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5.22 Lenz–Ising Constants

The Ising model is concerned with the physics of phase transitions, for example, the tendency of a magnet to lose strength as it is heated, with total loss occurring above a certain finite critical temperature. This essay can barely introduce the subject. Unlike hard squares [5.12] and percolation clusters [5.18], a concise complete problem statement here is not possible. We are concerned with large arrays of 1s and -1s whose joint distribution passes through a singularity as a parameter T increases. The definition and characterization of the joint distribution is elaborate; our treatment is combinatorial and focuses on series expansions. See [1–10] for background.

Let L denote the regular d-dimensional cubic lattice with $N = n^d$ sites. For example, in two dimensions, L is the $n \times n$ square lattice with $N = n^2$. To eliminate boundary effects, L is wrapped around to form a d-dimensional torus so that, without exception, every site has $2d$ nearest neighbors. This convention leads to negligible error for large N.

5.22.1 Low-Temperature Series Expansions

Suppose that the N sites of L are colored black or white at random. The dN edges of L fall into three categories: black-black, black-white, and white-white. What can be said jointly about the relative numbers of these? Over all possible such colorings, let $A(p, q)$ be the number of colorings for which there are exactly p black sites and exactly q black-white edges. (See Figure 5.20.)

Then, for large enough N [11–14],

$$\begin{array}{ll} A(0,0) = 1 & \text{(all white)},\\ A(1,2d) = N & \text{(one black)},\\ A(2,4d-2) = dN & \text{(two black, adjacent)},\\ A(2,4d) = \tfrac{1}{2}(N-2d-1)N & \text{(two black, not adjacent)},\\ A(3,6d-4) = (2d-1)dN & \text{(three black, adjacent)}. \end{array}$$

Properties of this sequence can be studied via the bivariate generating function

$$a(x, y) = \sum_{p,q} A(p, q)x^p y^q$$

and the formal power series

$$\alpha(x, y) = \lim_{n\to\infty} \frac{1}{N}\ln(a(x, y))$$
$$= xy^{2d} + dx^2y^{4d-2} - \frac{2d+1}{2}x^2y^{4d} + (2d-1)dx^3y^{6d-4} + \cdots$$

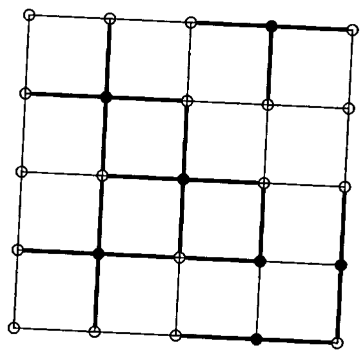

Figure 5.20. Sample coloring with $d = 2$, $N = 25$, $p = 7$, and $q = 21$ (ignoring wraparound).

obtained by merely collecting the coefficients that are linear in N. The latter is sometimes written as [15]

$$\exp(\alpha(x, y)) = 1 + xy^{2d} + dx^2y^{4d-2} - dx^2y^{4d} + (2d-1)dx^3y^{6d-4} + \cdots,$$

a series whose coefficients are integers only. This is what physicists call the **low-temperature series** for the **Ising free energy per site**. The letters x and y are not dummy variables but are related to temperature and magnetic field; the series $\alpha(x, y)$ is not merely a mathematical construct but is a thermodynamic function with properties that can be measured against physical experiment [16]. In the special case when $x = 1$, known as the **zero magnetic field case**, we write $\alpha(y) = \alpha(1, y)$ for convenience.

When $d = 2$, we have [11,17]

$$\exp(\alpha(y)) = 1 + y^4 + 2y^6 + 5y^8 + 14y^{10} + 44y^{12} + 152y^{14} + 566y^{16} + \cdots.$$

Onsager [18–23] discovered an astonishing closed-form expression:

$$\alpha(y) = \frac{1}{2}\int_0^1\int_0^1 \ln\left[(1+y^2)^2 - 2y(1-y^2)(\cos(2\pi u) + \cos(2\pi v))\right] du\, dv$$

that permits computation of series coefficients to arbitrary order [24] and much more.

When $d = 3$, we have [11,25–30]

$$\exp(\alpha(y)) = 1 + y^6 + 3y^{10} - 3y^{12} + 15y^{14} - 30y^{16} + 101y^{18} - 261y^{16} + - \cdots$$

No closed-form expression for this series has been found, and the required computations are much more involved than those for $d = 2$.

5.22.2 High-Temperature Series Expansions

The associated high-temperature series arises via a seemingly unrelated combinatorial problem. Let us assume that a nonempty *subgraph* of L is connected and contains at least one edge. Suppose that several subgraphs are drawn on L with the property that

- each edge of L is used at most once, and
- each site of L is used an *even* number of times (possibly zero).

