Exact Distribution of Energies in the Two-Dimensional Ising Model

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The low-temperature series expansion for the partition function of the two-dimensional Ising model on a square lattice can be determined exactly for finite lattices using Kaufman's generalization of Onsager's solution. The exact distribution function for the energy can then be determined from the coefficients of the partition function. This provides an exact solution with which one can compare energy histograms determined in Monte Carlo simulations. This solution should prove useful for detailed studies of statistical and systematic errors in histogram reweighting.

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This paper describes an exact determination of the low-temperature series expansion for the partition function of the two-dimensional Ising model on a square lattice. The expansion is based on Onsager's exact solution [1] as generalized by Kaufman [2]. The purpose of the calculation is to determine the exact distribution function of energies with which one can compare energy histograms generated by Monte Carlo simulations. Previously only low-order cumulants of the distribution were known exactly [3], so Monte Carlo tests depended on comparing the results of the simulations with only the exactly known values of the internal energy and the specific heat on finite square lattices [3]. Knowledge of the full energy distribution, however, is equivalent to knowing all cumulants for the model exactly so it potentially contains much more information than is typically used for checking the validity and convergence of new Monte Carlo methods. For example, subtle correlations in the pseudorandom numbers cause very easily discernible deviations of the energy histogram from the exact distribution. Another potential use of the exact solution for the energy distribution involves testing the range of accuracy of the histogram reweighting method [4]. Histogram reweighting is a widely used technique because of the savings in computer time that results from performing Monte Carlo simulations at one value of the applied fields (temperature, magnetic field, chemical potential, etc.) and reweighting the measured histograms to determine the thermal averages at nearby field values. The energy distribution function provides an exact benchmark for testing the evolution of statistical and systematic errors as a function of temperature.

The isotropic two-dimensional Ising model with nearest-neighbor interactions on a lattice with m rows and n columns with periodic boundary conditions in zero external field is defined by the Hamiltonian

$$H = -J \sum_{(ij)} s_i s_j , \tag{1}$$

where J is the coupling energy and $s_i = \pm 1$. The sum is over pairs of nearest-neighbor sites on the lattice. The partition function at any temperature T can be written as a low-temperature series expansion,

$$Z_{n,m}(K) = e^{2nmK} \sum_{k=0}^{nm} g_k x^{2k}, \tag{2}$$

where n is the number of columns, m is the number of rows, $K = J/k_B T$ is the coupling, k_B is Boltzmann's constant, $x = e^{-2K}$ is the low-temperature expansion variable, and the coefficient g_k is the number of configurations with energy $4kJ$ above the two ground states (all spins $+1$ or all spins -1). Only even orders appear in the expansion. If $m > 5$ and $n > 5$, the first few terms in the series are

$$\begin{aligned} Z_{n,m}(K) = e^{2nmK}\{2 &+ (2mn)x^4 + (4mn)x^6 \\ &+ [(mn)^2 + 9mn]x^8 \\ &+ [4(mn)^2 + 24mn]x^{10} + \cdots\}. \end{aligned} \tag{3}$$

If both m and n are even then ferromagnetic or antiferromagnetic symmetry ($J \to -J$ and $s_i \to -s_i$ on one sublattice) gives

$$g_k = g_{mn-k} . \tag{4}$$

[Due to the self-duality of the two-dimensional square lattice exactly the same coefficients g_k also appear in the high-temperature series expansion where the expansion variable is $\tanh(K)$.]

The energy distribution P_k is the probability of finding an equilibrium state with energy 4 kJ above the ground state. It is given simply by

$$P_k(K) = \frac{g_k x^{2k}}{\sum_{k=0}^{mn} g_k x^{2k}} . \tag{5}$$

Onsager's exact solution [1] of the two-dimensional Ising model was extended by Kaufman [2] in 1949 to give the exact solution for the partition function on a finite square lattice with periodic boundary conditions. One can cast this solution in the form of a low-temperature

