# The Ising Model susceptibility

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# Outline of talk

- History and significance of the Ising model
- Crash course in Statistical Mechanics
- Three key quantites, free energy, magnetisation, susceptibility
- Solution in 1 dimension
- Solution in 2 dimensions (Onsager, free energy; Yang, magnetisation)
- Progress in finding the susceptibility
- Concept of a *differentiably finite* or *D-finite* function. A linear ODE with polynomial coefficients.
- Direct analysis, based on correlation functions
- An analysis based on *n*-particle contributions (Feynman-type integrals)

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- Proposed as a model of ferromagnetism.
- Ferromagnetism known for millenia. After the discovery of the electron, a viable mechanism was proposed.
- Magnetism is due to the electron's spin.
- Short range interaction between electrons. How do local interactions have a global effect?
- More precisely, how could short range forces lead to long-range correlations?

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- The gas-liquid transition.
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- **Neurology** Hopfield
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# Statistical mechanics

- Write down the Hamiltonian $\mathcal{H}$. (Energy of a configuration)
- Then the partition function

$$Z(T,H) = \sum_{all\ configs.} \exp(-\mathcal{H}/kT).$$

  ($k$ is Boltzmann's constant, $T$ is temperature, $H$ is an external magnetic field.)
- The (Helmholtz) free energy $F(T,H) = -kT \log Z(T,H)$.
- We need $\mathcal{F}(T,H) = \lim_{N\to\infty} F(T,H)/N$.
- All quantities follow by differentiation. The three primary quantities are:
- The specific heat $C_0 = -T\frac{d^2\mathcal{F}(T,0)}{dT^2}$
- The (zero-field) magnetisation $m_0(T) = \frac{\partial\mathcal{F}(T,H)}{\partial H}|_{H=0}$
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# One-dimensional model

- A one-dimensional array of “spins" $\{\mu_i, i = 1 \ldots N\}$, “up" or “down”, $\mu_i = \pm 1$. The Hamiltonian $\mathcal{H}$ of a configuration of spins, denoted $\{\mu\}$, is

$$\mathcal{H}\{\mu\} = -J \sum_{\langle i,j \rangle} \mu_i \mu_j + H \sum_{i=1}^{N} \mu_i = -J \sum_{i} \mu_i \mu_{i+1} + H \sum_{i=1}^{N} \mu_i.$$

  $\sum_{\langle i,j \rangle}$ means a sum over nearest-neighbour pairs, $J$ is the strength of the interaction between adjacent spins. The second sum gives the interaction of each spin with an external magnetic field $H$.

# One-dimensional model

- The partition function is

$$Z_N = \sum_{\{\mu\}} \exp\left(-\beta \mathcal{H}\{\mu\}\right),$$

  where $\beta = 1/(k_B T)$.
- We want the Helmholtz free-energy, $\mathcal{F}/k_B T = -\lim_{N\to\infty} 1/N \log Z_N$.
- The zero-field free energy then follows (set H=0 in the above),
- the zero-field magnetisation, $\lim_{H\to 0} \partial(-\mathcal{F}/kT)/\partial H$,
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# One-dimensional model

- In 1 dimension, impose cyclic boundary conditions, so that $\mu_{N+1} = \mu_1$. Then symmetrise the energy function

$$\begin{aligned} \mathcal{H}\{\mu\} &= -J \sum_{i=1}^{N} \mu_i \mu_{i+1} + H \sum_{i=1}^{N} \mu_i \\ &= -J \sum_{i=1}^{N} \mu_i \mu_{i+1} + H/2 \sum_{i=1}^{N} (\mu_i + \mu_{i+1}). \end{aligned}$$

- The partition function sum $\sum_{\{\mu\}}$ can be written $\sum_{\mu_1=\pm 1} \sum_{\mu_2=\pm 1} \sum_{\mu_3=\pm 1} \cdots \sum_{\mu_N=\pm 1}$.

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- The summand is

$$e^{(-\beta\mathcal{H}\{\mu\})} = e^{[\beta J \sum_{i=1}^{N} \mu_i \mu_{i+1} + \beta H/2 \sum_{i=1}^{N} (\mu_i + \mu_{i+1})]}.$$

- Summing this over a particular value of $\mu_i$ is just taking a matrix product. Indeed, consider the matrix

$$T = \begin{pmatrix} e^{(\beta J + \beta H)} & e^{-\beta J} \\ e^{-\beta J} & e^{(\beta J - \beta H)} \end{pmatrix}$$

- Then

$$Z_N = \sum_{\mu_1 = \pm 1} T^N = \mathrm{Tr}(T^N) = \lambda_1^N + \lambda_2^N$$

- When $\beta J > 0$, $\lambda_1 > \lambda_2$, so in the TL we only consider $\lambda_1$.