Call such a configuration on L an **even polygonal drawing**. (See Figure 5.21.) An even polygonal drawing is the union of simple, closed, edge-disjoint polygons that need not be connected.

Let $B(r)$ be the number of even polygonal drawings for which there are exactly r edges. Then, for large enough N [4,11,31],

$$\begin{array}{ll} B(4) = \tfrac{1}{2}d(d-1)N & \text{(square)},\\ B(6) = \tfrac{1}{3}d(d-1)(8d-13)N & \text{(two squares, adjacent)},\\ B(8) = \tfrac{1}{8}d(d-1)\left(d(d-1)N + 216d^2 - 848d + 850\right)N & \text{(many possibilities)}. \end{array}$$

On the one hand, for $d \geq 3$, the drawings can intertwine and be knotted [32], so computing $B(r)$ for larger r is quite complicated! On the other hand, for $d = 2$, clearly

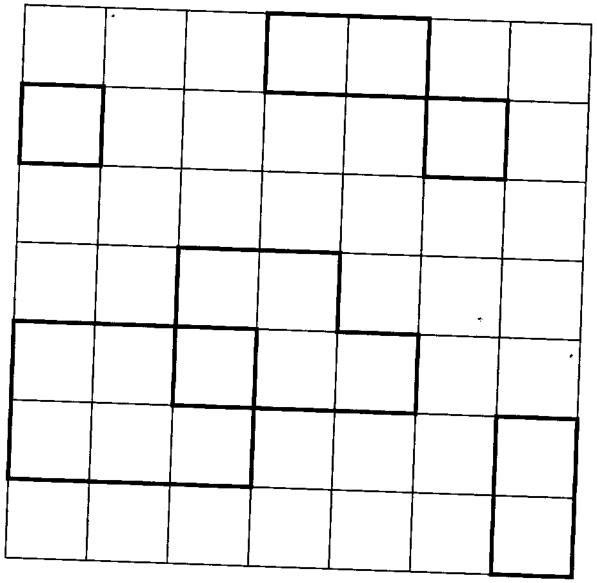

Figure 5.21. An even polygonal drawing for $d = 2$; other names include closed or Eulerian subgraph.

$B(q) = \sum_p A(p, q)$ always. As before, we define a (univariate) generating function

$$b(z) = 1 + \sum_r B(r) z^r$$

and a formal power series

$$\begin{aligned}\beta(z) &= \lim_{n\to\infty} \frac{1}{N} \ln(b(z)) \\ &= \frac{1}{2}d(d-1)z^4 + \frac{1}{3}d(d-1)(8d-13)z^6 + \frac{1}{4}d(d-1)(108d^2 - 424d + 425)z^8 \\ &\quad + \frac{2}{15}d(d-1)(2976d^3 - 19814d^2 + 44956d - 34419)z^{10} + \cdots\end{aligned}$$

called the **high-temperature zero-field series** for the **Ising free energy**. When $d = 3$ [11,25,29,33–36],

$$\exp(\beta(z)) = 1 + 3z^4 + 22z^6 + 192z^8 + 2046z^{10} + 24853z^{12} + 329334z^{14} + \cdots,$$

but again our knowledge of the series coefficients is limited.

5.22.3 Phase Transitions in Ferromagnetic Models

The two major unsolved problems connected to the Ising model are [4,31,37]:

- Find a closed-form expression for $\alpha(x, y)$ when $d = 2$.
- Find a closed-form expression for $\beta(z)$ when $d = 3$.

Why are these so important? We discuss now the underlying physics, as well its relationship to the aforementioned combinatorial problems.

Place a bar of iron in an external magnetic field at constant absolute temperature T. The field will induce a certain amount of magnetization into the bar. If the external field is then slowly turned off, we empirically observe that, for small T, the bar retains some of its internal magnetization, but for large T, the bar's internal magnetization disappears completely.

There is a unique **critical temperature,** T_c, also called the **Curie point**, where this qualitative change in behavior occurs. The Ising model is a simple means for explaining the physical phenomena from a microscopic point of view.

At each site of the lattice L, define a "spin variable" $\sigma_i = 1$ if site i is "up" and $\sigma_i = -1$ if site i is "down." This is known as the **spin-1/2 model**. We study the **partition function**

$$Z(T) = \sum_\sigma \exp\left[\frac{1}{\kappa T}\left(\sum_{(i,j)} \xi \sigma_i \sigma_j + \sum_k \eta \sigma_k\right)\right],$$

where ξ is the coupling (or interaction) constant between nearest neighbor spin variables, $\eta \geq 0$ is the intensity constant of the external magnetic field, and $\kappa > 0$ is Boltzmann's constant.

