n and M^2 at $T=T_c$. It is interesting that in the low-temperature phase the different S_n functions and M^2 are practically indistinguishable until $T/T_c \gtrsim 0.8$, whereas in the high-temperature phase there is a greater separation between these S_n's. This indicates that the disordering (or, viewed differently, short-range order), which occurs in the $\mathbf{Z}_2$ symmetric phase, $T>T_c$, depends more sensitively on n, at least for small n, than the approach to long-range order does in the phase with spontaneously broken $\mathbf{Z}_2$ symmetry, $T<T_c$.

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APPENDIX

The $\mathscr{P}_{n-l,l}^{(n,\pm)}$ are listed below for $n=5$. Because of the length of the expressions for $n>5$, we avoid giving results for S_n, $n>5$ here. (For $n=6$, see Ref. 8.) For $n=5$, $T>T_c$,

$$\mathscr{P}_{5,0}^{(5,+)}=262y_>^{10}+9340y_>^9-1\,411\,795y_>^8-1\,417\,235y_>^7-2\,293\,735y_>^6-7\,179\,887y_>^5$$
$$+26\,133\,515y_>^4-1\,102\,985y_>^3-133\,795y_>^2-20\,785y_>+12\,,$$

$$\mathscr{P}_{4,1}^{(5,+)}=5(12y_>^{10}+715y_>^9-301\,320y_>^8-205\,360y_>^7-475\,660y_>^6-2\,228\,562y_>^5$$
$$+16\,836\,940y_>^4-909\,560y_>^3-115\,920y_>^2-18\,385y_>+12)\,,$$

$$\mathscr{P}_{3,2}^{(5,+)}=-5(24y_>^9+111\,337y_>^8-89\,860y_>^7-41\,517y_>^6+943\,946y_>^5-21\,491\,273y_>^4$$
$$+14\,639\,28y_>^3+196\,741y_>^2+32\,330y_>-24)\,,$$

$$\mathscr{P}_{2,3}^{(5,+)}=-5(14\,157y_>^8-83\,180y_>^7-131\,273y_>^6-20\,398y_>^5-13\,698\,717y_>^4$$
$$+1\,145\,440y_>^3+162\,833y_>^2+28\,250y_>-24)\,,$$

$$\mathscr{P}_{1,4}^{(5,+)}=5(14\,169y_>^7+12\,352y_>^6+35\,277y_>^5+4\,382\,564y_>^4-434621y_>^3-65\,328y_>^2-12\,265y_>+12)\,,$$

$$\mathscr{P}_{0,5}^{(5,+)}=-17\,715y_>^6-65\,501y_>^5+2\,824\,190y_>^4-320\,730y_>^3-50\,375y_>^2-10\,585y_>+12\,,$$

and $n=5$, $T<T_c$,

$$\mathscr{P}_{5,0}^{(5,-)}=12y_<^{10}-20\,785y_<^9-133\,795y_<^8-1\,102\,985y_<^7+26\,133\,515y_<^6-7\,179\,887y_<^5$$
$$-2\,293\,735y_<^4-1\,417\,235y_<^3-1\,411\,795y_<^2+9340y_<+262\,,$$

$$\mathscr{P}_{4,1}^{(5,-)}=-125(96y_<^8+811y_<^7+8548y_<^6-363\,315y_<^5-165\,262y_<^4-92\,539y_<^3-44\,064y_<^2+355y_<+10)\,,$$

$$\mathscr{P}_{3,2}^{(5,-)}=-5(360y_<^9+651y_<^8+31\,658y_<^7-6\,410\,543y_<^6+6\,389\,472y_<^5+2\,643\,313y_<^4$$
$$+1\,923\,170y_<^3+1\,729\,647y_<^2-15\,796y_<-476)\,,$$

$$\mathscr{P}_{2,3}^{(5,-)}=-10(270y_<^8+2523y_<^7+1\,010\,246y_<^6-1\,920\,319y_<^5-870\,116y_<^4$$
$$-707\,955y_<^3-667\,762y_<^2+7159y_<+226)\,,$$

$$\mathscr{P}_{1,4}^{(5,-)}=-10(135y_<^7-122\,352y_<^6+551\,498y_<^5+258\,369y_<^4+239\,203y_<^3+256\,106y_<^2-3204y_<-107)\,,$$

$$\mathscr{P}_{0,5}^{(5,-)}=225y_<^6-616\,911y_<^5-284\,740y_<^4-286\,190y_<^3-391\,095y_<^2+5645y_<+202\,.$$

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[9]S_2 (but not S_n for $n>2$) has also bee calculated by J. H. H. Perk (private communication).