Susceptibility of the Two-Dimensional Ising Model

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6. The Ising susceptibility and the natural boundary conjecture

Only #6 reports on new developments—joint with Harold Widom

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$$\mathcal{E}_\Lambda(\sigma) = -J_1 \sum_{i,j\in\Lambda} \sigma_{i\,j}\sigma_{i\,j+1} - J_2 \sum_{i,j\in\Lambda} \sigma_{i\,j}\sigma_{i+1\,j} - h \sum_{i,j\in\Lambda} \sigma_{i\,j}$$

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- In practice we will take periodic boundary conditions which means the system is defined on a torus with m rows and n columns.
- This defines the 2D Ising model with nearest neighbor interactions on the square lattice in a magnetic field.

Thermodynamic quantities and correlation functions

- *Free energy* per lattice site

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- *Spin-spin correlation function*

$$\langle \sigma_{00}\sigma_{MN}\rangle = \lim_{|\Lambda|\to\infty} \mathbb{E}_\Lambda(\sigma_{00}\sigma_{MN}) = \lim_{|\Lambda|\to\infty} \frac{\sum_\sigma \sigma_{00}\sigma_{MN}\, e^{-\beta\mathcal{E}(\sigma)}}{\sum_\sigma e^{-\beta\mathcal{E}(\sigma)}}$$

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Second question a bit easier to answer:

$$M_0^2(\beta) = \lim_{N\to\infty} \langle \sigma_{00}\sigma_{NN} \rangle$$

$$\text{zero-field susceptibility: } \chi(\beta) = \sum_{M,N\in\mathbb{Z}} \left[\langle \sigma_{00}\sigma_{MN} \rangle - M_0^2 \right]$$

Method of Transfer Matrices

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$$Z_{mn}(\beta, h) = \mathrm{Tr}(V^m) \qquad (\star)$$

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To see this let $\vec{s}_\alpha$ represent the configuration of row α, $\vec{s}_\alpha = (s_1, s_2, \ldots, s_n)$, $s_j = \pm 1$. Define the $2^n \times 2^n$ matrix V_1 by incorporating the Boltzmann factors in *row* α:

$$V_1(\vec{s}, \vec{s}\,') = \delta_{\vec{s}, \vec{s}\,'} \cdot \prod_{\alpha=1}^{n} \mathrm{e}^{\beta J_1 s_\alpha s'_{\alpha+1}}$$

For Boltzmann factors on columns we introduce

$$V_2(\vec{s}, \vec{s}\,') = \prod_{j=1}^{n} \mathrm{e}^{\beta J_2 s_j s'_j}$$

and for the magnetic field

$$V_3(\vec{s}, \vec{s}\,') = \delta_{\vec{s}, \vec{s}\,'} \cdot \prod_{j=1}^{n} \mathrm{e}^{\beta h s_j}$$

Defining

$$V = V_1 V_2 V_3$$

it is easy to check that

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For $h = 0$; namely, $V_3 = I$, a diagonalization was first accomplished by Lars Onsager (1944). His analysis was subsequently simplified by Bruria Kaufman (1949).

It is Kaufman's point of view which we now summarize.

Kaufman's Analysis

Stated concisely here is what Kaufman realized:

> *The $2^n \times 2^n$ matrices V_1 and V_2; and hence $V = V_1 V_2$, are spin representations of rotations in the orthogonal group $\mathcal{O}(2n)$. Furthermore, V is a spin representative of a product of commuting plane rotations. Thus the spectral analysis is reduced to that of a $2n \times 2n$ orthogonal matrix. Indeed, due to the translational invariance of the interaction energy, the spectral theory reduces to solving quadratic equations!*[1]

V is not a spin-representative of a rotation when $h \neq 0$.

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[1] Actually, this statement is true for a certain direct sum decomposition $V = V^+ \oplus V^-$. The statements apply to $V^\pm$.

Combinatorial Approach to 2D Ising Model

Kasteleyn's theory (1963) of dimers on planar lattices: Partition function is expressible as a Pfaffian.[2]

Fisher (1966) building on work of Kac and Ward (1952) showed the 2D Ising model (as defined above) is equivalent to a dimer problem.