The function $Z(T)$ captures all of the thermodynamic features of the physical system and acts as a kind of "denominator" when calculating state probabilities. Observe that the first summation is over all 2^N possible values of the vector $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_N)$ and the second summation is over all edges of the lattice (sites i and j are distinct and adjacent). Henceforth we will assume $\xi > 0$, which corresponds to the **ferromagnetic case.** A somewhat different theory emerges in the antiferromagnetic case ($\xi < 0$), which we will not discuss.

How is Z connected to the combinatorial problems discussed earlier? If we assign a spin 1 to the color white and a spin -1 to the color black, then

$$\sum_{(i,j)} \sigma_i \sigma_j = (dN - q) \cdot 1 + q \cdot (-1) = dN - 2q,$$

$$\sum_k \sigma_k = (N - p) \cdot 1 + p \cdot (-1) = N - 2p,$$

and therefore

$$Z = x^{-\frac{1}{2}N} y^{-\frac{d}{2}N} a(x, y),$$

where

$$x = \exp\left(-\frac{2\eta}{\kappa T}\right), \quad y = \exp\left(-\frac{2\xi}{\kappa T}\right).$$

Since small T gives small values of x and y, the phrase low-temperature series for $\alpha(x, y)$ is justified. (Observe that $T = \infty$ corresponds to the case when lattice site colorings are assigned equal probability, which is precisely the combinatorial problem described earlier. The range $0 < T < \infty$ corresponds to unequal weighting, accentuating the states with small p and q. The point $T = 0$ corresponds to an ideal case when all spins are aligned; heat introduces disorder into the system.)

For the high-temperature case, rewrite Z as

$$Z = \left(\frac{4}{(1-z^2)^d(1-w^2)}\right)^{\frac{N}{2}} \frac{1}{2^N}\sum_{\sigma}\left(\prod_{(i,j)}(1+\sigma_i\sigma_j z)\cdot\prod_k(1+\sigma_k w)\right),$$

where

$$z = \tanh\left(\frac{\xi}{\kappa T}\right), \quad w = \tanh\left(\frac{\eta}{\kappa T}\right).$$

In the zero-field scenario ($\eta = 0$), this expression simplifies to

$$Z = \left(\frac{4}{(1-z^2)^d}\right)^{\frac{N}{2}} b(z),$$

and since large T gives small z, the phraseology again makes sense.

5.22.4 *Critical Temperature*

We turn attention to some interesting constants. The radius of convergence y_c in the complex plane of the low-temperature series $\alpha(y) = \sum_{k=0}^{\infty}\alpha_k y^k$ is given by [29]

$$y_c = \lim_{k\to\infty}|\alpha_{2k}|^{-\frac{1}{2k}} = \begin{cases}\sqrt{2}-1 = 0.4142135623\ldots & \text{if } d = 2,\\ \sqrt{0.2853\ldots} = 0.5341\ldots & \text{if } d = 3;\end{cases}$$

hence, if $d = 2$, the ferromagnetic critical temperature T_c satisfies

$$K_c = \frac{\xi}{\kappa T_c} = \frac{1}{2}\ln\left(\frac{1}{y_c}\right) = \frac{1}{2}\ln(\sqrt{2}+1) = 0.4406867935\ldots.$$

The two-dimensional result is a famous outcome of work by Kramers & Wannier [38] and Onsager [18]. For $d = 3$, the singularity at $y^2 = -0.2853\ldots$ is nonphysical and thus is not relevant to ferromagnetism; a second singularity at $y^2 = 0.412048\ldots$ is what we want but it is difficult to compute directly [29, 39]. To accurately obtain the critical temperature here, we examine instead the high-temperature series $\beta(z) = \sum_{k=0}^{\infty}\beta_k z^k$ and compute

$$z_c = \lim_{k\to\infty}\beta_{2k}{}^{-\frac{1}{2k}} = 0.218094\ldots, \quad K_c = \tfrac{1}{2}\ln\left(\frac{1+z_c}{1-z_c}\right) = 0.221654\ldots.$$

There is a huge literature of series and Monte Carlo analyses leading to this estimate [40–53]. (A conjectured exact expression for z_c in [54] appears to be false [55].) For $d > 3$, the following estimates are known [56–65]:

$$z_c = \begin{cases}0.14855\ldots & \text{if } d = 4,\\ 0.1134\ldots & \text{if } d = 5,\\ 0.0920\ldots & \text{if } d = 6,\\ 0.0775\ldots & \text{if } d = 7,\end{cases} \qquad K_c = \begin{cases}0.14966\ldots & \text{if } d = 4,\\ 0.1139\ldots & \text{if } d = 5,\\ 0.0923\ldots & \text{if } d = 6,\\ 0.0777\ldots & \text{if } d = 7.\end{cases}$$

An associated critical exponent γ will be discussed shortly.