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series (2) thereby giving an exact determination of $P_k(K)$. Kaufman's [2] solution for the partition function on a $m \times n$ square lattice is

$$Z_{m,n}(K) = 2^{mn/2-1}(Y_1 + Y_2 + Y_3 + Y_4), \quad (6)$$

where

$$Y_1 = \prod_{k=0}^{n-1} 2\cosh\left(\frac{m}{2}\gamma_{2k+1}\right) \sinh^{m/2}(2K), \quad (7a)$$

$$Y_2 = \prod_{k=0}^{n-1} 2\sinh\left(\frac{m}{2}\gamma_{2k+1}\right) \sinh^{m/2}(2K), \quad (7b)$$

$$Y_3 = \prod_{k=0}^{n-1} 2\cosh\left(\frac{m}{2}\gamma_{2k}\right) \sinh^{m/2}(2K), \quad (7c)$$

$$Y_4 = \prod_{k=0}^{n-1} 2\sinh\left(\frac{m}{2}\gamma_{2k}\right) \sinh^{m/2}(2K). \quad (7d)$$

For $0 < k < 2n$ the quantity γ_k is the positive root of

$$\cosh(\gamma_k) = \frac{\cosh^2(2K)}{\sinh(2K)} - \cos\left(\frac{\pi k}{n}\right), \quad (8)$$

The $k = 0$ case is

$$e^{\gamma_0} = e^{2K}\tanh(K). \quad (9)$$

Equations (6) and (7) can be simplified to the point that MATHEMATICA can be used to express the result (6)–(9) in the form (2), i.e., a polynomial in the variable x. The factors in Eqs. (7a)–(7d) can be simplified considerably using the following definitions:

$$\beta = 2x(1 - x^2), \quad (10a)$$

$$\alpha_k = (1 + x^2)^2 - \beta\cos\left(\frac{\pi k}{n}\right), \quad (10b)$$

$$c_0 = (1 - x)^m + x^m(1 + x)^m, \quad (10c)$$

$$s_0 = (1 - x)^m - x^m(1 + x)^m, \quad (10d)$$

$$c_n = (1 + x)^m + x^m(1 - x)^m, \quad (10e)$$

$$s_n = (1 + x)^m - x^m(1 - x)^m, \quad (10f)$$

$$c_k^2 = \frac{1}{2^{m-1}}\left(\sum_{j=0}^{[m/2]} \frac{m!}{(2j)!\,(m - 2j)!}(\alpha_k^2 - \beta^2)^j \alpha_k^{m-2j} + \beta^m\right), \quad (10g)$$

$$s_k^2 = \frac{1}{2^{m-1}}\left(\sum_{j=0}^{[m/2]} \frac{m!}{(2j)!\,(m - 2j)!}(\alpha_k^2 - \beta^2)^j \alpha_k^{m-2j} - \beta^m\right). \quad (10h)$$

The function $[z]$ denotes the largest integer less than or equal to z. The quantities c_k^2 and s_k^2 were expanded using the binomial series in order to explicitly remove all square roots that hide the polynomial nature of the final result (2). The partition function can then be written as

$$Z_{m,n}(K) = e^{2mnK}(Z_1 + Z_2 + Z_3 + Z_4). \quad (11)$$

If n is even

$$Z_1 = \frac{1}{2}\prod_{k=0}^{n/2-1} c_{2k+1}^2, \quad (12a)$$

$$Z_2 = \frac{1}{2}\prod_{k=0}^{n/2-1} s_{2k+1}^2, \quad (12b)$$

$$Z_3 = \frac{1}{2}c_0 c_n \prod_{k=1}^{n/2-1} c_{2k}^2, \quad (12c)$$

$$Z_4 = \frac{1}{2}s_0 s_n \prod_{k=1}^{n/2-1} s_{2k}^2. \quad (12d)$$

If n is odd

$$Z_1 = \frac{1}{2}c_n \prod_{k=0}^{(n-3)/2} c_{2k+1}^2, \quad (13a)$$

$$Z_2 = \frac{1}{2}s_n \prod_{k=0}^{(n-3)/2} s_{2k+1}^2, \quad (13b)$$

$$Z_3 = \frac{1}{2}c_0 \prod_{k=1}^{(n-1)/2} c_{2k}^2, \quad (13c)$$

$$Z_4 = \frac{1}{2}s_0 \prod_{k=1}^{(n-1)/2} s_{2k}^2. \quad (13d)$$

For any chosen lattice size one can use MATHEMATICA to expand the products of the polynomials in Eqs. (12) or (13) to give the form (2). If one is interested in the exact integer values for the coefficients g_k, one must set the numerical precision to about $mn\ln(2)/\ln(10)$ decimal digits. The

calculation can be checked against the low-order result (3) or with an exact enumeration of the energies on small lattices. The series for the 32×32 Ising model is

$$Z_{32,32}(K) = e^{2048\,K}(2 + 2048x^4 + 4096x^6 + 1057792x^8 + 4218880x^{10} + 371621888x^{12} + 2191790080x^{14} + 100903637504x^{16} + 768629792768x^{18} + 22748079183872x^{20} + \cdots + 4096x^{1018} + 2048x^{1020} + 2x^{1024}). \quad (14)$$