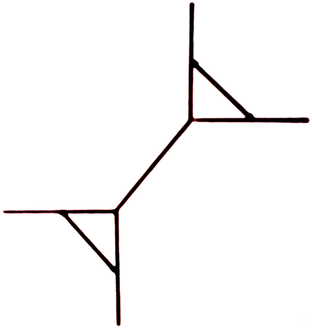

Figure: A six-site cluster that may be used to convert the Ising problem into a dimer problem. See McCoy & Wu, *The Two-Dimensional Ising Model* for details.

[2]For modern treatment see work of Rick Kenyon.

The Spontaneous Magnetization: Some history[3]

Onsager, well-known for being cryptic, announced in a discussion section at a conference in Florence (1949)[4] that he and Kaufman had recently obtained an exact formula for the spontaneous magnetization:

$$M_0 = (1-k^2)^{1/8}, \quad k := (\sinh 2\beta J_1 \sinh 2\beta J_2)^{-1} \qquad (\star\star)$$

Onsager gave no details to how he and Kaufman obtained $(\star\star)$.

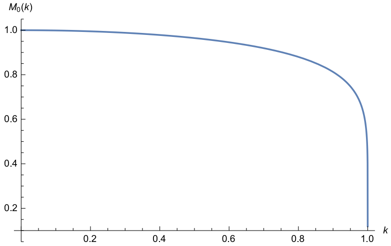

Figure: Spontaneous magnetization. $k = 1$ defines the critical temperature.

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[3] See, P. Deift, A. Its and I. Krasovsky, Toeplitz Matrices and Toeplitz Determinants under the Impetus of the Ising Model: Some History and Some Recent Results.

[4] And on a blackboard at Cornell on 23 August 1948.

What was later revealed was that Onsager and Kaufman first showed that $\langle \sigma_{00}\sigma_{0N} \rangle$ was expressible as a *Toeplitz determinant*. Unpublished, they also showed the diagonal correlation is a Toeplitz determinant and the expression is a bit simpler:

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$$\langle \sigma_{00}\sigma_{NN} \rangle = \det \left(\varphi_{m-n}\right)_{m,n=0,\dots,N-1}$$

with

$$\varphi_m = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{e}^{-\,\mathrm{i}\, m\theta}\,\varphi(\mathrm{e}^{\mathrm{i}\,\theta})\,d\theta,\ \ \varphi(z) = \left[\frac{1-k/z}{1-kz}\right]^{1/2}$$

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Today we know the *strong Szegö limit theorem* (plus some conditions on φ)

$$\lim_{N\to\infty}\frac{\det(\varphi_{m-n})}{\mu^N} = \exp\left(\sum_{k=1}^{\infty} k(\log\varphi)_k(\log\varphi)_{-k}\right)$$

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But Szegö had not yet proved his strong limit theorem (1952)!

- Onsager had, in fact, derived (nonrigorously) the limit formula. He communicated this result to *Shizuo Kakutani* who communicated the result to Szegö. (I verified this story when I met, many years later, Kakutani at Yale.)

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- Before all this was revealed(!), *C. N. Yang* (1952) gave an independent derivation which is a subtle perturbation argument. To quote Yang from his *Selected Works 1945–1980*:

> *I was thus led to a long calculation, the longest in my career. Full of local, tactical tricks, the calculation proceeded by twists and turns. There were many obstructions. But always, after a few days, a new trick was somehow found that pointed to a new path. The trouble was that I soon felt I was in a maze and was not sure whether in fact, after so many turns, I was anywhere nearer the goal than when I began. This kind of strategic overview was very depressing, and several times I almost gave up. But each time something drew me back, usually a new tactical trick that brightened the scene, even though only locally.*
>
> *Finally, after six months of work off and on, all the pieces suddenly fitted together, producing miraculous cancellations, and I was staring at the amazingly simple final result . . .*

Spin-spin correlation functions

- Though both the row and diagonal correlations are expressible as Toeplitz determinants, there is no Toeplitz representation for the general case $\langle\sigma_{00}\sigma_{MN}\rangle$.