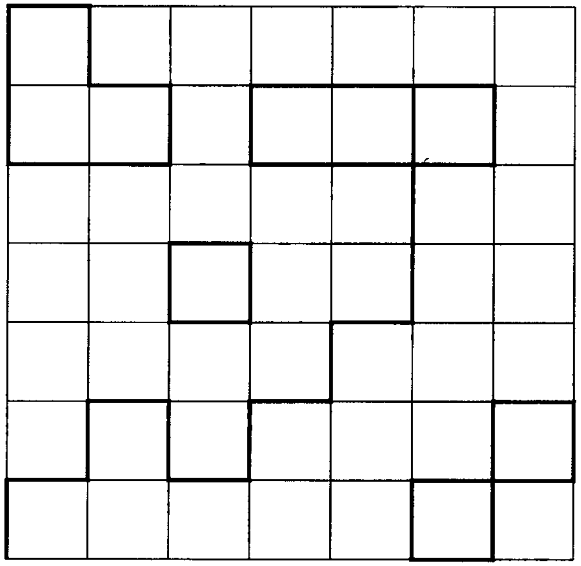

Figure 5.22. An odd polygonal drawing for $d = 2$.

5.22.5 *Magnetic Susceptibility*

Here is another combinatorial problem. Suppose that several subgraphs are drawn on L with the property that

- each edge of L is used at most once,
- all sites of L, except two, are even, and
- the two remaining sites are odd and must lie in the same (connected) subgraph.

Call this configuration an **odd polygonal drawing**. (See Figure 5.22.) Note that an odd polygonal drawing is the edge-disjoint union of an even polygonal drawing and an (undirected) self-avoiding walk [5.10] linking the two odd sites.

Let $C(r)$ be twice the number of odd polygonal drawings for which there are exactly r edges. Then, for large enough N [12, 66],

$$\begin{aligned}
&C(1) = 2dN && \text{(SAW)},\\
&C(2) = 2d(2d-1)N && \text{(SAW)},\\
&C(3) = 2d(2d-1)^2N && \text{(SAW)},\\
&C(4) = 2d\left(2d(2d-1)^3 - 2d(2d-2)\right)N && \text{(SAW)},\\
&C(5) = d^2(d-1)N^2 + 2d\left(16d^4 - 32d^3 + 16d^2 + 4d - 3\right)N && \text{(square and/or SAW)}.
\end{aligned}$$

As before, we may define a generating function and a formal power series

$$c(z) = N + \sum_r C(r)z^r, \quad \chi(z) = \lim_{n\to\infty}\frac{1}{N}\ln(c(z)) = \sum_{k=0}^{\infty}\chi_k z^k,$$

which is what physicists call the **high-temperature zero-field series** for the **Ising magnetic susceptibility per site**. The radius of convergence z_c of $\chi(z)$ is the same as that for $\beta(z)$ for $d > 1$. For example, when $d = 3$, analyzing the series [67–73]

$$\chi(z) = 1 + 6z + 30z^2 + 150z^3 + 726z^4 + 3510z^5 + 16710z^6 + \cdots$$

is the preferred way to obtain critical parameter estimates (being the best behaved of several available series). Further, the limit

$$\lim_{k\to\infty} \frac{\chi_k}{z_c^{-k} k^{\gamma-1}}$$

appears to exist and is nonzero for a certain positive constant γ depending on dimensionality. As an example, if $d = 2$, numerical evidence surrounding the series [67,74,75]

$$\chi(z) = 1 + 4z + 12z^2 + 36z^3 + 100z^4 + 276z^5 + 740z^6 + 1972z^7 + 5172z^8 + \cdots$$

suggests that the **critical susceptibility exponent** γ is 7/4 and that γ is *universal* (in the sense that it is independent of the choice of lattice). No analogous exact expressions appear to be valid for γ when $d \ge 3$; for $d = 3$, the consensus is that $\gamma = 1.238\ldots$ [40,44,46,49–52,71,73].

We finally make explicit the association of $\chi(z)$ with the Ising model [76]:

$$\lim_{n\to\infty} \frac{1}{N} \ln(Z(z, w)) = \ln(2) - \frac{d}{2}\ln(1 - z^2) - \frac{1}{2}\ln(1 - w^2) + \beta(z) + \frac{1}{2}(\chi(z) - 1)\,w^2 + O(w^4),$$

where the big O depends on z. Therefore $\chi(z)$ occurs when evaluating a second derivative with respect to w, specifically, when computing the variance of P (defined momentarily).