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# One-dimensional model

- So to solve the 1d Ising model we need only the eigenvalues of a $2 \times 2$ matrix
- Thus

$$\frac{\mathcal{F}(T,H)}{-kT} = \left[\beta J + \log\left(\cosh\beta H + \sqrt{\sinh^2\beta H + \exp(-4\beta J)}\right)\right].$$

- Thus

$$\mathcal{F}(T,0) = -kT\log(2\cosh\beta J),$$

- $m_0(T) = 0$ for $T > 0$, and $m_0(T) = \pm 1$ for $T = 0$.
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# Two-dimensional model

- Onsager's solution was refined by Kaufmann, who pointed out that a Clifford algebra could be used. Kac and Ward sought a simpler solution. Sherman pointed out a flaw. Feynman conjectured a fix. Sherman proved Feynman's conjecture.
- Later, Schutzenberger informed Sherman that his proof extended an identity of W. Witt on *“the dimension of the linear space of Lie elements of degree r in a free Lie algebra with k generators over a field of characteristic zero,"* and made some remarks on further extensions that might be of use in proving results in three dimensions.

# The two-dimensional model

- Let $\mu_{i,j}$ be the spin at lattice site $(i,j)$ of a lattice of $m$ rows and $n$ columns, wrapped as a cylinder. The Hamiltonian is

$$\mathcal{H}\{\mu\} = -J\sum_{i,j}\mu_{i,j}\mu_{i+1,j} - J\sum_{i,j}\mu_{i,j}\mu_{i,j+1} - H\sum_{i,j}\mu_{i,j}$$

The partition function

$$Z = \sum_{\{\mu\}}\exp(-\mathcal{H}\{\mu\}/kT)$$

can be calculated by diagonalising a $2^m \times 2^m$ matrix in the limit as $m \to \infty$.

- This was Onsager's triumphant achievement (with $H$ set to zero).

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- The final result for the internal energy is relatively simple:

$$U = -J \coth 2K \left[ 1 + (2\tanh^2 2K - 1)\frac{2}{\pi} K(k_1) \right]$$

$k_1 = 2\sinh 2K / \cosh^2 2K$, $K = J/kT$ and $K(k_1)$ is the complete elliptic integral of the first kind.

- Denote by $\mathcal{M}$ the magnetisation. It is zero for $T > T_c$ and, $\mathcal{M} = (1 - s^{-4})^{1/8}$ for $T < T_c$, where $s = \sinh(2J/kT)$ .
- The two-point correlation function is

$$C(m,n) = \langle \mu_{0,0} \mu_{m,n} \rangle.$$

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- However, considerable progress has been made.
- In 1976, Wu, McCoy, Tracy and Barouch showed that the susceptibility can be expressed as an infinite sum of *n-particle contributions.* The susceptibility is given by

$$kT\chi_H(w) = \frac{1}{s} \cdot (1 - s^4)^{\frac{1}{4}} \sum_n \tilde{\chi}^{(2n+1)}(w)$$

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$$\tilde{\chi}^{(n)}(w) = \frac{1}{n!} \cdot \Big( \prod_{j=1}^{n-1} \int_0^{2\pi} \frac{d\phi_j}{2\pi} \Big) \Big( \prod_{j=1}^{n} y_j \Big) \cdot R^{(n)} \cdot \Big( G^{(n)} \Big)^2,$$

$$G^{(n)} = \prod_{1 \le i < j \le n} h_{ij}, \quad h_{ij} = \frac{2 \sin\left((\phi_i - \phi_j)/2\right) \cdot \sqrt{x_i x_j}}{1 - x_i x_j},$$

$$R^{(n)} = \frac{1 + \prod_{i=1}^{n} x_i}{1 - \prod_{i=1}^{n} x_i},$$

$$x_i = \frac{2w}{1 - 2w\cos(\phi_i) + \sqrt{(1 - 2w\cos(\phi_i))^2 - 4w^2}},$$

$$y_i = \frac{2w}{\sqrt{(1 - 2w\cos(\phi_i))^2 - 4w^2}}, \qquad \sum_{j=1}^{n} \phi_j = 0$$

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- To evaluate $\tilde{\chi}^{(n)}$ convert to an $n$-fold integration with the explicit phase constraint $\sum \phi_i = 0$ now in the integrand. A Fourier transform decouples all $\phi_i$ integrations at the expense of a sum over the Fourier integer $k$. Next expand all denominator factors in the integrand, thereby converting it into a sum of $n$-fold products $\prod y_i x_i^{n_i}$. Each $i$ integration picks out the $k^{th}$ Fourier coefficient of $y_i x_i^{n_i}$. This coefficient is proportional to a ${}_4F_3$ hypergeometric function. The integrand becomes a nested sum of products of hypergeometric functions.