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- If we use the *Case-Geronimo-Borodin-Okounkov* (CGBO) formula that expresses a Toeplitz determinant as a Fredholm determinant (times a normalization constant), we arrive at new representations for these correlations. It is this type of expression that generalizes. For $T < T_c$ it takes the form

$$\langle \sigma_{00} \sigma_{MN} \rangle = \mathcal{M}_0^2 \det(I - K_{MN})$$

  This was first derived by Wu, McCoy, Barouch & CT (1976) and then put on a rigorous footing by Palmer and CT (1981).[5]

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Massive Scaling Functions & Universality

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- Precisely, let $\xi(T)$ denote the correlation length, which is known to diverge at $T \to T_c^{\pm}$, then the *massive scaling limit*[6] from below T_c is

$$F_{-}(r) := \lim_{\text{scaling}} \frac{\langle \sigma_{00} \sigma_{MN} \rangle}{M_0^2} = \det(I - K_{<})$$

where "$\lim_{\text{scaling}}$" is

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- Note that the scaling functions are rotationally invariant.
- The scaling functions $F_\pm$ are expected to be universal for a large class of 2D ferromagnetic systems. There is no proof (as far as I know), but it is generally accepted by physicists using nonrigorous renormalization group arguments.

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$$\frac{d^2\psi}{dr^2} + \frac{1}{r}\frac{d\psi}{dr} = \frac{1}{2}\sinh(2\psi), \quad \psi(r) \sim 2K_0(r), r \to \infty.$$

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- $\eta(r) = e^{-\psi(r)}$ is a Painlevé III function.
- M. Sato, T. Miwa & M. Jimbo (1978–79) gave an *isomonodromy deformation analysis* interpretation for the appearance of Painlevé III in the 2D Ising model. They also derived a total system of PDEs for the *n*-point scaling functions. The asymptotic analysis of these PDEs is an open problem.

The problem of the Ising susceptibility

The *zero-field susceptibility* $\chi(T)$ is defined by

$$\chi(T) := \left.\frac{\partial \mathcal{M}(T,H)}{\partial H}\right|_{H=0^+} .$$

To distinguish between $T < T_c$ and $T > T_c$ we write χ_- and χ_+, respectively.

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$$\beta^{-1}\chi(T) = \sum_{M,N\in\mathbb{Z}} \left[\langle \sigma_{00}\sigma_{MN} \rangle - \mathcal{M}_0^2 \right],$$

and

$$\langle \sigma_{00}\sigma_{MN} \rangle = \mathcal{M}_0^2 \det(I - K_{MN}), \ \ T < T_c,$$

we study

$$\sum_{M,N\in\mathbb{Z}} [\det(I - K_{MN}) - 1]$$

But first some history of the problem

•M. FISHER in 1959 initiated the analysis of the analytic structure of χ near the critical temperature T_c by relating it to the long-distance asymptotics of the correlation function at T_c (a result known to Kaufmann and Onsager).

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•WMTB (1973–76) derived the *exact form factor expansion* of χ and related the the coefficients $C_\pm$ in the asymptotic expansion

$$\chi_\pm(T) = C_\pm \left|1 - T/T_c\right|^{-7/4} + \mathrm{O}\left(\left|1 - T/T_c\right|^{-3/4}\right), \quad T \to T_c^\pm$$

to integrals involving a *Painlevé III* function.

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•B. NICKEL (1999,2000) analyzed the n-dimensional integrals appearing in the form factor expansion and identified a class of complex singularities, now called *Nickel singularities*, that lie on a curve and which become ever more dense with increasing n. This provides very strong support for the existence of a natural boundary for $\chi_\pm$—curve is $|k| = 1$.