5.22.6 *Q and P Moments*

Let us return to the random coloring problem, suitably generalized to incorporate temperature. Let

$$Q = d - \frac{2}{N}q = \frac{1}{N}\sum_{(i,j)} \sigma_i\sigma_j, \quad P = 1 - \frac{2}{N}p = \frac{1}{N}\sum_k \sigma_k$$

for convenience and assume henceforth that $d = 2$. To study the asymptotic distribution of Q, define

$$F(z) = \lim_{n\to\infty} \frac{1}{N}\ln(Z(z)).$$

Then clearly

$$\lim_{n\to\infty} \mathrm{E}(Q) = (\kappa T)\frac{dF}{d\xi}, \quad \lim_{n\to\infty} N\,\mathrm{Var}(Q) = (\kappa T)^2 \frac{d^2F}{d\xi^2}$$

via term-by-term differentiation of $\ln(Z)$. Exact expressions for both moments are

possible using Onsager's formula:

$$F(z) = \ln\left(\frac{2}{1 - z^2}\right) + \frac{1}{2}\int_0^1\int_0^1 \ln\left[(1 + z^2)^2 - 2z(1 - z^2)(\cos(2\pi u) + \cos(2\pi v))\right] du\,dv,$$

but we give results at only two special temperatures. In the case $T = \infty$, for which states are assigned equal weighting, $\mathrm{E}(Q) \to 0$ and $N\,\mathrm{Var}(Q) \to 2$, confirming reasoning in [77]. In the case $T = T_c$, note that the singularity is fairly subtle since F and its first derivative are both well defined [11]:

$$F(z_c) = \frac{\ln(2)}{2} + \frac{2G}{\pi} = 0.9296953983\ldots = \frac{1}{2}(\ln(2) + 1.1662436161\ldots),$$

$$\lim_{n\to\infty} \mathrm{E}(Q) = \sqrt{2},$$

where G is Catalan's constant [1.7]. The second derivative of F, however, is unbounded in the vicinity of $z = z_c$ and, in fact [5],

$$\lim_{n\to\infty} N\,\mathrm{Var}(Q) \approx -\frac{8}{\pi}\left(\ln\left|\frac{T}{T_c} - 1\right| + g\right),$$

where g is the constant

$$g = 1 + \frac{\pi}{4} + \ln\left(\frac{\sqrt{2}}{4}\ln(\sqrt{2} + 1)\right) = 0.6194036984\ldots.$$

This is related to what physicists call the **logarithmic divergence** of the **Ising specific heat.** (See Figure 5.23.)

As an aside, we mention that corresponding values of $F(z_c)$ on the triangular and hexagonal planar lattices are, respectively [11],

$$\ln(2) + \frac{\ln(3)}{4} + \frac{H}{2} = 0.8795853862\ldots,$$

$$\frac{3\ln(2)}{4} + \frac{\ln(3)}{2} + \frac{H}{4} = 1.0250590965\ldots.$$

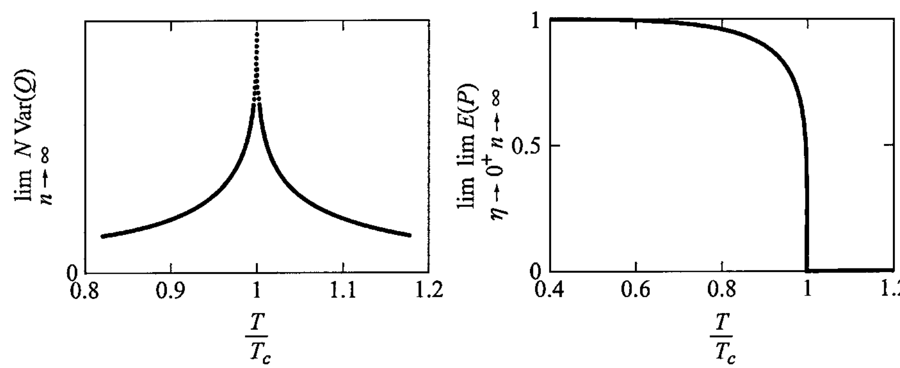

Figure 5.23. Graphs of Ising specific heat and spontaneous magnetization.

Both results feature a new constant [78, 79]:

$$H = \frac{5\sqrt{3}}{6\pi}\psi'\left(\frac{1}{3}\right) - \frac{5\sqrt{3}}{9}\pi - \ln(6) = \frac{\sqrt{3}}{6\pi}\psi'\left(\frac{1}{6}\right) - \frac{\sqrt{3}}{3}\pi - \ln(6)$$
$$= -0.1764297331\ldots,$$

where $\psi'(x)$ is the trigamma function (derivative of the digamma function $\psi(x)$ [1.5.4]). See [80–82] for other occurrences of H; note that the formula

$$\ln(2) + \ln(3) + H = \frac{1}{4\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \ln\left[6 - 2\cos(\theta) - 2\cos(\varphi) - 2\cos(\theta+\varphi)\right] d\theta\, d\varphi$$
$$= \frac{3\sqrt{3}}{\pi}\left(1 - \frac{1}{5^2} + \frac{1}{7^2} - \frac{1}{11^2} + \frac{1}{13^2} - \frac{1}{17^2} + - \cdots\right)$$
$$= 1.6153297360\ldots$$

parallels nicely similar results in [3.10] and [5.23].