The largest coefficient for the 32×32 Ising model is

$$g_{512} = 6,342,873,169,001,916,568,766,443,273,025,000,331,593,063,924,436,135,196,680,443,689,656,478,072,741,300,511,612,123,900,652,711,596,311,283,701,724,071,226,144,241,851,411,641,714,893,727,789,741,510,169,213,344,005,116,385,197,594,692,089,556,614,547,788,150,860,200,720,413,211,442,412,355,672,291,841,364,265,145,274,980,444,405,423,129,672,679,584,959,498,234,944,801,613,246,300,853,599,317,229,362,316 \approx 6.342873169 \times 10^{306}.$$

A plot of the coefficients for the 32×32 Ising model is shown in Fig. 1.

A final verification of the correctness of the calculation is to ensure that the reduced free energy per spin gives the same power series as the thermodynamic limit series

$$\lim_{N\to\infty} \frac{\log(\frac{1}{2}Z_N)}{N} = 2K + x^4 + 2x^6 + \frac{9}{2}x^8 + 12x^{10} + \frac{112}{3}x^{12} + 130x^{14} + \frac{1961}{4}x^{16} + \frac{5876}{3}x^{18} + \frac{40871}{5}x^{20} + 35302x^{22} + 156740x^{24} + 712052x^{26} + \frac{23084692}{7}x^{28} + \frac{77637922}{5}x^{30} + \cdots. \quad (15)$$

Equation (15) is derived by expanding the integrand in Onsager's solution for the free energy per spin in the thermodynamic limit as a power series in x and evaluating the resulting integrals term by term using MATHEMATICA. The expansion of the logarithm of Eq. (14) using MATHEMATICA gives the same series as (15) up to order x^{30}.

The histograms of energies generated from Monte Carlo simulations can be compared with this exact distribution function (5) in order to ensure that the Monte Carlo results converge to the exact solution. This provides a good test of the convergence of new Monte Carlo methods. As an example, we show results for the now famous case of incorrect Monte Carlo results arising from using the R250 feedback shift-register pseudorandom number generator in conjunction with the Wolff cluster update

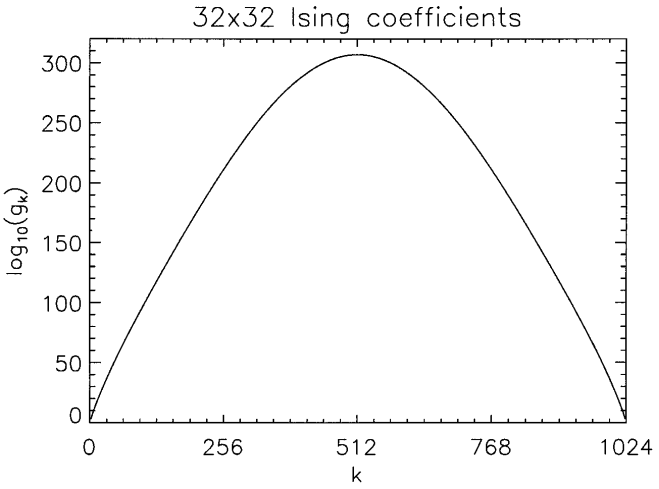

FIG. 1. The base-10 logarithm of the partition function coefficients of the 32×32 Ising model. The largest coefficient is $g_{512} \approx 6.342873169 \times 10^{306}$.