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- In 1996, Guttmann and Enting gave compelling arguments (though not a proof) that the Ising susceptibility was in a different class of functions to that of most solutions of exactly solved lattice models.
- In particular, both the Ising free-energy and magnetisation are holonomic functions (i.e. *differentiably finite* or *D-finite* functions), while the susceptibility, they argued, was not.
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- In 2001, Orrick, Nickel, Guttmann and Perk gave a *polynomial time* algorithm for the generation of the coefficients of the series expansion of the susceptibility, in time O($N^6$).
- From an algebraic-combinatorics viewpoint, a polynomial time algorithm is considered a solution.
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# The susceptibility directly from correlation functions

Recall

$$kT \cdot \chi = \sum_m \sum_n (C(m,n) - \mathcal{M}^2),$$

- Quadratic partial difference equations give $C(m,n)$ efficiently for high- and low-temperature series. A series of $N$ terms requires $C(m,n)$ for $m+n \leq 2N,\ m<n$.
- The diagonal $C(n,n)$ is the initial value data.
- Subsequently, by using modular arithmetic and FFT to perform multiplications of polynomials we reduced the complexity to $O(N^4 \log(N))$.
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- In 2004, Zenine, Boukraa, Hassani and Maillard obtained the Fuchsian linear ODE for $\tilde{\chi}^{(3)}$. In 2005, the same group found the Fuchsian linear ODE for $\tilde{\chi}^{(4)}$ by similar methods.
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# The susceptibility

- A number of computational "tricks" were used, including a partial fraction rearrangement of the denominators, recursion relations for the summations and FFT to perform multiplications.
- This produces an algorithm of complexity $O(N^4 \log(N))$.
- We calculated the series for $\chi^{(5)}$ to order 2000, and for $\chi^{(6)}$ to order 3260 in $w$.
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Returning to the full susceptibility, we found the following asymptotic behaviour:

- $$kT\chi = const.|\tau|^{-7/4}F_{\pm} + B_f$$

  where $\tau = (1/s - s)/2$, is a parameterisation of the temperature deviation from criticality, $1 - T_c/T$.

- First, note the $(1 - T_c/T)^{-7/4}$ leading order behaviour of the susceptibility. All the more subtle behaviour is contained in the two terms $F_{\pm}$ and $B_f$.
- We found

  $$F_{\pm} = 1+\tau/2+5\tau^2/8+3\tau^3/16-23\tau^4/384-35\tau^5/768+f_{\pm}^{(6)}\tau^7+O(\tau$$

  and $f_{+}^{(6)} = -0.1326933\ldots$, while $f_{-}^{(6)} = -6.3307469\ldots$. We have this expansion through to order $\tau^{15}$.

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$$B_f = \sum_{q=0}^{\infty} \sum_{p=0}^{\sqrt{q}} b^{(p,q)} \tau^q (\log|\tau|)^p.$$

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$$s + 1/s = \cos(\frac{2\pi k}{n}) + \cos(\frac{2\pi m}{n}), \; 0 \leq k, m < n,$$

  on the unit circle in the complex $s$-plane. (Leads to a proof of non-D-finiteness)
- There are others found, unique to each integral.

# The susceptibility from $n$-particle contributions

We consider only Fuchsian ODEs. So $x = 0$ and $x = \infty$ are regular singular points. We use operators of the form

$$L_{MD} = \sum_{m=0}^{M} \sum_{d=0}^{D} a_{md} x^d (x \frac{\mathrm{d}}{\mathrm{d}x})^m, \ a_{M0} \neq 0, \ a_{MD} \neq 0.$$

The operator $x \frac{\mathrm{d}}{\mathrm{d}x}$ ensures that the origin is a regular singular point. There are $N_{MD} = (M+1)(D+1)$ unknown coefficients. Given more terms, we can find the ODE. Just solve a system of $N_{MD}$ linear equations

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# The susceptibility from *n*-particle contributions

- From the integral representation, we generate the series. Then we searched for a Fuchsian ODE.
- Identified by integer coefficients (that predict subsequent ones).
- For $\chi^{(3)}$ an ODE of order 7 with polynomials of degree 12.
- For $\chi^{(4)}$ an ODE of order 9 with polynomials of degree 7.
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# The susceptibility from *n*-particle contributions

- We tried one prime with 10000 terms, and found the ODE for $\chi^{(5)}$ *modulo* a prime.
- We found an ODE of order 56 with polynomials of degree 129. This is sufficient to check for all predicted singularities.
- We have very recently found the ODE for $\chi^{(6)}$ *modulo* a prime.
- Analysing the differential operators we found that combinations of $\chi^{(2n)}$ and $\chi^{(2n-2)}$ simplify the problem.
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# The susceptibility and the susceptibility from $n$-particle contributions

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- The power/log behaviour of each $\chi^{(n)}$ is not the same as the behaviour of the full $\chi$.

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# Conclusion

- We have provided an $\mathrm{O}(N^4 \log N)$ complexity algorithm for the susceptibility of the Ising model, and $n$-particle contributions.
- This enables us to generate some 2000 terms in the series, and subsequent analysis provides a complete description of the asymptotics (scaling function).
- This is arguably more useful than a complete solution.
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- We now know the ODEs for the first 6 such integrals.
- This is sufficient to answer many of the questions as to how the full susceptibility develops from the contributions, including how logarithmic singularites resum to a constant.
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- Despite all this, it would be intellectually satisfying to have a closed form solution, even though it is likely to be extremely ugly!
- The Ising model is still a very active research topic, and likely to continue to be so, even in 2020, on the occasion of its $100^{th}$ birthday.
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