A more difficult analysis allows us to compute the corresponding two moments of P and also to see more vividly the significance of magnetic susceptibility and critical exponents. Let

$$F(z, w) = \lim_{n\to\infty} \frac{1}{N}\ln(Z(z, w));$$

then clearly

$$\lim_{\eta\to 0^+}\lim_{n\to\infty} \mathrm{E}(P) = (\kappa T)\left.\frac{\partial F}{\partial \eta}\right|_{\eta=0}, \quad \lim_{\eta\to 0^+}\lim_{n\to\infty} N\,\mathrm{Var}(P) = (\kappa T)^2\left.\frac{\partial^2 F}{\partial \eta^2}\right|_{\eta=0}$$

as before. Of course, we do not know $F(z, w)$ exactly when $w \neq 0$. Its derivative at $w = 0$, however, has a simple expression valid for all z:

$$\lim_{\eta\to 0^+}\lim_{n\to\infty} \mathrm{E}(P) = \begin{cases} \left[1 - \sinh\left(\frac{2\xi}{\kappa T}\right)^{-4}\right]^{\frac{1}{8}} & \text{if } T < T_c, \\ 0 & \text{if } T > T_c, \end{cases}$$
$$= \begin{cases} (1+y^2)^{\frac{1}{4}}(1-6y^2+y^4)^{\frac{1}{8}}(1-y^2)^{-\frac{1}{2}} & \text{if } T < T_c, \\ 0 & \text{if } T > T_c \end{cases}$$

due to Onsager and Yang [83–85]. A rigorous justification is found in [86–88]. For the special temperature $T = \infty$, we have $\mathrm{E}(P) \to 0$ and $N\,\mathrm{Var}(P) \to 1$ since p is Binomial $(N, 1/2)$ distributed. At criticality, $\mathrm{E}(P) \to 0$ as well, but the second derivative exhibits fascinatingly complicated behavior:

$$\lim_{\eta\to 0^+}\lim_{n\to\infty} N\,\mathrm{Var}(P) = \chi(z) \approx c_0^+ t^{-\frac{7}{4}} + c_1^+ t^{-\frac{3}{4}} + d_0 + c_2^+ t^{\frac{1}{4}} + e_0\, t\ln(t) + d_1 t + c_3^+ t^{\frac{5}{4}},$$

where $0 < t = 1 - T_c/T$, $c_0^+ = 0.9625817323\ldots$, $d_0 = -0.1041332451\ldots$, $e_0 = 0.0403255003\ldots$, $d_1 = -0.14869\ldots$, and

$$c_1^+ = \tfrac{\sqrt{2}}{8} K_c c_0^+, \quad c_2^+ = \tfrac{151}{192} K_c^2 c_0^+, \quad c_3^+ = \tfrac{615\sqrt{2}}{512} K_c^3 c_0^+.$$

Wu, McCoy, Tracy & Barouch [89–99] determined exact expressions for these series coefficients in terms of the solution to a Painlevé III differential equation (described in the next section). Different numerical values of the coefficients apply for $T < T_c$, as well as for the antiferromagnetic case [100, 101]. For example, when $t < 0$, the corresponding leading coefficient is $c_0^- = 0.0255369745\ldots$. The study of magnetic susceptibility $\chi(z)$ is far more involved than the other thermodynamic functions mentioned in this essay, and there are still gaps in the rigorous line of thought [102]. Also, in a recent breakthrough [103, 104], the entire asymptotic structure of $\chi(z)$ has now largely been determined.

5.22.7 Painlevé III Equation

Let $f(x)$ be the solution of the Painlevé III differential equation [105]

$$\frac{f''(x)}{f(x)} = \left(\frac{f'(x)}{f(x)}\right)^2 - \frac{1}{x}\frac{f'(x)}{f(x)} + f(x)^2 - \frac{1}{f(x)^2}$$

satisfying the boundary conditions

$$f(x) \sim 1 - \frac{e^{-2x}}{\sqrt{\pi x}} \text{ as } x \to \infty, \quad f(x) \sim x\,(2\ln(2) - \gamma - \ln(x)) \text{ as } x \to 0^+,$$

where γ is Euler's constant [1.5]. Define

$$g(x) = \left[\frac{x f'(x)}{2 f(x)} + \frac{x^2}{4 f(x)^2}\left(\left(1 - f(x)^2\right)^2 - f'(x)^2\right)\right]\ln(x).$$

Then exact expressions for c_0^+ and c_0^- are

$$c_0^+ = 2^{\frac{5}{8}}\pi \ln(\sqrt{2}+1)^{-\frac{7}{4}} \int_0^\infty y(1 - f(y))$$
$$\times \exp\left[\int_y^\infty x\ln(x)\left(1 - f(x)^2\right) dx - g(y)\right] dy,$$
$$c_0^- = 2^{\frac{5}{8}}\pi \ln(\sqrt{2}+1)^{-\frac{7}{4}} \int_0^\infty y$$
$$\times \left\{(1 + f(y))\exp\left[\int_y^\infty x\ln(x)\left(1 - f(x)^2\right) dx - g(y)\right] - 2\right\} dy.$$

Painlevé II arises in our discussion of the longest increasing subsequence problem [5.20], and Painlevé V arises in connection with the GUE hypothesis [2.15.3].