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$$\mathcal{B} = \sum_{q=0}^{\infty} \sum_{p=0}^{\lfloor \sqrt{q} \rfloor} b^{(p,q)} (\log |\tau|)^p \tau^q$$

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with numerical approximations to $b^{(p,q)}$, $p \leq 5$, and

$$\mathcal{F}_{\pm} = k^{\frac{1}{4}} \Big[1 + \frac{\tau^2}{2} - \frac{\tau^4}{12} + \left(\frac{647}{15360} - \frac{7 C_{6\pm}}{5} \right) \tau^6 - \left(\frac{296813}{11059200} - \frac{4973 C_{6\pm}}{3600} \right) \tau^8 + \left(\frac{23723921}{1238630400} - \frac{100261 C_6 \pm}{115200} - \frac{793 C_{10\pm}}{210} \right) \tau^{10} + \cdots \Big]$$

with high-precision decimal estimates for $C_{6\pm}$ and $C_{10\pm}$.

Diagonal susceptibility: A simpler problem[7]

From now on we restrict to $T < T_c$:

$$\beta\chi_d = \sum_{N\in\mathbb{Z}} \left[\langle\sigma_{00}\sigma_{NN}\rangle - \mathcal{M}_0^2\right]$$

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$$\langle\sigma_{00}\sigma_{NN}\rangle = \det(T_N(\varphi)) \stackrel{\mathrm{GCBO}}{=} \mathcal{M}_0^2 \det(I - K_N)$$

$$K_N = H_N(\Lambda)H_N(\Lambda^{-1}),\ \Lambda(\xi) = \varphi_-(\xi)/\varphi_+(\xi) = \sqrt{(1-k\xi)(1-k/\xi)}.$$

Here $\varphi = \varphi_+ \cdot \varphi_-$ is the Wiener-Hopf factorization of φ and $H_N(\psi)$ is the Hankel operator with entries $(\psi_{N+i+j+1})_{i,j\geq 0}$.

Sum to be analyzed:

$$\mathcal{S} := \sum_{N=1}^{\infty} \left[\det(I - K_N) - 1\right].$$

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Proposition (T–Widom): Let $H_N(du)$ and $H_N(dv)$ be two Hankel matrices acting on $\ell^2(\mathbb{Z}^+)$ with i,j entries

$$\int x^{N+i+j}\,du(x),\ \int y^{N+i+j}\,dv(y)$$

respectively, where u and v are measures supported inside the unit circle. Set $K_N = H_N(du)H_N(dv)$. Then

$$\sum_{N=1}^{\infty}[\det(I-K_N)-1] = \sum_{n=1}^{\infty}\frac{(-1)^n}{(n!)^2}\int\cdots\int\frac{\prod_i x_i y_i}{1-\prod_i x_i y_i}\times \left(\det\left(\frac{1}{1-x_i y_j}\right)\right)^2\prod_i du(x_i)dv(y_i)$$

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Ideas in proof:

1. First use Fredholm expansion of $\det(I - K_N)$.
2. Then use the Andréief identity:

$$\int \cdots \int \det(\phi_j(x_k))_{j,k=1,\dots,N} \cdot \det(\psi_j(x_k))_{j,k=1,\dots,N}\, dx_1 \cdots dx_N = N! \det\Big(\int \phi_j(x)\psi_k(x)\, dx\Big)_{j,k=1,\dots,N}$$

3. Symmetrization argument

Applying this to $K_N = H_N(\Lambda)H_N(\Lambda^{-1})$ followed by a deformation of contours gives $\mathcal{S} = \sum_{n=1}^{\infty} \mathcal{S}_n$ with

$$\mathcal{S}_n = \frac{1}{(n!)^2}\frac{\kappa^{2n}}{\pi^{2n}}\int_0^1 \cdots \int_0^1 \frac{\prod_i x_i y_i}{1-\kappa^n \prod_i x_i y_i}\left(\det\left(\frac{1}{1-\kappa x_i y_j}\right)\right)^2 \times \prod_i \frac{\Lambda_1(x_i)}{\Lambda_1(y_i)} \prod_i dx_i dy_i$$

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Alternate representation of $\mathcal{S}_n$ (Cauchy determinant identity):

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Theorem (T–Widom): The unit circle $|\kappa| = 1$ is a natural boundary for $\mathcal{S}$.

Proof proceeds by four lemmas.