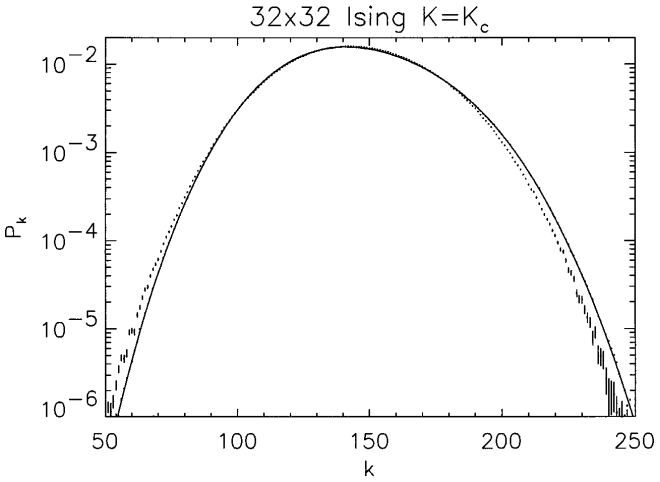

FIG. 2. The exact distribution of energies for the 32×32 Ising model at the critical temperature (solid line) and the distribution calculated from 10^7 configurations using the Wolff algorithm [6] with the R250 feedback shift-register pseudorandom number generator [5] (error bars). The distribution calculated from 5×10^7 configurations using the Wolff algorithm [6] with a double precision version of *Numerical Recipes'* [7] ran2( ) is also shown, but is almost indistinguishable from the solid curve at this scale.

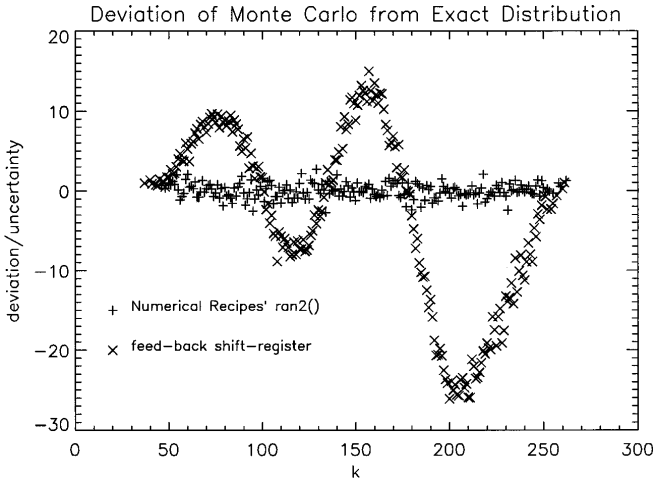

FIG. 3. This plot shows the deviation of the Monte Carlo results in Fig. 2 from the exact distribution in units of the statistical uncertainty of each point. The +'s indicate the ran2( ) results and the ×'s indicate the feedback shift-register results. The χ^2 for the two cases are 190 for 210 nonzero points and 28 000 for 217 nonzero points, respectively. The ran2( ) results are -0.95σ from the expected value and the feedback shift-register results are $+1300\sigma$ from the expected value.

algorithm [5,6]. The deviation of the energy histogram from the exact energy distribution (5) for the 32×32 Ising model at the critical point caused by subtle correlations present in the pseudorandom numbers is very clear in Fig. 2. The results are derived from 10^7 independent configurations. By comparison, the energy distribution that results from 5×10^7 configurations generated by the Wolff [6] algorithm with a double precision version of *Numerical Recipes'* ran2( ) pseudorandom number generator [7] gives a histogram that is almost indistinguishable from the exact distribution on the scale in this figure. (In both cases the energy correlation factor [8] for the model is $2\tau + 1 \approx 8$ so only every 20th configuration was used in order to assure approximate statistical independence of configurations used in the calculation of the histogram.) The deviation of the Monte Carlo results from the exact distribution of energies is shown in Fig. 3. The χ^2 for the two cases are 190 for 210 nonzero points using ran2( ) and 28 000 for 217 nonzero points using R250. The ran2( ) results are -0.95σ from the expected value of 209.5 and the feedback shift-register results are $+1300\sigma$ from the expected value of 216.5. The small but perhaps significant deviation of the ran2( ) results from the expected χ^2 value is probably attributable to the residual correlations in the configurations that survive after 20 cluster updates.

The exact distribution function (5) should also prove useful for more detailed studies of statistical errors in histogram reweighting [4]. Using the exact distribution, one can easily draw samples from the exact distribution at one temperature [7] without resorting to Monte Carlo simulations. The deviation of the reweighted histogram from the exact distribution at another temperature is then trivial to calculate. Using the full energy distribution rather than just the first two moments of the distribution will also provide much more information for use in monitoring the evolution of statistical errors.

The partition function coefficients for several lattice sizes and the MATHEMATICA code that performs the calculation of those coefficients can be found at the anonymous ftp site bly.colorado.edu in director /pub/cml_pubs/beale. Log in using ftp with the login name *anonymous.* Use your full e-mail or login address as your password.

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