Here is a slight variation of these results. Define

$$h(x) = -\ln\left(f\left(\frac{x}{c}\right)\right)$$

for any constant $c > 0$; then the function $h(x)$ satisfies what is known as the sinh-Gordon differential equation:

$$h''(x) + \frac{1}{x}h'(x) = \frac{2}{c^2}\sinh(2h(x)),$$

$$h(x) \sim \sqrt{\frac{c}{\pi x}}\exp\left(-\frac{2x}{c}\right) \quad \text{as } x \to \infty.$$

Finally, we mention a beautiful formula:

$$\int_0^\infty x\ln(x)\left(1 - f(x)^2\right)dx = \frac{1}{4} + \frac{7}{12}\ln(2) - 3\ln(A),$$

where A is Glaisher's constant [2.15]. Conceivably, c_0^+ and c_0^- may someday be related to A as well.

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5.23 Monomer-Dimer Constants

Let L be a graph [5.6]. A **dimer** consists of two adjacent vertices of L and the (non-oriented) bond connecting them. A **dimer arrangement** is a collection of disjoint dimers on L. Uncovered vertices are called **monomers**, so dimer arrangements are also known as **monomer-dimer coverings**. We will discuss such coverings only briefly at the beginning of the next section.

A **dimer covering** is a dimer arrangement whose union contains all the vertices of L. Dimer coverings and the closely-related topic of tilings will occupy the remainder of this essay.

5.23.1 2D Domino Tilings

Let a_n denote the number of distinct monomer-dimer coverings of an $n \times n$ square lattice L and $N = n^2$; then $a_1 = 1$, $a_2 = 7$, $a_3 = 131$, $a_4 = 10012$ [1,2], and asymptotically [3–6]

$$A = \lim_{n\to\infty} a_n^{\frac{1}{N}} = 1.940215351\ldots = (3.764435608\ldots)^{\frac{1}{2}}.$$

No exact expression for the constant A is known. Baxter's approach for estimating A was based on the corner transfer matrix variational approach, which also played a

role in [5.12]. A natural way for physicists to discuss the monomer-dimer problem is to associate an activity z with each dimer; A thus corresponds to the case $z = 1$. The mean number ρ of dimers per vertex is 0 if $z = 0$ and $1/2$ if $z = \infty$; when $z = 1$, ρ is $0.3190615546\ldots$, for which again there is no closed-form expression [3]. Unlike other lattice models (see [5.12], [5.18], and [5.22]), monomer-dimer systems do not have a phase transition [7].

Computing a_n is equivalent to counting (not necessarily perfect) **matchings** in L, that is, to counting independent sets of edges in L. This is related to the difficult problem of computing permanents of certain binary incidence matrices [8–14]. Kenyon, Randall & Sinclair [15] gave a randomized polynomial-time approximation algorithm for computing the number of monomer-dimer coverings of L, assuming ρ to be given.

Let us turn our attention henceforth to the zero monomer density case, that is, $z = \infty$. If b_n is the number of distinct dimer coverings of L, then $b_n = 0$ if n is odd and

$$b_n = 2^{N/2}\prod_{j=1}^{n/2}\prod_{k=1}^{n/2}\left(\cos^2\frac{j\pi}{n+1} + \cos^2\frac{k\pi}{n+1}\right)$$

if n is even. This exact expression is due to Kastelyn [16] and Fisher & Temperley [17,18]. Further,

$$\lim_{\substack{n\to\infty\\ n\text{ even}}} \frac{1}{N}\ln(b_n) = \frac{1}{16\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \ln\left[4 + 2\cos(\theta) + 2\cos(\varphi)\right]\, d\theta\, d\varphi$$
$$= \frac{G}{\pi} = 0.2915609040\ldots;$$

that is,

$$B = \lim_{\substack{n\to\infty\\ n\text{ even}}} b_n^{\frac{1}{N}} = \exp\left(\frac{G}{\pi}\right) = 1.3385151519\ldots = (1.7916228120\ldots)^{\frac{1}{2}},$$

where G is Catalan's constant [1.7]. This is a remarkable solution, in graph theoretic terms, of the problem of counting **perfect matchings** on the square lattice. It is also an answer to the following question: What is the number of ways of tiling an $n \times n$ chessboard with 2×1 or 1×2 **dominoes**? See [19–26] for more details. The constant B^2 is called δ in [3.10] and appears in [1.8] too; the expression $4G/\pi$ arises in [5.22], $G/(\pi \ln(2))$ in [5.6], and $8G/\pi^2$ in [7.7].