Let $\epsilon \neq 1$ be a nth root of unity and we wish to consider behavior of $\mathcal{S}$ as $\kappa \to \epsilon$ radially. Look at $d^\ell \mathcal{S}_n / d\kappa^\ell$—main contribution will come from

$$\bigstar\bigstar \quad \int_0^1 \cdots \int_0^1 \frac{\prod_i x_i y_i}{(1 - \kappa^n \prod_i x_i y_i)^{\ell+1}} \frac{\Delta(x)^2 \Delta(y)^2}{\prod_{i,j}(1 - \kappa x_i y_j)^2} \prod_i \frac{\Lambda_1(x_i)}{\Lambda_1(y_i)} dx_i dy_i$$

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Lemma 1: The integral $\bigstar\bigstar$ is bounded when $\ell < 2n^2 - 1$ and it is of order $\log(1-|\kappa|)^{-1}$ when $\ell = 2n^2 - 1$.

Main idea: Various approximations bound $\bigstar\bigstar$ by the integral

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Lemma 2:

$$(\frac{d}{d\kappa})^{2n^2-1} \mathcal{S}_n \approx \log(1-\kappa)^{-1}$$

In differentiating $\bigstar$ the other terms are $\mathrm{O}(1)$.

Lemma 3: If $\epsilon^m \neq 1$, then

$$\left(\frac{d}{d\kappa}\right)^{2n^2-1} \mathcal{S}_m = \mathrm{O}(1).$$

All integrals are bounded as $\kappa \to \epsilon$.

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Lemma 4: (Main lemma)

$$\sum_{m>n} \left(\frac{d}{d\kappa}\right)^{2n^2-1} \mathcal{S}_m = \mathrm{O}(1)$$

For κ sufficiently close to ϵ, all integrals we get by differentiating the integrals for $\mathcal{S}_m$ are at most $A^m m^m$. (A can depend upon n but not on m.) The extra $(m!)^2$ appearing in ★ gives a bounded sum.

What about χ?

For $T < T_c$:

$$\begin{aligned}\beta^{-1}\chi_- &= \sum_{M,N\in\mathbb{Z}} \left[\langle\sigma_{00}\sigma_{MN}\rangle - \mathcal{M}_0^2\right] = \mathcal{M}_0^2 \sum_{M,N\in\mathbb{Z}} \left[\det(I - K_{M,N}) - 1\right] \\ &= \mathcal{M}_0^2 \sum_{n=1}^{\infty} \chi^{(2n)}\end{aligned}$$

In the last equality we used the Fredholm expansion and product formulas for the determinants appearing in the integrands to find

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$$\chi^{(n)}(s) = \frac{1}{n!}\frac{1}{(2\pi\,\mathrm{i})^{2n}} \int_{\mathcal{C}_r} \cdots \int_{\mathcal{C}_r} \frac{(1+\prod_j x_j^{-1})(1+\prod_j y_j^{-1})}{(1-\prod_j x_j)(1-\prod_j y_j)} \times \prod_{j<k} \frac{(x_j - x_k)(y_j - y_k)}{(x_j x_k - 1)(y_j y_k - 1)} \prod_j \frac{dx_j dy_j}{D(x_j, y_j; s)}$$

$$D(x, y; s) = s + s^{-1} - (x + x^{-1})/2 - (y + y^{-1})/2, \quad s := 1/\sqrt{k}$$

Nickel Singularities

Standard estimates show that $\chi_-(s)$ is holomorphic for $|s| > 1$ ($|k| < 1$).

Definition: A *Nickel singularity* of order n is a point s^0 on the unit circle such that the real part of s^0 is the average of the real parts of two nth roots of unity.

Note that $D(x, y; s)$ vanishes when

$$\Re(s) = \frac{\Re(x) + \Re(y)}{2}$$

Theorem (T–Widom) When n is even $\chi^{(n)}$ extends to a C^∞ function on the unit circle except at the Nickel singularities of order n.

Some ideas in the proof

- A partition of unity allows one to localize.

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- Application of the divergence theorem gives the bound $\mathrm{O}(1)$—same bound after differentiating with with respect to s any number of times.
- Follows that $\chi^{(n)}$ extends to a C^∞ function excluding the Nickel singularities.

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Thank you for your attention!