If we wrap the square lattice around to form a torus, the counts b_n differ somewhat, but the limiting constant B remains the same [16,27]. If, instead, we assume the chessboard to be shaped like an Aztec diamond [28], then the associated constant $B = 2^{1/4} = 1.189\ldots < 1.338\ldots = e^{G/\pi}$. Hence, even though the square chessboard has slightly less area than the diamond chessboard, the former possesses many more domino tilings [29]. Lattice boundary effects are thus seen to be nontrivial.

5.23.2 Lozenges and Bibones

The analog of $\exp(2G/\pi)$ for dimers on a hexagonal (honeycomb) lattice with wraparound is [30–32]

$$C^2 = \lim_{n\to\infty} c_n^{\frac{2}{N}} = \exp\left(\frac{1}{8\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \ln\left[3+2\cos(\theta)+2\cos(\varphi)+2\cos(\theta+\varphi)\right]\,d\theta\,d\varphi\right)$$
$$= 1.3813564445\ldots.$$

This constant is called β in [3.10] and can be expressed by other formulas too. It characterizes lozenge tilings on a chessboard with triangular cells satisfying periodic boundary conditions. See [33–38] as well.

If there is no wraparound, then the sequence [39]

$$c_n = \prod_{j=1}^{n}\prod_{k=1}^{n}\frac{n+j+k-1}{j+k-1}$$

emerges, and a different growth constant $3\sqrt{3}/4$ applies. We have assumed that the hexagonal grid is center-symmetric with sides n, n, and n (i.e., the simplest possible boundary conditions). The sequence further enumerates plane partitions contained within an $n \times n \times n$ box [40,41].

The corresponding analog for dimers on a triangular lattice with wraparound is [30,42,43]

$$D^2 = \lim_{n\to\infty} d_n^{\frac{2}{N}} = \exp\left(\frac{1}{8\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \ln\left[6+2\cos(\theta)+2\cos(\varphi)+2\cos(\theta+\varphi)\right]\,d\theta\,d\varphi\right)$$
$$= 2.3565273533\ldots.$$

The expression $4\ln(D)$ bears close similarity to a constant $\ln(6)+H$ described in [5.22]. It also characterizes bibone tilings on a chessboard with hexagonal cells satisfying periodic boundary conditions. The case of no wraparound [1,44,45] apparently remains open.

5.23.3 3D Domino Tilings

Let h_n denote the number of distinct dimer coverings of an $n \times n \times n$ cubic lattice L and $N = n^3$. Then $h_n = 0$ if n is odd, $h_2 = 9$, and $h_4 = 5051532105$ [46,47]. An important unsolved problem in solid-state chemistry is the estimation of

$$\lim_{\substack{n\to\infty\\ n\text{ even}}} h_n^{\frac{1}{N}} = \exp(\lambda)$$

or, equivalently,

$$\lambda = \lim_{\substack{n\to\infty\\ n\text{ even}}} \frac{1}{N}\ln(h_n).$$

Hammersley [48] proved that λ exists and $\lambda \geq 0.29156$. Lower bounds were improved by Fisher [49] to 0.30187, Hammersley [50,51] to 0.418347, and Priezzhev [52,53] to 0.419989. In a review of [54], Minc pointed out that a conjecture due to Schrijver & Valiant on lower bounds for permanents of certain binary matrices would imply that $\lambda \geq 0.44007584$. Schrijver [55] proved this conjecture, and this is the best-known result.

Fowler & Rushbrooke [56] gave an upper bound of 0.54931 for λ over sixty years ago (assuming λ exists). Upper bounds have been improved by Minc [8,57,58] to 0.5482709, Ciucu [59] to 0.463107, and Lundow [60] to 0.457547.

A sequence of nonrigorous numerical estimates by Nagle [30], Gaunt [31], and Beichl & Sullivan [61] has culminated with $\lambda = 0.4466\ldots$. As with a_n, computing h_n for even small values of n is hard and matrix permanent approximation schemes offer the only hope. The field is treacherously difficult: Conjectured exact asymptotic formulas for h_n in [62,63] are incorrect.

A related topic is the number, k_n, of dimer coverings of the n-dimensional unit cube, whose 2^n vertices consist of all n-tuples drawn from $\{0, 1\}$ [47,64]. The term $k_6 = 16332454526976$ was computed independently by Lundow [46] and Weidemann [65]. In this case, we know the asymptotic behavior of k_n rather precisely [44,65,66]:

$$\lim_{n\to\infty}\frac{1}{n}k_n^{2^{1-n}} = \frac{1}{e} = 0.3678794411\ldots,$$

where e is the natural logarithmic base [1.3].

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